Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:51 AM GMT

PDB ID	:	2BO8
Title	:	DISSECTION OF MANNOSYLGLYCERATE SYNTHASE: AN ARCHETYPAL MANNOSYLTRANSFERASE
Authors	:	Flint, J.; Taylor, E.; Yang, M.; Bolam, D.N.; Tailford, L.E.; Martinez-Fleites, C.; Dodson, E.J.; Davis, B.G.; Gilbert, H.J.; Davies, G.J.
Deposited on	:	2005-04-08
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

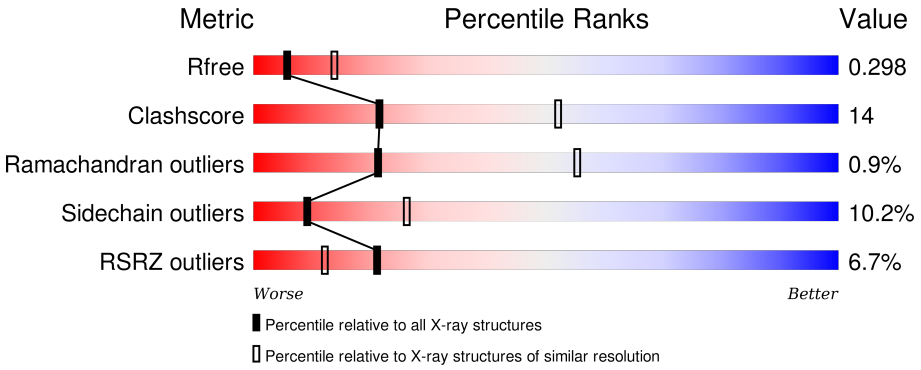
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	397	3% 66% 21% 7%
1	B	397	% 64% 24% 6%
1	C	397	3% 70% 19% 6%
1	D	397	2% 72% 16% 6%
1	E	397	3% 73% 18% 5%

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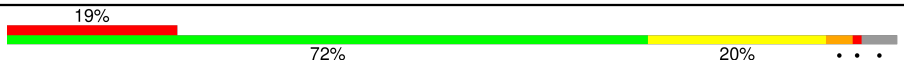
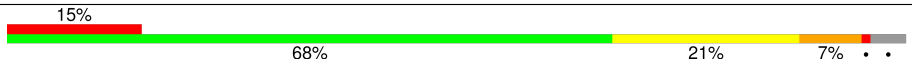
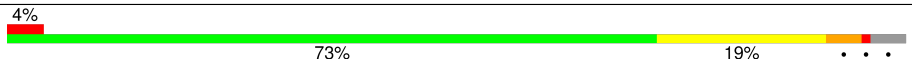
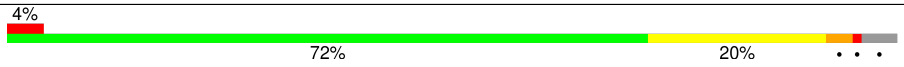
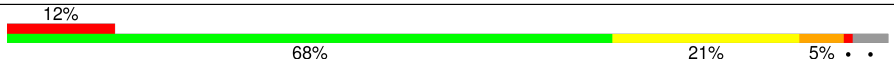
Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	
1	I	397	
1	J	397	

2 Entry composition

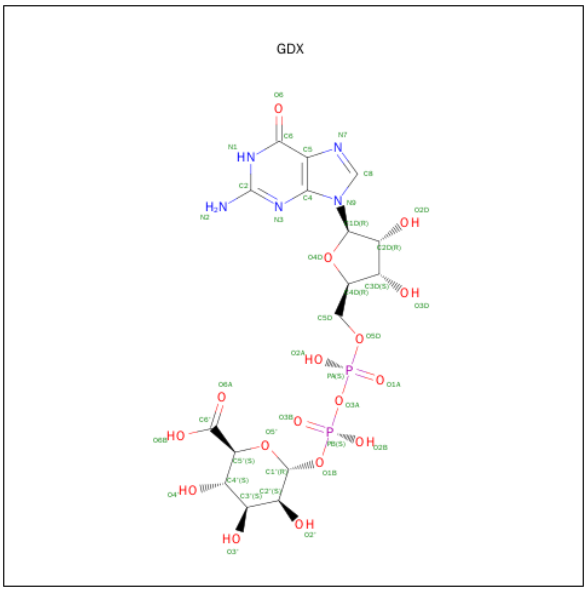
There are 5 unique types of molecules in this entry. The entry contains 32098 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MANNOSYLGLYCERATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	B	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	C	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	D	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	E	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	F	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	G	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	H	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	I	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	J	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			

- Molecule 2 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (three-letter code: GDX) (formula: $C_{16}H_{23}N_5O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	B	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	C	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	D	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	E	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	F	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	G	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	H	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	I	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	J	1	Total	C	N	O	P	0	0
			39	16	5	16	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	J	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	H	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	I	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	I	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is water.

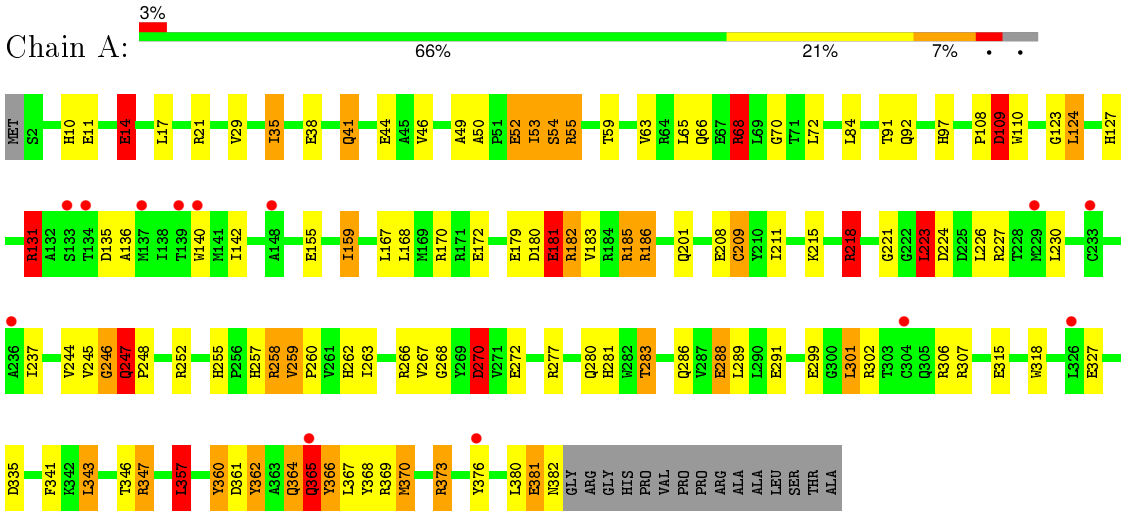
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	78	Total O 78 78	0	0
5	B	80	Total O 80 80	0	0
5	C	38	Total O 38 38	0	0
5	D	27	Total O 27 27	0	0
5	E	34	Total O 34 34	0	0
5	F	3	Total O 3 3	0	0
5	G	23	Total O 23 23	0	0
5	H	6	Total O 6 6	0	0
5	I	13	Total O 13 13	0	0
5	J	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

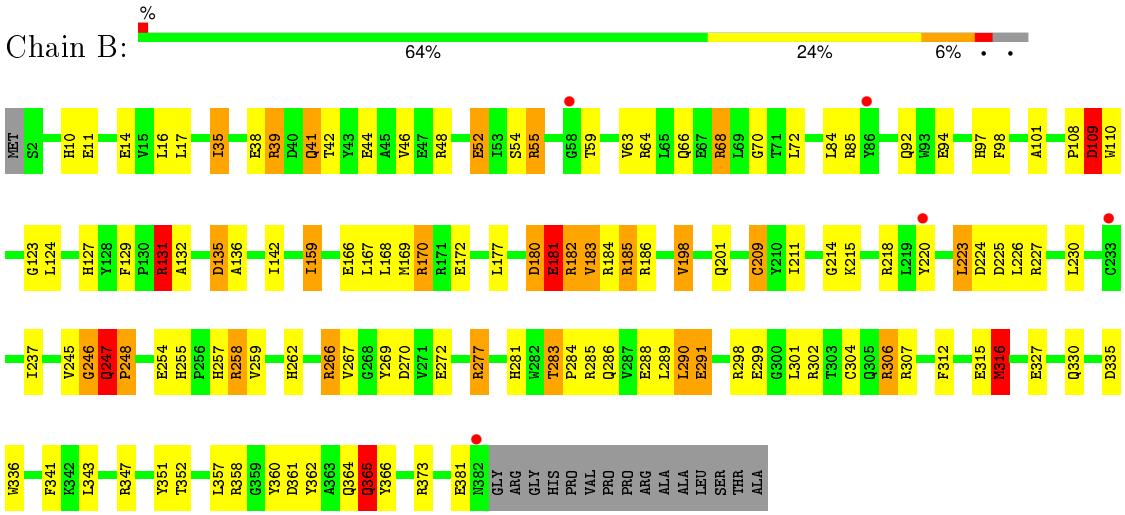
- Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain A:



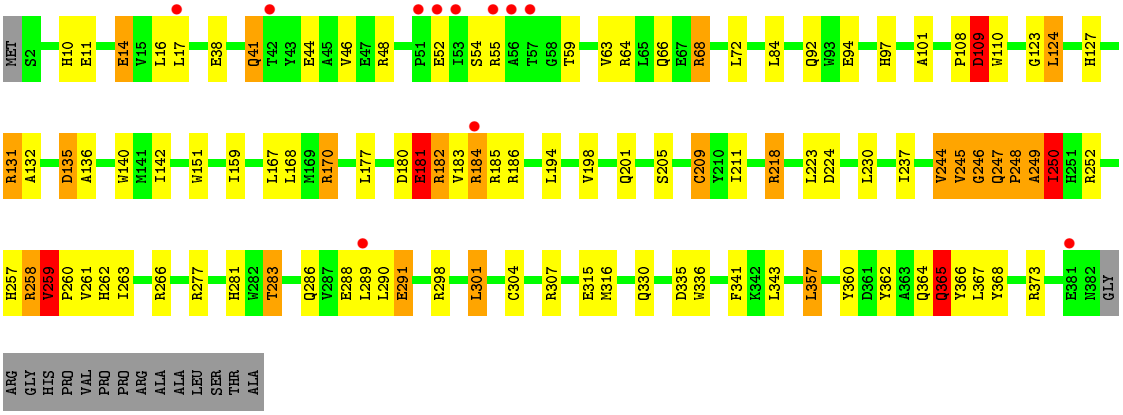
- Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain B:



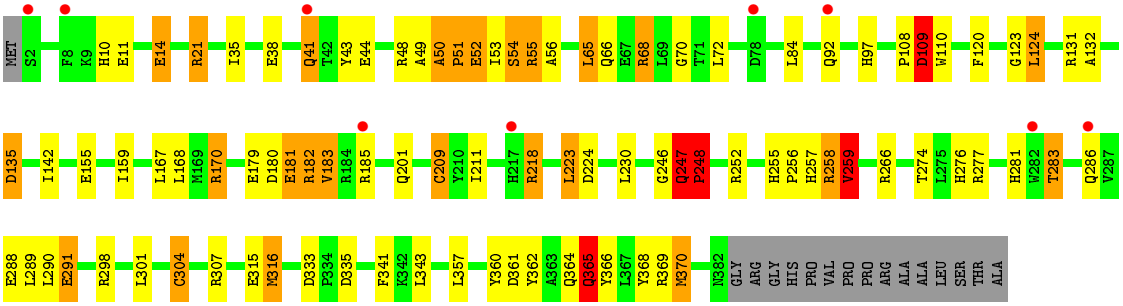
- Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain C:



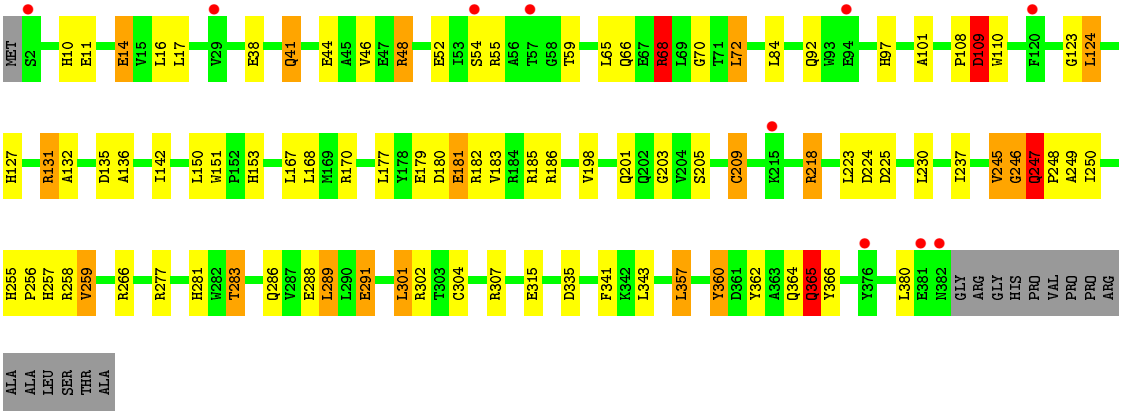
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain D:



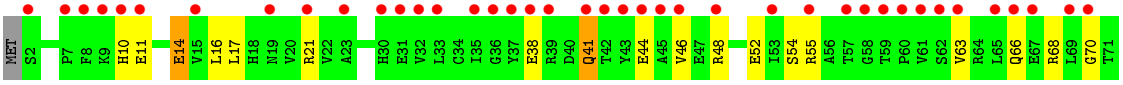
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

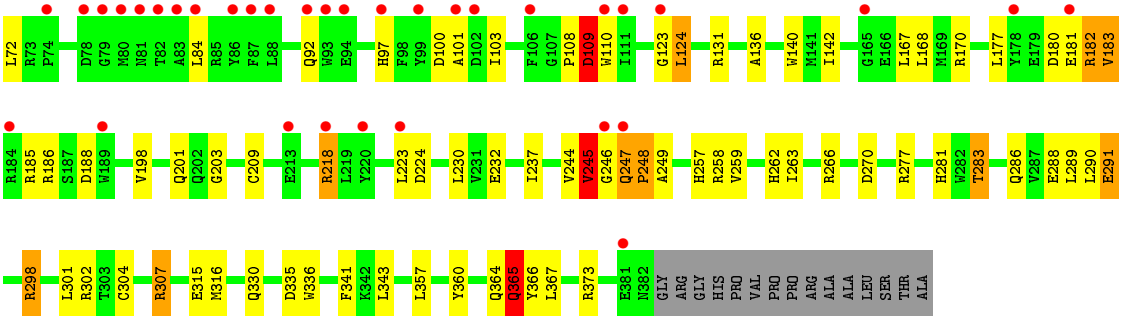
Chain E:



• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

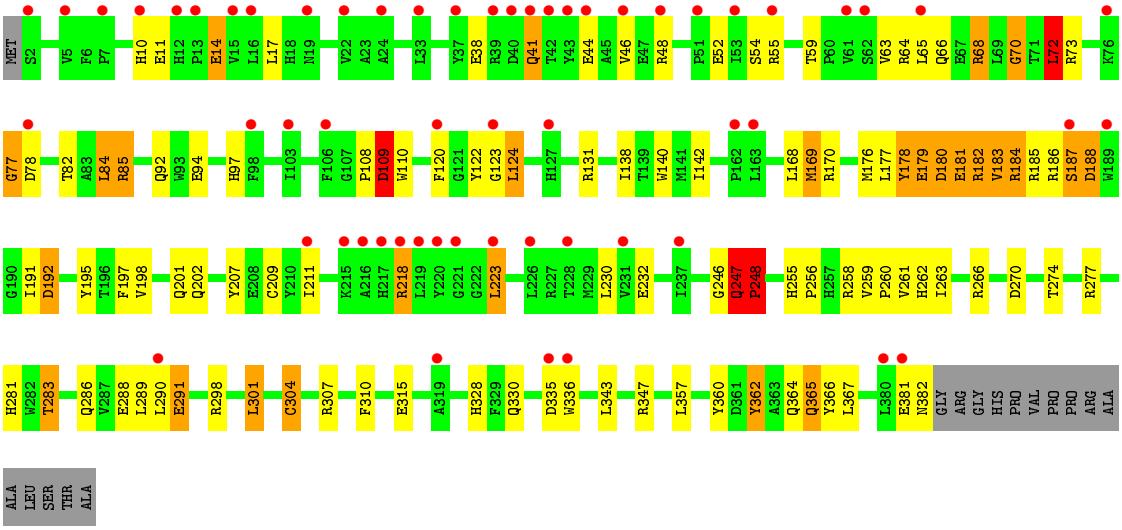
Chain F:





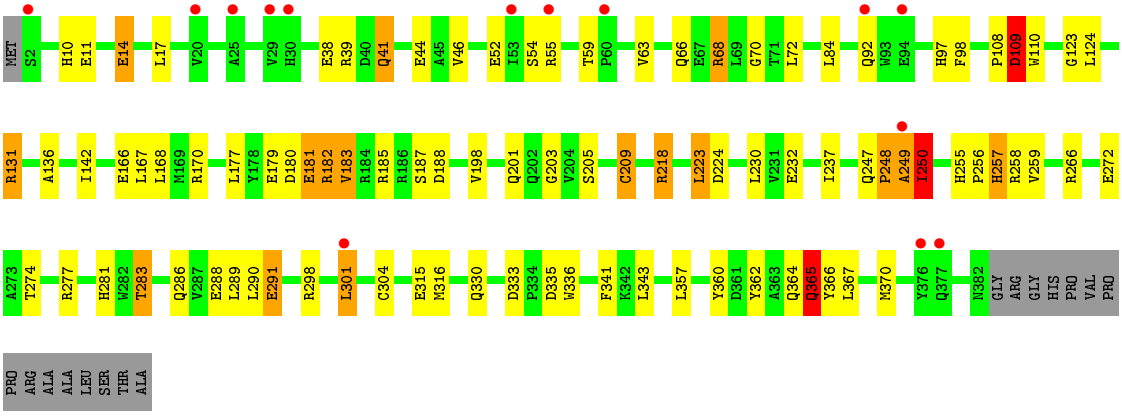
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain G:



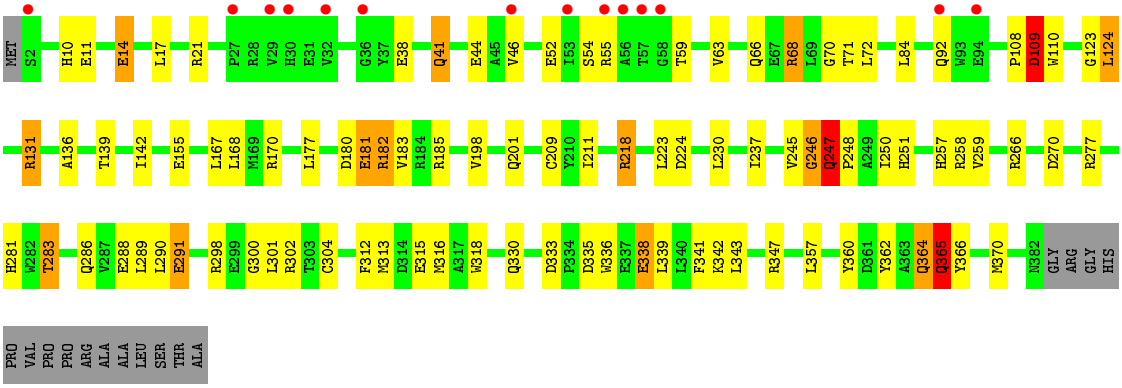
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain H:

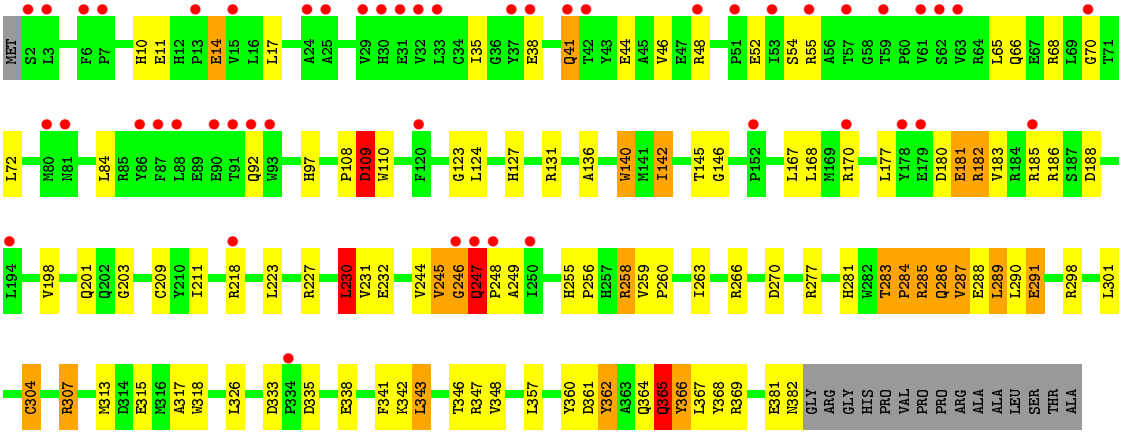


• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain I:



- Molecule 1: MANNOSYLGLYCERATE SYNTHASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	405.09Å 161.43Å 108.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.12 – 2.80 74.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (74.12-2.80) 97.4 (74.10-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.216 0.287 , 0.298	Depositor DCC
R_{free} test set	8687 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 171318 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	32098	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDX, MN, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.51	24/3229 (0.7%)	1.24	28/4394 (0.6%)
1	B	1.50	28/3229 (0.9%)	1.22	29/4394 (0.7%)
1	C	1.09	7/3229 (0.2%)	0.97	13/4394 (0.3%)
1	D	1.16	9/3229 (0.3%)	0.95	10/4394 (0.2%)
1	E	1.00	4/3229 (0.1%)	0.92	7/4394 (0.2%)
1	F	0.75	3/3229 (0.1%)	0.77	4/4394 (0.1%)
1	G	1.17	15/3229 (0.5%)	0.97	8/4394 (0.2%)
1	H	0.80	2/3229 (0.1%)	0.82	4/4394 (0.1%)
1	I	0.90	5/3229 (0.2%)	0.88	9/4394 (0.2%)
1	J	1.14	24/3229 (0.7%)	0.98	7/4394 (0.2%)
All	All	1.13	121/32290 (0.4%)	0.98	119/43940 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	6
1	D	0	3
1	E	0	4
1	F	0	4
1	G	0	4
1	H	0	4
1	I	1	3
1	J	0	3
All	All	1	36

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	CYS	CB-SG	-17.09	1.53	1.82
1	A	209	CYS	CB-SG	-14.65	1.57	1.82
1	A	365	GLN	CB-CG	14.57	1.91	1.52
1	B	209	CYS	CB-SG	-14.55	1.57	1.82
1	I	209	CYS	CB-SG	-13.87	1.58	1.82
1	C	209	CYS	CB-SG	-13.41	1.59	1.82
1	H	209	CYS	CB-SG	-13.39	1.59	1.82
1	G	72	LEU	C-O	11.47	1.45	1.23
1	F	209	CYS	CB-SG	-10.43	1.64	1.82
1	J	338	GLU	CG-CD	9.86	1.66	1.51
1	J	347	ARG	C-O	9.78	1.42	1.23
1	G	169	MET	CG-SD	9.69	2.06	1.81
1	J	209	CYS	CB-SG	-9.18	1.66	1.82
1	C	365	GLN	CB-CG	8.99	1.76	1.52
1	G	188	ASP	CG-OD1	8.98	1.46	1.25
1	D	120	PHE	CE1-CZ	8.84	1.54	1.37
1	E	209	CYS	CB-SG	-8.82	1.67	1.82
1	J	341	PHE	C-O	8.77	1.40	1.23
1	B	316	MET	CG-SD	8.75	2.03	1.81
1	B	365	GLN	CB-CG	8.53	1.75	1.52
1	A	181	GLU	CD-OE2	8.31	1.34	1.25
1	D	120	PHE	CD1-CE1	8.31	1.55	1.39
1	B	181	GLU	CD-OE1	8.13	1.34	1.25
1	J	318	TRP	CE3-CZ3	8.09	1.52	1.38
1	D	365	GLN	CB-CG	7.90	1.73	1.52
1	D	120	PHE	CG-CD2	7.80	1.50	1.38
1	J	365	GLN	CB-CG	7.54	1.72	1.52
1	F	365	GLN	CB-CG	7.45	1.72	1.52
1	B	220	TYR	CD2-CE2	7.44	1.50	1.39
1	G	187	SER	CB-OG	7.39	1.51	1.42
1	J	230	LEU	CG-CD1	-7.36	1.24	1.51
1	D	304	CYS	CB-SG	-7.35	1.69	1.82
1	J	347	ARG	CZ-NH1	7.25	1.42	1.33
1	J	145	THR	C-N	7.19	1.46	1.33
1	A	373	ARG	CZ-NH1	7.17	1.42	1.33
1	A	306	ARG	CZ-NH1	7.11	1.42	1.33
1	J	348	VAL	C-O	7.09	1.36	1.23
1	D	120	PHE	CD2-CE2	7.07	1.53	1.39
1	G	186	ARG	C-O	7.01	1.36	1.23
1	J	368	TYR	N-CA	6.86	1.60	1.46
1	J	140	TRP	CB-CG	-6.61	1.38	1.50
1	A	131	ARG	CG-CD	6.59	1.68	1.51
1	J	231	VAL	CA-CB	6.58	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	ARG	CZ-NH1	6.55	1.41	1.33
1	B	172	GLU	CD-OE2	6.48	1.32	1.25
1	I	365	GLN	CB-CG	6.43	1.70	1.52
1	A	268	GLY	C-O	6.41	1.33	1.23
1	J	346	THR	CB-CG2	-6.41	1.31	1.52
1	I	338	GLU	CD-OE1	6.34	1.32	1.25
1	B	220	TYR	CD1-CE1	6.32	1.48	1.39
1	G	77	GLY	CA-C	6.25	1.61	1.51
1	B	299	GLU	CD-OE2	6.12	1.32	1.25
1	B	373	ARG	CZ-NH1	6.12	1.41	1.33
1	H	365	GLN	CB-CG	6.09	1.69	1.52
1	C	261	VAL	CB-CG1	-6.00	1.40	1.52
1	B	172	GLU	CD-OE1	5.99	1.32	1.25
1	B	269	TYR	C-O	-5.99	1.11	1.23
1	A	373	ARG	CZ-NH2	5.99	1.40	1.33
1	B	129	PHE	CB-CG	-5.90	1.41	1.51
1	A	218	ARG	CG-CD	5.88	1.66	1.51
1	G	209	CYS	CB-SG	-5.86	1.72	1.81
1	F	365	GLN	CG-CD	5.84	1.64	1.51
1	A	172	GLU	CD-OE1	5.81	1.32	1.25
1	A	362	TYR	CG-CD2	5.79	1.46	1.39
1	A	299	GLU	CG-CD	5.76	1.60	1.51
1	B	52	GLU	CD-OE2	5.76	1.31	1.25
1	B	181	GLU	CG-CD	5.75	1.60	1.51
1	A	288	GLU	CD-OE1	5.74	1.31	1.25
1	D	316	MET	CG-SD	5.74	1.96	1.81
1	A	299	GLU	CD-OE2	5.73	1.31	1.25
1	B	215	LYS	CE-NZ	5.72	1.63	1.49
1	G	192	ASP	C-O	5.71	1.34	1.23
1	J	317	ALA	C-O	5.71	1.34	1.23
1	G	85	ARG	CG-CD	-5.68	1.37	1.51
1	B	304	CYS	CB-SG	-5.68	1.72	1.81
1	G	70	GLY	C-O	5.68	1.32	1.23
1	J	366	TYR	CD1-CE1	5.67	1.47	1.39
1	E	59	THR	CB-CG2	5.66	1.71	1.52
1	C	94	GLU	CD-OE2	5.66	1.31	1.25
1	G	362	TYR	CE2-CZ	5.65	1.45	1.38
1	J	347	ARG	N-CA	-5.64	1.35	1.46
1	B	254	GLU	CB-CG	-5.63	1.41	1.52
1	B	180	ASP	C-O	-5.60	1.12	1.23
1	B	272	GLU	CB-CG	-5.58	1.41	1.52
1	A	360	TYR	CB-CG	-5.51	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	300	GLY	N-CA	5.51	1.54	1.46
1	J	366	TYR	CE2-CZ	5.50	1.45	1.38
1	A	272	GLU	CG-CD	5.47	1.60	1.51
1	A	14	GLU	CG-CD	5.45	1.60	1.51
1	B	351	TYR	CD2-CE2	-5.41	1.31	1.39
1	I	365	GLN	CG-CD	5.39	1.63	1.51
1	B	267	VAL	CB-CG2	5.38	1.64	1.52
1	C	181	GLU	CD-OE2	5.35	1.31	1.25
1	A	381	GLU	CB-CG	-5.33	1.42	1.52
1	J	362	TYR	CE1-CZ	5.30	1.45	1.38
1	B	312	PHE	CG-CD2	5.29	1.46	1.38
1	A	221	GLY	N-CA	5.28	1.53	1.46
1	B	185	ARG	CZ-NH2	5.26	1.39	1.33
1	G	94	GLU	CG-CD	5.24	1.59	1.51
1	A	208	GLU	CG-CD	-5.23	1.44	1.51
1	B	135	ASP	CG-OD2	5.23	1.37	1.25
1	B	327	GLU	CD-OE1	5.23	1.31	1.25
1	B	381	GLU	CD-OE1	5.20	1.31	1.25
1	J	304	CYS	CB-SG	5.19	1.91	1.82
1	B	352	THR	C-O	-5.18	1.13	1.23
1	G	82	THR	CA-CB	5.17	1.66	1.53
1	C	365	GLN	CG-CD	5.16	1.62	1.51
1	C	131	ARG	CG-CD	5.15	1.64	1.51
1	J	140	TRP	CE3-CZ3	-5.14	1.29	1.38
1	A	376	TYR	CE1-CZ	5.12	1.45	1.38
1	J	146	GLY	N-CA	5.10	1.53	1.46
1	E	360	TYR	CE2-CZ	5.10	1.45	1.38
1	J	142	ILE	CA-CB	-5.09	1.43	1.54
1	A	306	ARG	CZ-NH2	5.07	1.39	1.33
1	E	365	GLN	CB-CG	5.05	1.66	1.52
1	A	327	GLU	CG-CD	5.04	1.59	1.51
1	G	197	PHE	CE2-CZ	5.03	1.47	1.37
1	G	184	ARG	C-O	5.02	1.32	1.23
1	B	94	GLU	CG-CD	5.01	1.59	1.51
1	A	366	TYR	CG-CD2	-5.01	1.32	1.39
1	J	338	GLU	CD-OE2	5.01	1.31	1.25

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	68	ARG	NE-CZ-NH2	12.44	126.52	120.30
1	J	347	ARG	NE-CZ-NH1	10.73	125.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	135	ASP	CB-CG-OD1	-10.67	108.69	118.30
1	J	347	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	A	347	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	85	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	B	68	ARG	NE-CZ-NH2	9.41	125.01	120.30
1	A	270	ASP	CB-CG-OD1	9.14	126.52	118.30
1	C	109	ASP	CB-CG-OD1	-8.66	110.50	118.30
1	J	307	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	D	68	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	E	68	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	C	68	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	D	109	ASP	CB-CG-OD1	-7.96	111.14	118.30
1	D	170	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	347	ARG	NH1-CZ-NH2	7.66	127.82	119.40
1	B	306	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	131	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	35	ILE	CG1-CB-CG2	-7.50	94.90	111.40
1	B	227	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	B	270	ASP	CB-CG-OD1	7.43	124.99	118.30
1	E	124	LEU	CA-CB-CG	7.35	132.21	115.30
1	G	124	LEU	CA-CB-CG	7.34	132.19	115.30
1	A	347	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	B	180	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	302	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	B	109	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	D	135	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	A	209	CYS	N-CA-CB	-6.90	98.18	110.60
1	C	170	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	C	259	VAL	CB-CA-C	-6.78	98.51	111.40
1	A	259	VAL	CB-CA-C	-6.78	98.52	111.40
1	C	184	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	306	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	211	ILE	CG1-CB-CG2	-6.62	96.83	111.40
1	C	209	CYS	N-CA-CB	-6.62	98.69	110.60
1	A	109	ASP	N-CA-CB	-6.54	98.82	110.60
1	C	211	ILE	CG1-CB-CG2	-6.44	97.24	111.40
1	A	343	LEU	CB-CG-CD1	6.43	121.94	111.00
1	I	68	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	B	306	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	170	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	F	307	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	I	131	ARG	NE-CZ-NH2	-6.27	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	211	ILE	CG1-CB-CG2	-6.22	97.71	111.40
1	B	302	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	B	347	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	E	68	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	A	357	LEU	CB-CG-CD2	-6.14	100.57	111.00
1	F	124	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	185	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	170	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	124	LEU	CA-CB-CG	6.09	129.31	115.30
1	D	370	MET	CG-SD-CE	6.09	109.94	100.20
1	A	21	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	I	304	CYS	CA-CB-SG	-6.08	103.05	114.00
1	G	188	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	109	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	I	109	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	A	131	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	346	THR	CA-C-O	-5.95	107.61	120.10
1	H	131	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	227	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	307	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	F	298	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	135	ASP	CB-CG-OD2	5.86	123.58	118.30
1	G	347	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	301	LEU	CB-CG-CD2	5.79	120.85	111.00
1	I	211	ILE	CG1-CB-CG2	-5.77	98.71	111.40
1	C	186	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	68	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	B	358	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	C	135	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	B	211	ILE	CG1-CB-CG2	-5.70	98.85	111.40
1	D	209	CYS	N-CA-CB	-5.70	100.34	110.60
1	J	227	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	124	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	211	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	H	109	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	B	209	CYS	N-CA-CB	-5.58	100.56	110.60
1	I	124	LEU	CA-CB-CG	5.55	128.06	115.30
1	D	259	VAL	CB-CA-C	-5.54	100.87	111.40
1	A	370	MET	CG-SD-CE	5.52	109.04	100.20
1	C	252	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	E	302	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	E	131	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	185	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	198	VAL	CG1-CB-CG2	5.43	119.59	110.90
1	I	209	CYS	N-CA-CB	-5.43	100.83	110.60
1	I	270	ASP	CB-CG-OD2	5.42	123.18	118.30
1	G	180	ASP	CB-CG-OD2	5.42	123.17	118.30
1	J	343	LEU	CA-CB-CG	5.39	127.69	115.30
1	G	68	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
1	A	159	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	H	68	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	124	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	307	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	285	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	J	211	ILE	CG1-CB-CG2	-5.31	99.72	111.40
1	D	109	ASP	N-CA-CB	-5.30	101.05	110.60
1	B	277	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	G	109	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	272	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	I	68	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	B	184	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	290	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	J	342	LYS	CD-CE-NZ	-5.18	99.79	111.70
1	B	182	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	285	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	H	209	CYS	N-CA-CB	-5.14	101.34	110.60
1	B	39	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	259	VAL	CB-CA-C	-5.07	101.77	111.40
1	B	159	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	E	209	CYS	N-CA-CB	-5.06	101.49	110.60
1	C	64	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	F	373	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	35	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	A	302	ARG	NH1-CZ-NH2	5.03	124.93	119.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	245	VAL	CA

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PRO	Peptide
1	A	247	GLN	Peptide
1	B	108	PRO	Peptide
1	B	246	GLY	Peptide
1	B	247	GLN	Peptide
1	C	108	PRO	Peptide
1	C	244	VAL	Peptide
1	C	246	GLY	Peptide
1	C	247	GLN	Peptide
1	C	248	PRO	Peptide
1	C	249	ALA	Peptide
1	D	108	PRO	Peptide
1	D	247	GLN	Peptide
1	D	248	PRO	Peptide
1	E	108	PRO	Peptide
1	E	245	VAL	Peptide
1	E	246	GLY	Peptide
1	E	247	GLN	Peptide
1	F	108	PRO	Peptide
1	F	245	VAL	Peptide
1	F	247	GLN	Peptide
1	F	248	PRO	Peptide
1	G	108	PRO	Peptide
1	G	246	GLY	Peptide
1	G	247	GLN	Peptide
1	G	248	PRO	Peptide
1	H	108	PRO	Peptide
1	H	248	PRO	Peptide
1	H	249	ALA	Peptide
1	H	250	ILE	Peptide
1	I	108	PRO	Peptide
1	I	246	GLY	Peptide
1	I	247	GLN	Peptide
1	J	108	PRO	Peptide
1	J	246	GLY	Peptide
1	J	247	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3138	0	3037	102	2
1	B	3138	0	3037	91	1
1	C	3138	0	3037	96	0
1	D	3138	0	3037	101	0
1	E	3138	0	3037	70	0
1	F	3138	0	3037	81	0
1	G	3138	0	3037	106	1
1	H	3138	0	3037	79	0
1	I	3138	0	3037	78	0
1	J	3138	0	3036	100	0
2	A	39	0	20	4	0
2	B	39	0	20	4	0
2	C	39	0	20	3	0
2	D	39	0	20	4	0
2	E	39	0	20	3	0
2	F	39	0	20	3	0
2	G	39	0	20	3	0
2	H	39	0	20	3	0
2	I	39	0	20	3	0
2	J	39	0	20	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	F	1	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	1	0
4	I	1	0	0	1	0
4	J	1	0	0	1	0
5	A	78	0	0	17	0
5	B	80	0	0	12	0
5	C	38	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	27	0	0	3	0
5	E	34	0	0	6	0
5	F	3	0	0	1	0
5	G	23	0	0	9	0
5	H	6	0	0	2	0
5	I	13	0	0	6	0
5	J	6	0	0	0	0
All	All	32098	0	30569	880	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (880) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:GLN:CB	1:C:365:GLN:CG	1.76	1.61
1:B:365:GLN:CG	1:B:365:GLN:CB	1.75	1.55
1:B:316:MET:SD	1:B:316:MET:CG	2.03	1.46
1:J:247:GLN:CB	1:J:248:PRO:HD3	1.43	1.44
1:A:365:GLN:CB	1:A:365:GLN:CG	1.91	1.44
1:G:169:MET:CG	1:G:169:MET:SD	2.06	1.42
1:B:247:GLN:HB2	1:B:248:PRO:CD	1.54	1.31
1:F:247:GLN:CG	1:F:248:PRO:HD3	1.62	1.28
1:F:247:GLN:HG2	1:F:248:PRO:CD	1.62	1.27
1:B:247:GLN:HB2	1:B:248:PRO:CG	1.66	1.25
1:J:247:GLN:CG	1:J:248:PRO:HG3	1.68	1.23
1:D:50:ALA:HB3	1:D:51:PRO:CD	1.67	1.22
1:G:178:TYR:CE2	1:G:184:ARG:NH2	2.08	1.21
1:C:365:GLN:HB3	5:C:2032:HOH:O	1.41	1.19
1:E:247:GLN:HB2	1:E:248:PRO:HD2	1.20	1.17
1:J:285:ARG:HH11	1:J:285:ARG:HG2	1.04	1.16
1:I:201:GLN:HE21	1:I:245:VAL:HG11	1.07	1.15
1:I:365:GLN:HB3	5:I:2009:HOH:O	1.46	1.15
1:J:247:GLN:CG	1:J:248:PRO:HD3	1.75	1.14
1:E:247:GLN:HB2	1:E:248:PRO:CD	1.77	1.12
1:I:201:GLN:HE21	1:I:245:VAL:CG1	1.63	1.10
1:H:205:SER:HA	1:H:250:ILE:CG2	1.80	1.10
1:B:185:ARG:HD3	5:B:2035:HOH:O	1.51	1.10
1:C:244:VAL:HG12	1:C:245:VAL:H	1.11	1.10
1:J:247:GLN:CG	1:J:248:PRO:CD	2.30	1.10
1:J:247:GLN:CB	1:J:248:PRO:CD	2.31	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASP:HB2	5:C:2008:HOH:O	1.51	1.08
1:J:247:GLN:CG	1:J:248:PRO:CG	2.30	1.08
1:J:247:GLN:HG2	1:J:248:PRO:HG3	1.30	1.08
1:J:247:GLN:HG2	1:J:248:PRO:CG	1.84	1.08
1:D:50:ALA:HB3	1:D:51:PRO:HD3	1.30	1.06
1:I:283:THR:HG22	1:I:286:GLN:H	1.20	1.05
1:J:283:THR:HG21	1:J:335:ASP:OD2	1.55	1.03
1:F:283:THR:HG22	1:F:286:GLN:H	1.23	1.03
1:B:247:GLN:HB2	1:B:248:PRO:HD3	1.31	1.03
1:A:218:ARG:HB3	5:A:2077:HOH:O	1.55	1.02
1:E:283:THR:HG22	1:E:286:GLN:H	1.24	1.02
1:I:201:GLN:NE2	1:I:245:VAL:HG11	1.73	1.02
1:J:247:GLN:HB3	1:J:248:PRO:HD3	1.01	0.99
1:J:247:GLN:HG3	1:J:248:PRO:HG3	1.41	0.99
1:G:178:TYR:CD2	1:G:184:ARG:NH2	2.29	0.99
1:F:247:GLN:HG2	1:F:248:PRO:HD2	1.43	0.99
1:F:247:GLN:CG	1:F:248:PRO:CD	2.30	0.99
1:G:66:GLN:HE22	2:G:400:GDX:HN1	1.08	0.99
1:A:283:THR:HG22	1:A:286:GLN:H	1.29	0.98
1:H:66:GLN:HE22	2:H:400:GDX:HN1	1.09	0.98
1:G:283:THR:HG22	1:G:286:GLN:H	1.29	0.98
1:C:283:THR:HG22	1:C:286:GLN:H	1.27	0.98
1:D:283:THR:HG22	1:D:286:GLN:H	1.27	0.98
1:J:247:GLN:HB3	1:J:248:PRO:CD	1.93	0.97
1:H:283:THR:HG22	1:H:286:GLN:H	1.28	0.97
1:B:247:GLN:CB	1:B:248:PRO:CD	2.43	0.97
1:I:259:VAL:HG21	1:I:360:TYR:CE1	2.00	0.97
1:D:50:ALA:CB	1:D:51:PRO:CD	2.37	0.96
1:E:109:ASP:HB3	1:E:110:TRP:HD1	1.30	0.96
1:F:66:GLN:HE22	2:F:400:GDX:HN1	1.07	0.96
1:C:250:ILE:HG22	1:C:250:ILE:O	1.63	0.96
1:I:246:GLY:C	1:I:247:GLN:HG3	1.86	0.96
1:B:283:THR:HG22	1:B:286:GLN:H	1.32	0.95
1:I:66:GLN:HE22	2:I:400:GDX:HN1	1.08	0.95
1:I:201:GLN:HG3	1:I:245:VAL:HG11	1.47	0.95
1:C:66:GLN:HE22	2:C:400:GDX:HN1	1.15	0.94
1:J:285:ARG:NH1	1:J:285:ARG:HG2	1.79	0.94
1:E:66:GLN:HE22	2:E:400:GDX:HN1	1.04	0.94
1:I:246:GLY:O	1:I:247:GLN:HG3	1.68	0.93
1:D:66:GLN:HE22	2:D:400:GDX:HN1	1.10	0.93
1:C:247:GLN:HB3	1:C:248:PRO:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:328:HIS:HD2	5:G:2019:HOH:O	1.52	0.93
1:F:247:GLN:CB	1:F:248:PRO:CD	2.46	0.93
1:J:283:THR:HG22	1:J:283:THR:O	1.67	0.92
1:H:205:SER:HA	1:H:250:ILE:HG23	1.52	0.92
1:H:259:VAL:HG21	1:H:360:TYR:CE1	2.05	0.92
1:D:52:GLU:O	1:D:55:ARG:HG2	1.69	0.92
1:D:50:ALA:HB3	1:D:51:PRO:HD2	1.49	0.92
1:J:286:GLN:O	1:J:288:GLU:N	2.01	0.92
1:G:178:TYR:HE2	1:G:184:ARG:NH2	1.66	0.92
1:A:66:GLN:HE22	2:A:400:GDX:HN1	1.18	0.92
1:J:286:GLN:O	1:J:289:LEU:N	2.04	0.90
1:F:245:VAL:O	1:F:245:VAL:HG12	1.69	0.90
1:G:259:VAL:HG21	1:G:360:TYR:CE1	2.07	0.90
1:B:247:GLN:HB3	1:B:248:PRO:HB3	1.51	0.90
1:J:259:VAL:HG21	1:J:360:TYR:CE1	2.06	0.90
1:B:365:GLN:HB3	5:B:2073:HOH:O	1.72	0.89
1:F:247:GLN:CB	1:F:248:PRO:HD3	1.89	0.89
1:B:247:GLN:CB	1:B:248:PRO:HB3	2.03	0.89
1:B:59:THR:HG21	5:B:2001:HOH:O	1.71	0.89
1:J:247:GLN:HG3	1:J:248:PRO:CG	1.99	0.89
1:B:247:GLN:CB	1:B:248:PRO:HD3	2.00	0.89
1:H:205:SER:CA	1:H:250:ILE:CG2	2.50	0.89
1:H:250:ILE:O	1:H:250:ILE:HG23	1.72	0.89
1:B:66:GLN:HE22	2:B:400:GDX:HN1	1.16	0.88
1:J:66:GLN:HE22	2:J:400:GDX:HN1	1.18	0.88
1:F:259:VAL:HG21	1:F:360:TYR:CE1	2.08	0.88
1:D:369:ARG:HD3	5:D:2025:HOH:O	1.73	0.88
1:H:205:SER:CB	1:H:250:ILE:CG2	2.52	0.87
1:C:109:ASP:HB3	1:C:110:TRP:HD1	1.37	0.87
1:G:109:ASP:HB3	1:G:110:TRP:HD1	1.37	0.87
1:I:59:THR:HG21	5:I:2002:HOH:O	1.74	0.87
1:D:52:GLU:C	1:D:52:GLU:CD	2.33	0.87
1:E:247:GLN:CB	1:E:248:PRO:CD	2.45	0.86
1:I:246:GLY:C	1:I:247:GLN:CG	2.44	0.86
1:A:41:GLN:HA	1:A:41:GLN:HE21	1.40	0.86
1:B:247:GLN:HB2	1:B:248:PRO:CB	2.05	0.86
1:H:109:ASP:HB3	1:H:110:TRP:HD1	1.40	0.85
1:A:373:ARG:HD2	5:A:2074:HOH:O	1.74	0.85
1:I:109:ASP:HB3	1:I:110:TRP:HD1	1.40	0.85
1:C:244:VAL:CG1	1:C:245:VAL:H	1.90	0.84
1:C:259:VAL:HG21	1:C:360:TYR:CE1	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:SER:HB2	1:C:250:ILE:HG21	1.57	0.84
1:A:369:ARG:HD2	5:A:2072:HOH:O	1.77	0.84
1:J:247:GLN:HG2	1:J:248:PRO:CD	2.06	0.83
1:G:176:MET:SD	1:G:202:GLN:HG3	2.17	0.83
1:C:59:THR:HG21	5:C:2004:HOH:O	1.78	0.83
1:D:369:ARG:CD	5:D:2025:HOH:O	2.24	0.83
1:B:247:GLN:CB	1:B:248:PRO:CB	2.56	0.83
1:A:179:GLU:HG3	5:A:2033:HOH:O	1.79	0.83
1:C:244:VAL:HG12	1:C:245:VAL:N	1.86	0.83
1:J:109:ASP:HB3	1:J:110:TRP:HD1	1.42	0.83
1:F:66:GLN:NE2	2:F:400:GDX:HN1	1.76	0.82
1:B:284:PRO:HB3	1:F:288:GLU:HG3	1.60	0.82
1:F:109:ASP:HB3	1:F:110:TRP:HD1	1.43	0.82
1:B:259:VAL:HG21	1:B:360:TYR:CZ	2.15	0.82
1:C:283:THR:HG21	1:C:335:ASP:OD2	1.81	0.81
1:I:66:GLN:NE2	2:I:400:GDX:HN1	1.77	0.81
1:C:123:GLY:HA2	1:C:170:ARG:HD3	1.61	0.81
1:D:109:ASP:HB3	1:D:110:TRP:HD1	1.45	0.81
1:G:178:TYR:CD2	1:G:178:TYR:O	2.33	0.81
1:H:205:SER:CB	1:H:250:ILE:HG21	2.10	0.81
1:C:205:SER:HB2	1:C:250:ILE:CG2	2.11	0.81
1:G:365:GLN:HG3	1:G:366:TYR:N	1.95	0.81
1:G:178:TYR:HD2	1:G:184:ARG:HH21	1.29	0.81
1:J:259:VAL:HG21	1:J:360:TYR:CZ	2.17	0.80
1:G:59:THR:HG21	5:G:2003:HOH:O	1.78	0.80
1:B:109:ASP:HB3	1:B:110:TRP:HD1	1.44	0.80
1:H:205:SER:HB3	1:H:250:ILE:HG21	1.63	0.80
1:J:283:THR:CG2	1:J:283:THR:O	2.30	0.79
1:A:109:ASP:HB3	1:A:110:TRP:HD1	1.48	0.79
1:B:247:GLN:CB	1:B:248:PRO:CG	2.56	0.79
1:I:246:GLY:O	1:I:247:GLN:CG	2.30	0.79
1:I:259:VAL:HG21	1:I:360:TYR:CZ	2.17	0.79
1:H:283:THR:HG21	1:H:335:ASP:OD2	1.82	0.79
1:F:247:GLN:HG2	1:F:248:PRO:HD3	1.26	0.79
1:D:66:GLN:NE2	2:D:400:GDX:HN1	1.80	0.79
1:I:59:THR:CG2	5:I:2002:HOH:O	2.29	0.79
1:A:10:HIS:HA	5:A:2002:HOH:O	1.83	0.79
1:B:283:THR:HG21	1:B:335:ASP:OD2	1.83	0.78
1:I:201:GLN:CG	1:I:245:VAL:HG11	2.14	0.78
1:C:250:ILE:CG2	1:C:250:ILE:O	2.30	0.78
1:G:180:ASP:HB3	1:G:183:VAL:HG13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ALA:HB1	5:C:2018:HOH:O	1.81	0.78
1:E:66:GLN:NE2	2:E:400:GDX:HN1	1.81	0.78
1:B:142:ILE:CD1	1:B:230:LEU:CD1	2.62	0.78
1:C:41:GLN:HE21	1:C:41:GLN:HA	1.49	0.77
1:D:259:VAL:HG21	1:D:360:TYR:CE1	2.18	0.77
1:H:205:SER:HA	1:H:250:ILE:HG22	1.64	0.77
1:E:123:GLY:HA2	1:E:170:ARG:HD3	1.66	0.77
1:E:259:VAL:HG21	1:E:360:TYR:CE1	2.19	0.77
1:G:66:GLN:NE2	2:G:400:GDX:HN1	1.82	0.77
1:H:66:GLN:NE2	2:H:400:GDX:HN1	1.82	0.77
1:G:178:TYR:CE2	1:G:184:ARG:CZ	2.68	0.76
1:C:66:GLN:NE2	2:C:400:GDX:HN1	1.81	0.76
1:H:205:SER:CA	1:H:250:ILE:HG23	2.15	0.76
1:I:357:LEU:HD13	1:J:357:LEU:HD13	1.68	0.76
1:J:66:GLN:NE2	2:J:400:GDX:HN1	1.84	0.75
1:B:247:GLN:HB2	1:B:248:PRO:HG3	1.66	0.75
1:B:259:VAL:HG21	1:B:360:TYR:CE1	2.22	0.75
1:H:205:SER:CB	1:H:250:ILE:HG23	2.17	0.74
1:I:142:ILE:CD1	1:I:230:LEU:HD11	2.16	0.74
1:F:283:THR:HG21	1:F:335:ASP:OD2	1.88	0.74
1:G:180:ASP:OD1	1:G:182:ARG:HB2	1.88	0.74
1:A:66:GLN:NE2	2:A:400:GDX:HN1	1.83	0.74
1:G:41:GLN:HE21	1:G:41:GLN:HA	1.53	0.74
1:H:123:GLY:HA2	1:H:170:ARG:HD3	1.69	0.74
1:A:283:THR:HG21	1:A:335:ASP:OD2	1.88	0.74
1:G:283:THR:HG21	1:G:335:ASP:OD2	1.87	0.74
1:H:259:VAL:HG21	1:H:360:TYR:CZ	2.22	0.74
1:C:205:SER:CB	1:C:250:ILE:HG21	2.19	0.73
1:J:123:GLY:HA2	1:J:170:ARG:HD3	1.70	0.73
1:F:180:ASP:HB3	1:F:183:VAL:HG13	1.70	0.73
1:E:41:GLN:HA	1:E:41:GLN:HE21	1.54	0.73
1:A:267:VAL:HB	5:A:2053:HOH:O	1.86	0.73
1:E:357:LEU:HD13	1:F:357:LEU:HD13	1.70	0.73
1:B:66:GLN:NE2	2:B:400:GDX:HN1	1.86	0.73
1:A:259:VAL:HG21	1:A:360:TYR:CE1	2.23	0.73
1:D:283:THR:HG21	1:D:335:ASP:OD2	1.88	0.73
1:B:123:GLY:HA2	1:B:170:ARG:HD3	1.71	0.72
1:E:109:ASP:HB3	1:E:110:TRP:CD1	2.21	0.72
1:F:246:GLY:HA2	1:F:247:GLN:CB	2.20	0.72
1:F:259:VAL:HG21	1:F:360:TYR:CZ	2.24	0.72
1:H:203:GLY:HA2	1:H:249:ALA:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:GLN:HG3	1:I:245:VAL:CG1	2.17	0.72
1:F:123:GLY:HA2	1:F:170:ARG:HD3	1.72	0.72
1:A:357:LEU:HD13	1:B:357:LEU:HD13	1.71	0.71
1:J:41:GLN:HA	1:J:41:GLN:HE21	1.55	0.71
1:G:177:LEU:HD23	1:G:198:VAL:HG22	1.71	0.71
1:C:52:GLU:OE1	1:C:55:ARG:NH1	2.23	0.71
1:G:85:ARG:HB2	1:G:178:TYR:HE1	1.56	0.71
1:E:365:GLN:HG3	1:E:366:TYR:N	2.04	0.71
1:B:41:GLN:HA	1:B:41:GLN:HE21	1.55	0.71
1:C:244:VAL:CG1	1:C:245:VAL:N	2.52	0.71
1:F:41:GLN:HE21	1:F:41:GLN:HA	1.55	0.71
1:D:52:GLU:C	1:D:52:GLU:OE2	2.30	0.70
1:B:262:HIS:HE1	5:B:2044:HOH:O	1.74	0.70
1:G:178:TYR:O	1:G:178:TYR:HD2	1.72	0.70
1:I:283:THR:HB	1:I:286:GLN:NE2	2.07	0.70
1:C:142:ILE:CD1	1:C:230:LEU:CD1	2.69	0.70
1:G:123:GLY:HA2	1:G:170:ARG:HD3	1.72	0.70
1:G:315:GLU:HB2	5:G:2018:HOH:O	1.90	0.70
1:D:50:ALA:CB	1:D:51:PRO:HD3	2.11	0.70
1:B:142:ILE:CD1	1:B:230:LEU:HD11	2.22	0.69
1:C:142:ILE:CD1	1:C:230:LEU:HD11	2.22	0.69
1:C:259:VAL:HG21	1:C:360:TYR:CZ	2.27	0.69
1:A:52:GLU:C	1:A:52:GLU:OE2	2.30	0.69
1:E:218:ARG:HH11	1:E:218:ARG:HG2	1.57	0.69
1:D:52:GLU:O	1:D:52:GLU:CD	2.31	0.69
1:I:246:GLY:O	1:I:247:GLN:CD	2.30	0.69
1:I:365:GLN:HG3	1:I:366:TYR:N	2.06	0.69
1:A:252:ARG:NH1	1:D:155:GLU:OE1	2.26	0.69
1:I:123:GLY:HA2	1:I:170:ARG:HD3	1.75	0.69
1:A:68:ARG:HD3	5:E:2010:HOH:O	1.93	0.68
1:A:180:ASP:HB3	1:A:183:VAL:HG13	1.76	0.68
1:E:245:VAL:HG12	1:E:246:GLY:N	2.09	0.68
1:H:52:GLU:OE1	1:H:55:ARG:NH1	2.27	0.68
1:I:283:THR:HG21	1:I:335:ASP:OD2	1.94	0.68
1:I:41:GLN:HE21	1:I:41:GLN:HA	1.58	0.68
1:H:41:GLN:HA	1:H:41:GLN:HE21	1.58	0.68
1:G:142:ILE:CD1	1:G:230:LEU:HD11	2.24	0.68
1:H:250:ILE:CG2	1:H:250:ILE:O	2.42	0.68
1:J:182:ARG:NH2	1:J:201:GLN:OE1	2.26	0.68
1:J:286:GLN:O	1:J:287:VAL:C	2.32	0.68
1:D:123:GLY:HA2	1:D:170:ARG:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ARG:NH2	1:D:201:GLN:OE1	2.25	0.68
1:H:250:ILE:C	1:H:250:ILE:CD1	2.62	0.68
1:A:262:HIS:HE1	5:A:2039:HOH:O	1.77	0.68
1:B:52:GLU:OE1	1:B:55:ARG:NH1	2.27	0.68
1:F:283:THR:HB	1:F:286:GLN:NE2	2.09	0.67
1:E:136:ALA:HA	4:E:1382:CL:CL	2.31	0.67
1:E:283:THR:HG21	1:E:335:ASP:OD2	1.94	0.67
1:I:142:ILE:CD1	1:I:230:LEU:CD1	2.73	0.67
1:J:180:ASP:HB3	1:J:183:VAL:HG13	1.76	0.67
1:F:245:VAL:CG1	1:F:245:VAL:O	2.43	0.66
1:D:180:ASP:HB3	1:D:183:VAL:HG13	1.77	0.66
1:C:109:ASP:CB	5:C:2008:HOH:O	2.24	0.66
1:D:50:ALA:CB	1:D:51:PRO:HD2	2.15	0.66
1:J:246:GLY:H	1:J:247:GLN:HB2	1.60	0.66
1:D:49:ALA:O	1:D:50:ALA:O	2.12	0.66
1:A:142:ILE:CD1	1:A:230:LEU:HD11	2.25	0.66
1:E:182:ARG:NH2	1:E:201:GLN:OE1	2.29	0.66
1:J:285:ARG:NH1	1:J:335:ASP:OD1	2.29	0.66
1:H:250:ILE:C	1:H:250:ILE:HD13	2.15	0.66
1:E:218:ARG:HH11	1:E:218:ARG:CG	2.08	0.65
1:B:10:HIS:HE1	1:B:38:GLU:OE2	1.79	0.65
1:A:52:GLU:OE1	1:A:55:ARG:NH1	2.30	0.65
1:J:283:THR:O	1:J:285:ARG:N	2.30	0.65
1:C:59:THR:CG2	5:C:2004:HOH:O	2.39	0.65
1:E:259:VAL:HG21	1:E:360:TYR:CZ	2.31	0.65
1:E:180:ASP:HB3	1:E:183:VAL:HG13	1.79	0.65
1:G:52:GLU:OE1	1:G:55:ARG:NH1	2.29	0.65
1:I:52:GLU:OE1	1:I:55:ARG:NH1	2.30	0.65
1:D:50:ALA:O	1:D:52:GLU:N	2.30	0.65
1:A:52:GLU:OE2	1:A:53:ILE:N	2.30	0.65
1:G:177:LEU:O	1:G:179:GLU:N	2.30	0.64
1:A:259:VAL:HG21	1:A:360:TYR:CZ	2.32	0.64
1:F:244:VAL:HG12	1:F:245:VAL:N	2.12	0.64
1:A:142:ILE:CD1	1:A:230:LEU:CD1	2.76	0.64
1:H:205:SER:HB2	1:H:250:ILE:HG23	1.77	0.64
1:A:131:ARG:O	1:A:360:TYR:HE2	1.80	0.64
1:F:201:GLN:HG3	1:F:245:VAL:HG22	1.79	0.64
1:J:247:GLN:HG3	1:J:248:PRO:CD	2.24	0.64
1:G:142:ILE:CD1	1:G:230:LEU:CD1	2.74	0.64
1:E:247:GLN:CB	1:E:248:PRO:HD3	2.27	0.64
1:A:381:GLU:HG2	1:A:382:ASN:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:GLU:OE1	1:J:55:ARG:NH1	2.30	0.64
1:G:109:ASP:HB3	1:G:110:TRP:CD1	2.28	0.64
1:I:364:GLN:HB3	5:I:2010:HOH:O	1.98	0.64
1:I:247:GLN:N	1:I:247:GLN:OE1	2.30	0.63
1:C:357:LEU:HD13	1:D:357:LEU:HD13	1.78	0.63
1:D:53:ILE:C	1:D:55:ARG:H	2.01	0.63
1:B:266:ARG:NH1	5:B:2056:HOH:O	2.32	0.63
1:J:285:ARG:HH11	1:J:285:ARG:CG	1.92	0.63
1:H:180:ASP:HB3	1:H:183:VAL:HG13	1.78	0.63
1:G:259:VAL:HG21	1:G:360:TYR:CZ	2.32	0.63
1:C:259:VAL:CG2	1:C:360:TYR:CE1	2.81	0.63
1:G:191:ILE:HG23	1:G:192:ASP:N	2.14	0.63
1:C:109:ASP:HB3	1:C:110:TRP:CD1	2.28	0.63
1:E:48:ARG:HD3	5:E:2006:HOH:O	1.98	0.63
1:E:380:LEU:HD23	5:E:2033:HOH:O	1.98	0.63
1:D:41:GLN:HE21	1:D:41:GLN:HA	1.63	0.63
1:C:249:ALA:HB1	1:C:250:ILE:HB	1.82	0.62
1:A:123:GLY:HA2	1:A:170:ARG:HD3	1.79	0.62
1:H:142:ILE:CD1	1:H:230:LEU:CD1	2.76	0.62
1:H:142:ILE:CD1	1:H:230:LEU:HD11	2.30	0.62
1:F:365:GLN:HG3	1:F:366:TYR:N	2.14	0.62
1:G:169:MET:CB	1:G:169:MET:SD	2.87	0.62
1:A:142:ILE:HD13	1:A:230:LEU:HD12	1.81	0.62
1:E:247:GLN:CB	1:E:248:PRO:HD2	2.11	0.62
1:B:181:GLU:OE1	1:B:185:ARG:NH2	2.33	0.62
1:F:142:ILE:CD1	1:F:230:LEU:CD1	2.77	0.62
1:H:365:GLN:HG3	1:H:366:TYR:N	2.14	0.62
1:B:365:GLN:NE2	5:B:2075:HOH:O	2.29	0.61
1:J:285:ARG:NH1	1:J:285:ARG:CG	2.57	0.61
1:C:283:THR:HB	1:C:286:GLN:NE2	2.15	0.61
1:D:52:GLU:OE2	1:D:53:ILE:N	2.33	0.61
1:C:180:ASP:HB3	1:C:183:VAL:HG13	1.82	0.61
1:D:369:ARG:HD2	5:D:2025:HOH:O	1.95	0.61
1:B:283:THR:CG2	1:B:286:GLN:H	2.10	0.61
1:I:259:VAL:CG2	1:I:360:TYR:CE1	2.81	0.61
1:F:52:GLU:OE1	1:F:55:ARG:NH1	2.33	0.61
1:J:247:GLN:HG2	1:J:248:PRO:HD3	1.65	0.60
1:E:52:GLU:OE1	1:E:55:ARG:NH1	2.35	0.60
1:G:304:CYS:HA	1:G:307:ARG:O	2.00	0.60
1:D:246:GLY:O	1:D:247:GLN:HG2	2.01	0.60
1:I:283:THR:HG22	1:I:286:GLN:N	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ILE:CD1	1:F:230:LEU:HD11	2.30	0.60
1:E:277:ARG:CZ	1:E:281:HIS:HD2	2.15	0.60
1:H:136:ALA:HA	4:H:1382:CL:CL	2.38	0.60
1:C:205:SER:HA	1:C:250:ILE:HG22	1.83	0.60
1:D:142:ILE:CD1	1:D:230:LEU:CD1	2.79	0.60
1:D:53:ILE:O	1:D:55:ARG:N	2.32	0.60
1:J:285:ARG:HH12	1:J:335:ASP:HB2	1.66	0.60
1:J:136:ALA:HA	4:J:1382:CL:CL	2.39	0.60
1:J:142:ILE:CD1	1:J:230:LEU:CD1	2.80	0.60
1:D:55:ARG:HG3	1:D:56:ALA:N	2.16	0.59
1:J:283:THR:HG22	1:J:286:GLN:H	1.66	0.59
1:F:283:THR:HG22	1:F:286:GLN:N	2.07	0.59
1:A:168:LEU:HD23	1:A:168:LEU:C	2.23	0.59
1:G:247:GLN:O	1:G:248:PRO:C	2.41	0.59
1:C:365:GLN:HG3	1:C:366:TYR:N	2.17	0.59
1:D:283:THR:HB	1:D:286:GLN:NE2	2.17	0.59
1:G:283:THR:HB	1:G:286:GLN:NE2	2.18	0.59
1:B:131:ARG:CB	5:B:2023:HOH:O	2.51	0.59
1:F:246:GLY:HA2	1:F:247:GLN:CG	2.33	0.59
1:B:142:ILE:HD11	1:B:230:LEU:HD11	1.85	0.59
1:D:10:HIS:HE1	1:D:38:GLU:OE2	1.86	0.59
1:J:10:HIS:HE1	1:J:38:GLU:OE2	1.86	0.59
1:A:142:ILE:HD13	1:A:230:LEU:CD1	2.33	0.58
1:I:365:GLN:NE2	5:I:2011:HOH:O	2.35	0.58
1:H:10:HIS:HE1	1:H:38:GLU:OE2	1.87	0.58
1:E:245:VAL:HG12	1:E:246:GLY:H	1.68	0.58
1:I:201:GLN:CD	1:I:245:VAL:HG11	2.23	0.58
1:J:201:GLN:HG3	1:J:245:VAL:HG13	1.84	0.58
1:G:180:ASP:CG	1:G:182:ARG:HH11	2.07	0.58
1:F:109:ASP:HB3	1:F:110:TRP:CD1	2.33	0.58
1:E:180:ASP:OD2	1:E:182:ARG:NH1	2.36	0.58
1:F:244:VAL:O	1:F:245:VAL:HG23	2.04	0.58
5:A:2008:HOH:O	1:E:68:ARG:HD3	2.04	0.58
1:G:177:LEU:CD2	1:G:198:VAL:HG22	2.32	0.58
1:F:246:GLY:HA2	1:F:247:GLN:HG3	1.83	0.58
1:D:142:ILE:CD1	1:D:230:LEU:HD11	2.34	0.58
1:G:178:TYR:O	1:G:184:ARG:NH2	2.37	0.58
1:H:182:ARG:NH2	1:H:201:GLN:OE1	2.36	0.58
1:J:315:GLU:HG3	1:J:366:TYR:OH	2.04	0.57
1:D:259:VAL:HG21	1:D:360:TYR:CZ	2.37	0.57
1:H:283:THR:HB	1:H:286:GLN:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ASP:OD2	1:D:182:ARG:NH1	2.37	0.57
1:J:365:GLN:HG3	1:J:366:TYR:N	2.19	0.57
1:G:177:LEU:C	1:G:179:GLU:H	2.06	0.57
1:I:182:ARG:NH2	1:I:201:GLN:OE1	2.34	0.57
1:I:180:ASP:HB3	1:I:183:VAL:HG13	1.85	0.57
1:B:168:LEU:C	1:B:168:LEU:HD23	2.25	0.57
1:C:245:VAL:O	1:C:245:VAL:HG13	2.05	0.57
1:A:258:ARG:HG3	1:D:361:ASP:OD1	2.05	0.57
1:F:10:HIS:HE1	1:F:38:GLU:OE2	1.87	0.57
1:G:169:MET:CE	1:G:169:MET:CG	2.83	0.57
1:D:290:LEU:HB3	1:D:298:ARG:HG3	1.86	0.57
1:G:247:GLN:HG2	1:G:247:GLN:O	2.05	0.57
1:G:97:HIS:CE1	1:G:168:LEU:HD12	2.39	0.57
1:B:131:ARG:HB2	5:B:2023:HOH:O	2.05	0.57
1:A:270:ASP:OD2	1:A:270:ASP:C	2.42	0.57
1:F:182:ARG:NH2	1:F:201:GLN:OE1	2.38	0.56
1:A:373:ARG:CD	5:A:2074:HOH:O	2.43	0.56
1:B:288:GLU:O	1:B:291:GLU:HB2	2.05	0.56
1:D:50:ALA:O	1:D:51:PRO:C	2.43	0.56
1:B:177:LEU:HD23	1:B:198:VAL:HG22	1.86	0.56
1:I:168:LEU:HD23	1:I:168:LEU:C	2.25	0.56
1:C:365:GLN:NE2	5:C:2034:HOH:O	2.38	0.56
1:G:365:GLN:HG3	1:G:366:TYR:H	1.69	0.56
1:A:182:ARG:NH2	1:A:201:GLN:OE1	2.36	0.56
1:J:142:ILE:HD13	1:J:230:LEU:HD12	1.88	0.56
1:B:180:ASP:HB3	1:B:183:VAL:HG13	1.87	0.56
1:E:203:GLY:CA	1:E:249:ALA:HB2	2.35	0.56
1:H:109:ASP:HB3	1:H:110:TRP:CD1	2.30	0.56
1:G:259:VAL:CG2	1:G:360:TYR:CE1	2.88	0.56
1:H:59:THR:HG21	5:H:2002:HOH:O	2.05	0.56
1:D:257:HIS:N	1:D:257:HIS:CD2	2.74	0.56
1:G:180:ASP:HB3	1:G:183:VAL:CG1	2.36	0.56
1:C:131:ARG:O	1:C:360:TYR:HE2	1.88	0.56
1:H:168:LEU:C	1:H:168:LEU:HD23	2.27	0.56
1:I:218:ARG:HH11	1:I:218:ARG:HG2	1.71	0.56
1:B:284:PRO:CB	1:F:288:GLU:HG3	2.32	0.56
1:G:365:GLN:HB3	5:G:2020:HOH:O	2.06	0.56
1:C:205:SER:CB	1:C:250:ILE:CG2	2.80	0.55
1:A:66:GLN:HE21	2:A:400:GDX:HN21	1.54	0.55
1:C:109:ASP:CG	5:C:2008:HOH:O	2.38	0.55
1:B:142:ILE:CD1	1:B:230:LEU:HD12	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:ARG:CG	1:I:218:ARG:HH11	2.19	0.55
1:B:66:GLN:HE21	2:B:400:GDX:HN21	1.55	0.55
1:C:315:GLU:HG3	1:C:366:TYR:OH	2.06	0.55
1:J:70:GLY:HA2	1:J:185:ARG:HA	1.89	0.55
1:A:224:ASP:HB3	1:A:341:PHE:CZ	2.41	0.55
1:A:52:GLU:HG2	1:A:55:ARG:HH11	1.70	0.55
1:G:277:ARG:CZ	1:G:281:HIS:HD2	2.20	0.55
1:C:304:CYS:HA	1:C:307:ARG:O	2.07	0.55
1:A:369:ARG:CD	5:A:2072:HOH:O	2.46	0.55
1:C:142:ILE:HD13	1:C:230:LEU:HD12	1.87	0.55
1:G:131:ARG:O	1:G:360:TYR:HE2	1.90	0.55
1:A:179:GLU:CG	5:A:2033:HOH:O	2.48	0.55
1:E:288:GLU:O	1:E:291:GLU:HB2	2.07	0.54
1:D:181:GLU:OE1	1:D:185:ARG:NH2	2.40	0.54
1:D:362:TYR:O	1:D:365:GLN:HG3	2.07	0.54
1:B:224:ASP:HB3	1:B:341:PHE:CZ	2.42	0.54
1:J:201:GLN:O	1:J:246:GLY:O	2.24	0.54
1:E:283:THR:HG23	5:E:2029:HOH:O	2.06	0.54
1:A:52:GLU:O	1:A:55:ARG:N	2.34	0.54
1:F:247:GLN:CG	1:F:248:PRO:HD2	2.19	0.54
1:A:223:LEU:O	1:A:226:LEU:HB2	2.07	0.54
1:G:138:ILE:HB	4:G:1382:CL:CL	2.44	0.54
1:F:97:HIS:CE1	1:F:168:LEU:HD12	2.43	0.54
1:A:288:GLU:O	1:A:291:GLU:HB2	2.08	0.54
1:C:182:ARG:NH2	1:C:201:GLN:OE1	2.36	0.54
1:H:259:VAL:CG2	1:H:360:TYR:CE1	2.86	0.54
1:F:180:ASP:OD2	1:F:182:ARG:NH1	2.41	0.54
1:D:110:TRP:H	1:D:110:TRP:HD1	1.53	0.54
1:C:290:LEU:HB3	1:C:298:ARG:HG3	1.90	0.54
1:B:142:ILE:HD13	1:B:230:LEU:HD12	1.89	0.53
1:A:142:ILE:HD11	1:A:230:LEU:HD11	1.91	0.53
1:C:181:GLU:OE1	1:C:185:ARG:NH2	2.40	0.53
1:D:50:ALA:O	1:D:53:ILE:N	2.42	0.53
1:D:66:GLN:HE21	2:D:400:GDX:HN21	1.55	0.53
1:C:218:ARG:HB3	5:C:2038:HOH:O	2.09	0.53
1:G:177:LEU:C	1:G:179:GLU:N	2.59	0.53
1:H:205:SER:HB2	1:H:250:ILE:CG2	2.35	0.53
1:G:328:HIS:CD2	5:G:2019:HOH:O	2.40	0.53
1:E:123:GLY:HA2	1:E:170:ARG:CD	2.38	0.53
1:E:10:HIS:HE1	1:E:38:GLU:OE2	1.91	0.53
1:I:180:ASP:OD2	1:I:182:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:LEU:HB3	1:G:298:ARG:HG3	1.90	0.53
1:F:70:GLY:HA2	1:F:185:ARG:HA	1.91	0.53
1:C:177:LEU:HD23	1:C:198:VAL:HG22	1.90	0.53
1:D:131:ARG:O	1:D:360:TYR:HE2	1.91	0.53
1:D:132:ALA:HB3	1:D:135:ASP:OD2	2.09	0.53
1:H:59:THR:CG2	5:H:2002:HOH:O	2.56	0.53
1:I:277:ARG:CZ	1:I:281:HIS:HD2	2.22	0.53
1:J:259:VAL:CG2	1:J:360:TYR:CE1	2.87	0.53
1:I:131:ARG:O	1:I:360:TYR:HE2	1.91	0.53
1:F:244:VAL:CG1	1:F:245:VAL:N	2.71	0.53
1:D:142:ILE:HD13	1:D:230:LEU:HD12	1.90	0.53
1:H:257:HIS:N	1:H:257:HIS:CD2	2.76	0.53
1:C:184:ARG:HG2	1:C:184:ARG:NH1	2.23	0.53
1:E:151:TRP:CD1	1:E:245:VAL:HG23	2.44	0.52
1:C:180:ASP:OD2	1:C:182:ARG:NH1	2.42	0.52
1:E:304:CYS:HA	1:E:307:ARG:O	2.09	0.52
1:G:182:ARG:NH2	1:G:201:GLN:OE1	2.40	0.52
1:C:142:ILE:HD13	1:C:230:LEU:CD1	2.38	0.52
1:A:180:ASP:OD1	1:A:182:ARG:HB2	2.07	0.52
1:G:142:ILE:HD11	1:G:230:LEU:HD11	1.90	0.52
1:B:258:ARG:HH21	1:C:258:ARG:HE	1.56	0.52
1:C:123:GLY:HA2	1:C:170:ARG:CD	2.35	0.52
1:G:85:ARG:HB2	1:G:178:TYR:CE1	2.42	0.52
1:A:52:GLU:CD	1:A:55:ARG:NH1	2.62	0.52
1:C:10:HIS:HE1	1:C:38:GLU:OE2	1.92	0.52
1:D:49:ALA:O	1:D:50:ALA:C	2.47	0.52
1:I:109:ASP:HB3	1:I:110:TRP:CD1	2.30	0.52
1:F:136:ALA:HA	4:F:1382:CL:CL	2.46	0.52
1:G:177:LEU:HB3	1:G:183:VAL:HG21	1.92	0.52
1:I:142:ILE:HD11	1:I:230:LEU:HD11	1.92	0.52
1:I:155:GLU:HG3	1:I:251:HIS:ND1	2.24	0.52
1:D:52:GLU:O	1:D:55:ARG:CG	2.51	0.52
1:J:246:GLY:N	1:J:247:GLN:HB2	2.25	0.52
1:E:283:THR:HB	1:E:286:GLN:NE2	2.25	0.52
1:B:262:HIS:CE1	5:B:2044:HOH:O	2.55	0.51
1:A:49:ALA:O	1:A:53:ILE:HG13	2.11	0.51
1:I:181:GLU:OE1	1:I:185:ARG:NH2	2.44	0.51
1:A:10:HIS:HE1	1:A:38:GLU:OE2	1.93	0.51
1:J:283:THR:CG2	1:J:335:ASP:OD2	2.45	0.51
1:J:304:CYS:HA	1:J:307:ARG:O	2.10	0.51
1:E:131:ARG:O	1:E:360:TYR:HE2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HE2	5:A:2078:HOH:O	2.11	0.51
1:H:301:LEU:O	1:H:304:CYS:HB2	2.10	0.51
1:A:362:TYR:O	1:A:365:GLN:HG3	2.10	0.51
1:H:180:ASP:OD2	1:H:182:ARG:NH1	2.44	0.51
1:F:315:GLU:HG3	1:F:366:TYR:OH	2.11	0.51
1:C:136:ALA:HA	4:C:1382:CL:CL	2.48	0.51
1:H:70:GLY:HA2	1:H:185:ARG:HA	1.92	0.51
1:G:70:GLY:HA2	1:G:185:ARG:HA	1.92	0.51
1:G:177:LEU:HD23	1:G:198:VAL:CG2	2.38	0.50
1:C:262:HIS:HE1	5:C:2020:HOH:O	1.93	0.50
1:A:70:GLY:HA2	1:A:185:ARG:HA	1.93	0.50
1:F:330:GLN:HB2	1:F:336:TRP:CD1	2.46	0.50
1:B:109:ASP:HB3	1:B:110:TRP:CD1	2.35	0.50
1:B:142:ILE:HD13	1:B:230:LEU:CD1	2.41	0.50
1:B:283:THR:HB	1:B:286:GLN:NE2	2.26	0.50
1:D:109:ASP:HB3	1:D:110:TRP:CD1	2.37	0.50
1:D:97:HIS:CE1	1:D:168:LEU:HD12	2.47	0.50
1:H:288:GLU:O	1:H:291:GLU:HB2	2.11	0.50
1:H:290:LEU:HB3	1:H:298:ARG:HG3	1.93	0.50
1:I:257:HIS:CD2	1:I:257:HIS:N	2.79	0.50
1:D:53:ILE:C	1:D:55:ARG:N	2.64	0.50
1:J:286:GLN:C	1:J:288:GLU:N	2.61	0.50
1:H:123:GLY:HA2	1:H:170:ARG:CD	2.41	0.50
1:D:132:ALA:HB3	1:D:135:ASP:CG	2.32	0.50
1:A:245:VAL:O	1:A:246:GLY:O	2.30	0.50
1:E:257:HIS:N	1:E:257:HIS:CD2	2.79	0.50
1:E:246:GLY:O	1:E:247:GLN:O	2.30	0.50
1:C:97:HIS:CE1	1:C:168:LEU:HD12	2.45	0.50
1:A:68:ARG:HD2	5:A:2009:HOH:O	2.11	0.50
1:G:247:GLN:CG	1:G:247:GLN:O	2.60	0.50
1:A:365:GLN:HG3	1:A:366:TYR:N	2.27	0.50
1:B:246:GLY:O	1:B:247:GLN:O	2.30	0.50
1:D:50:ALA:N	1:D:51:PRO:HD2	2.23	0.50
1:I:247:GLN:O	1:I:248:PRO:O	2.30	0.50
1:F:142:ILE:HD13	1:F:230:LEU:HD12	1.94	0.50
1:I:10:HIS:HE1	1:I:38:GLU:OE2	1.95	0.50
1:J:381:GLU:HG2	1:J:382:ASN:N	2.26	0.50
1:D:51:PRO:O	1:D:55:ARG:HB3	2.12	0.50
1:B:70:GLY:HA2	1:B:185:ARG:HA	1.93	0.50
1:I:246:GLY:O	1:I:247:GLN:OE1	2.30	0.50
1:G:247:GLN:O	1:G:248:PRO:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:GLU:O	1:G:291:GLU:HB2	2.12	0.50
1:G:123:GLY:HA2	1:G:170:ARG:CD	2.38	0.49
1:D:142:ILE:HD13	1:D:230:LEU:CD1	2.42	0.49
1:J:66:GLN:HE21	2:J:400:GDX:HN21	1.59	0.49
1:J:123:GLY:HA2	1:J:170:ARG:CD	2.41	0.49
1:H:142:ILE:HD13	1:H:230:LEU:CD1	2.42	0.49
1:H:142:ILE:HD13	1:H:230:LEU:HD12	1.94	0.49
1:H:181:GLU:OE1	1:H:185:ARG:NH2	2.45	0.49
1:F:244:VAL:O	1:F:245:VAL:CG2	2.59	0.49
1:A:318:TRP:HB2	1:A:347:ARG:HD3	1.92	0.49
1:D:304:CYS:HA	1:D:307:ARG:O	2.12	0.49
1:D:52:GLU:O	1:D:52:GLU:OE1	2.30	0.49
1:I:247:GLN:OE1	1:I:247:GLN:O	2.30	0.49
1:D:315:GLU:HG3	1:D:366:TYR:OH	2.12	0.49
1:B:245:VAL:O	1:B:245:VAL:HG12	2.12	0.49
1:D:365:GLN:HG3	1:D:366:TYR:N	2.26	0.49
1:A:260:PRO:HG2	1:A:263:ILE:HD12	1.93	0.49
1:J:142:ILE:CD1	1:J:230:LEU:HD11	2.42	0.49
1:J:270:ASP:OD2	1:J:270:ASP:C	2.51	0.49
1:A:362:TYR:O	1:A:365:GLN:CG	2.61	0.49
1:F:66:GLN:HE21	2:F:400:GDX:HN21	1.61	0.49
1:B:131:ARG:CZ	5:B:2018:HOH:O	2.59	0.49
1:D:70:GLY:HA2	1:D:185:ARG:HA	1.95	0.49
1:F:168:LEU:HD23	1:F:168:LEU:C	2.33	0.49
1:A:277:ARG:CZ	1:A:281:HIS:HD2	2.25	0.49
1:I:290:LEU:HB3	1:I:298:ARG:HG3	1.93	0.49
1:B:177:LEU:CD2	1:B:198:VAL:HG22	2.43	0.49
1:F:244:VAL:C	1:F:245:VAL:HG23	2.33	0.48
1:A:41:GLN:CA	1:A:41:GLN:HE21	2.10	0.48
1:E:16:LEU:HD13	1:E:101:ALA:HB1	1.95	0.48
1:B:315:GLU:HG3	1:B:366:TYR:OH	2.14	0.48
1:I:312:PHE:CE2	1:I:313:MET:HB2	2.48	0.48
1:D:288:GLU:O	1:D:291:GLU:HB2	2.12	0.48
1:H:218:ARG:HH11	1:H:218:ARG:CG	2.26	0.48
1:C:362:TYR:O	1:C:365:GLN:HG3	2.12	0.48
1:C:247:GLN:HA	1:C:248:PRO:HD2	1.43	0.48
1:D:315:GLU:HG2	1:D:370:MET:HG3	1.94	0.48
1:J:109:ASP:HB3	1:J:110:TRP:CD1	2.32	0.48
1:D:110:TRP:N	1:D:110:TRP:CD1	2.80	0.48
1:J:142:ILE:CD1	1:J:230:LEU:HD12	2.43	0.48
1:C:184:ARG:HA	1:C:184:ARG:HD3	1.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:HIS:CD2	1:G:256:PRO:HD2	2.48	0.48
1:B:362:TYR:O	1:B:365:GLN:HG3	2.14	0.48
1:A:50:ALA:O	1:A:54:SER:OG	2.32	0.48
1:A:315:GLU:HG3	1:A:366:TYR:OH	2.14	0.48
1:F:247:GLN:HB3	1:F:248:PRO:CD	2.41	0.48
1:D:255:HIS:CD2	1:D:256:PRO:HD2	2.49	0.48
1:C:132:ALA:HB3	1:C:135:ASP:OD2	2.13	0.48
1:B:17:LEU:HD21	1:B:46:VAL:HA	1.96	0.48
1:E:218:ARG:NH1	1:E:218:ARG:CG	2.71	0.48
1:I:70:GLY:HA2	1:I:185:ARG:HA	1.96	0.48
1:G:10:HIS:HE1	1:G:38:GLU:OE2	1.96	0.48
1:J:17:LEU:HD21	1:J:46:VAL:HA	1.96	0.48
1:E:17:LEU:HD21	1:E:46:VAL:HA	1.96	0.48
1:C:262:HIS:CD2	1:C:263:ILE:HG13	2.48	0.47
1:H:39:ARG:HB2	1:I:71:THR:HB	1.95	0.47
1:F:17:LEU:HD21	1:F:46:VAL:HA	1.96	0.47
1:H:255:HIS:CD2	1:H:256:PRO:HD2	2.49	0.47
1:E:205:SER:HB2	1:E:250:ILE:HB	1.96	0.47
1:F:257:HIS:N	1:F:257:HIS:CD2	2.82	0.47
1:G:362:TYR:O	1:G:365:GLN:HG3	2.14	0.47
1:C:257:HIS:CD2	1:C:257:HIS:N	2.82	0.47
1:I:142:ILE:HD13	1:I:230:LEU:CD1	2.44	0.47
1:E:315:GLU:HG3	1:E:366:TYR:OH	2.14	0.47
1:A:262:HIS:CE1	5:A:2039:HOH:O	2.59	0.47
1:A:258:ARG:HH21	1:D:258:ARG:HE	1.63	0.47
1:C:177:LEU:CD2	1:C:198:VAL:HG22	2.44	0.47
1:G:357:LEU:HD13	1:H:357:LEU:HD13	1.96	0.47
1:E:142:ILE:CD1	1:E:230:LEU:HD11	2.44	0.47
1:A:14:GLU:CD	1:A:14:GLU:H	2.17	0.47
1:G:188:ASP:HB2	1:G:232:GLU:OE2	2.15	0.47
1:A:315:GLU:HG2	1:A:370:MET:HG3	1.96	0.47
1:F:288:GLU:O	1:F:291:GLU:HB2	2.14	0.47
1:B:142:ILE:HD12	1:B:230:LEU:CD1	2.44	0.47
1:C:218:ARG:CG	1:C:218:ARG:HH11	2.28	0.47
1:A:258:ARG:HE	1:D:258:ARG:HH21	1.63	0.47
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.80	0.47
1:D:132:ALA:N	1:D:135:ASP:OD2	2.40	0.47
1:G:181:GLU:OE1	1:G:185:ARG:NH2	2.48	0.47
1:C:247:GLN:CB	1:C:248:PRO:O	2.52	0.47
1:A:368:TYR:CD2	1:D:255:HIS:CE1	3.03	0.47
1:C:17:LEU:HD21	1:C:46:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:CD2	1:E:198:VAL:HG22	2.45	0.47
1:A:247:GLN:HA	1:A:248:PRO:HD3	1.39	0.47
1:C:277:ARG:CZ	1:C:281:HIS:HD2	2.28	0.47
1:D:277:ARG:CZ	1:D:281:HIS:HD2	2.28	0.47
1:H:142:ILE:HD11	1:H:230:LEU:HD11	1.97	0.47
1:B:132:ALA:HB3	1:B:135:ASP:OD2	2.15	0.47
1:G:191:ILE:CG2	1:G:192:ASP:N	2.78	0.47
1:G:178:TYR:HA	5:G:2012:HOH:O	2.14	0.47
1:J:283:THR:O	1:J:286:GLN:N	2.48	0.47
1:J:285:ARG:NH1	1:J:335:ASP:HB2	2.29	0.47
1:H:97:HIS:CE1	1:H:168:LEU:HD12	2.50	0.47
1:C:151:TRP:CD1	1:C:245:VAL:HG11	2.49	0.46
1:B:66:GLN:NE2	2:B:400:GDX:HN21	2.12	0.46
1:C:288:GLU:O	1:C:291:GLU:HB2	2.15	0.46
1:I:288:GLU:O	1:I:291:GLU:HB2	2.15	0.46
1:H:223:LEU:HD22	1:H:274:THR:HG21	1.96	0.46
1:G:330:GLN:HB2	1:G:336:TRP:CD1	2.50	0.46
1:G:84:LEU:HB3	1:G:178:TYR:HD1	1.81	0.46
1:J:188:ASP:HB2	1:J:232:GLU:OE2	2.15	0.46
1:G:17:LEU:HD21	1:G:46:VAL:HA	1.96	0.46
1:H:14:GLU:H	1:H:14:GLU:CD	2.19	0.46
1:I:136:ALA:HA	4:I:1382:CL:CL	2.53	0.46
1:A:155:GLU:OE1	1:D:252:ARG:NH1	2.47	0.46
1:C:110:TRP:O	1:C:127:HIS:HE1	1.99	0.46
1:D:168:LEU:HD23	1:D:168:LEU:C	2.36	0.46
1:J:97:HIS:CE1	1:J:168:LEU:HD12	2.51	0.46
1:J:180:ASP:OD2	1:J:182:ARG:NH1	2.48	0.46
1:D:21:ARG:HD3	1:D:53:ILE:HG12	1.97	0.46
1:C:66:GLN:HE21	2:C:400:GDX:HN21	1.64	0.46
1:G:362:TYR:O	1:G:365:GLN:CG	2.64	0.46
1:C:168:LEU:HD23	1:C:168:LEU:C	2.36	0.46
1:G:310:PHE:CZ	1:H:272:GLU:HB2	2.51	0.46
1:D:218:ARG:CG	1:D:218:ARG:HH11	2.29	0.46
1:B:16:LEU:HD13	1:B:101:ALA:HB1	1.96	0.46
1:A:110:TRP:O	1:A:127:HIS:HE1	1.98	0.46
1:F:142:ILE:HD11	1:F:230:LEU:HD11	1.97	0.46
1:A:97:HIS:CE1	1:A:168:LEU:HD12	2.51	0.46
1:I:318:TRP:HB2	1:I:347:ARG:HD3	1.97	0.46
1:F:203:GLY:HA2	1:F:249:ALA:HB2	1.98	0.46
1:B:39:ARG:NE	5:B:2004:HOH:O	2.48	0.46
1:F:131:ARG:O	1:F:360:TYR:HE2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLU:HG3	1:A:182:ARG:N	2.26	0.46
1:A:277:ARG:HA	1:A:280:GLN:OE1	2.16	0.46
1:E:177:LEU:HD23	1:E:198:VAL:HG22	1.97	0.46
1:E:150:LEU:HB2	1:E:151:TRP:CE3	2.51	0.46
1:H:188:ASP:HB2	1:H:232:GLU:OE2	2.16	0.46
1:G:85:ARG:CB	1:G:178:TYR:HE1	2.25	0.45
1:I:180:ASP:OD1	1:I:182:ARG:HB2	2.16	0.45
1:B:259:VAL:CG2	1:B:360:TYR:CE1	2.97	0.45
1:A:180:ASP:OD2	1:A:182:ARG:NH1	2.49	0.45
1:C:373:ARG:NH1	5:C:2037:HOH:O	2.39	0.45
1:J:285:ARG:HG2	1:J:335:ASP:OD1	2.16	0.45
1:H:66:GLN:HE21	2:H:400:GDX:HN21	1.64	0.45
1:B:224:ASP:HB3	1:B:341:PHE:HZ	1.80	0.45
1:F:304:CYS:HA	1:F:307:ARG:O	2.17	0.45
1:A:135:ASP:O	1:A:136:ALA:HB3	2.15	0.45
1:G:110:TRP:CD1	1:G:110:TRP:N	2.85	0.45
1:F:291:GLU:OE1	1:F:302:ARG:NH2	2.48	0.45
1:A:127:HIS:HA	1:A:209:CYS:HB3	1.98	0.45
1:F:142:ILE:CD1	1:F:230:LEU:HD12	2.47	0.45
1:I:338:GLU:HG3	1:I:342:LYS:NZ	2.32	0.45
1:B:306:ARG:HG2	5:F:2001:HOH:O	2.15	0.45
1:A:140:TRP:CD2	1:A:367:LEU:HD13	2.51	0.45
1:C:201:GLN:NE2	1:C:244:VAL:O	2.41	0.45
1:H:110:TRP:N	1:H:110:TRP:CD1	2.84	0.45
1:J:290:LEU:HB3	1:J:298:ARG:HG3	1.97	0.45
1:J:283:THR:O	1:J:284:PRO:C	2.54	0.45
1:I:110:TRP:CD1	1:I:110:TRP:N	2.84	0.45
1:J:168:LEU:C	1:J:168:LEU:HD23	2.37	0.45
1:I:17:LEU:HD21	1:I:46:VAL:HA	1.98	0.45
1:I:66:GLN:NE2	2:I:400:GDX:N1	2.57	0.45
1:A:66:GLN:NE2	2:A:400:GDX:HN21	2.13	0.45
1:F:259:VAL:CG2	1:F:360:TYR:CE1	2.91	0.45
1:D:259:VAL:CG2	1:D:360:TYR:CE1	2.95	0.45
1:A:29:VAL:O	1:A:59:THR:HG21	2.17	0.45
1:G:68:ARG:NH1	1:G:187:SER:OG	2.50	0.45
1:B:258:ARG:HE	1:C:258:ARG:HH21	1.63	0.45
1:G:260:PRO:HA	5:G:2016:HOH:O	2.17	0.45
1:J:177:LEU:HD23	1:J:198:VAL:HG22	1.99	0.45
1:G:14:GLU:H	1:G:14:GLU:CD	2.20	0.45
1:E:245:VAL:CG1	1:E:246:GLY:N	2.79	0.44
1:A:109:ASP:HB3	1:A:110:TRP:CD1	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:LEU:HD21	1:H:46:VAL:HA	1.99	0.44
1:G:77:GLY:O	1:G:78:ASP:C	2.55	0.44
1:F:123:GLY:HA2	1:F:170:ARG:CD	2.43	0.44
1:C:142:ILE:HD11	1:C:230:LEU:HD11	1.96	0.44
1:A:215:LYS:CE	5:A:2078:HOH:O	2.65	0.44
1:B:255:HIS:CE1	1:C:368:TYR:CD2	3.06	0.44
1:I:315:GLU:HG2	1:I:370:MET:HG3	1.98	0.44
1:H:70:GLY:HA3	1:H:187:SER:HB3	2.00	0.44
1:H:218:ARG:HG2	1:H:218:ARG:HH11	1.82	0.44
1:F:262:HIS:CD2	1:F:263:ILE:HG13	2.53	0.44
1:B:257:HIS:N	1:B:257:HIS:CD2	2.84	0.44
1:D:246:GLY:C	1:D:247:GLN:CG	2.85	0.44
1:J:177:LEU:CD2	1:J:198:VAL:HG22	2.47	0.44
1:E:132:ALA:HB3	1:E:135:ASP:OD2	2.17	0.44
1:G:301:LEU:HA	1:G:301:LEU:HD23	1.84	0.44
1:J:131:ARG:O	1:J:360:TYR:HE2	2.01	0.44
1:J:203:GLY:HA2	1:J:249:ALA:HB2	1.99	0.44
1:H:131:ARG:HD2	1:H:131:ARG:HA	1.87	0.44
1:B:365:GLN:HG3	1:B:366:TYR:N	2.33	0.44
1:C:218:ARG:HG2	1:C:218:ARG:HH11	1.83	0.44
1:E:142:ILE:CD1	1:E:230:LEU:CD1	2.95	0.44
1:E:110:TRP:O	1:E:127:HIS:HE1	2.01	0.44
1:J:365:GLN:HG3	1:J:366:TYR:H	1.82	0.44
1:B:136:ALA:HA	4:B:1382:CL:CL	2.54	0.44
1:I:14:GLU:CD	1:I:14:GLU:H	2.21	0.44
1:D:123:GLY:HA2	1:D:170:ARG:CD	2.45	0.44
1:J:142:ILE:HD11	1:J:230:LEU:HD11	2.00	0.44
1:C:307:ARG:HD2	1:D:276:HIS:CD2	2.53	0.44
1:A:283:THR:HB	1:A:286:GLN:NE2	2.33	0.44
1:A:267:VAL:C	5:A:2053:HOH:O	2.56	0.44
1:E:225:ASP:HB3	5:E:2024:HOH:O	2.18	0.44
1:G:168:LEU:HD23	1:G:168:LEU:C	2.38	0.43
1:A:365:GLN:HB3	5:A:2066:HOH:O	2.18	0.43
1:C:245:VAL:HA	1:C:246:GLY:HA3	1.89	0.43
1:G:66:GLN:HE21	2:G:400:GDX:HN21	1.66	0.43
1:A:110:TRP:N	1:A:110:TRP:CD1	2.87	0.43
1:G:223:LEU:HD22	1:G:274:THR:HG21	1.99	0.43
1:E:255:HIS:CD2	1:E:256:PRO:HD2	2.53	0.43
1:G:218:ARG:CG	1:G:218:ARG:HH11	2.31	0.43
1:J:277:ARG:CZ	1:J:281:HIS:HD2	2.31	0.43
1:G:122:TYR:CG	1:G:207:TYR:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:LEU:CD2	1:F:198:VAL:HG22	2.48	0.43
1:A:17:LEU:HD21	1:A:46:VAL:HA	2.00	0.43
1:A:257:HIS:N	1:A:257:HIS:CD2	2.84	0.43
1:G:178:TYR:CD2	1:G:178:TYR:C	2.88	0.43
1:B:290:LEU:HB3	1:B:298:ARG:HG3	2.00	0.43
1:B:35:ILE:HD12	1:B:35:ILE:HG23	1.32	0.43
1:B:365:GLN:CG	1:B:365:GLN:CA	2.84	0.43
1:E:365:GLN:HG3	1:E:366:TYR:H	1.82	0.43
1:H:98:PHE:O	1:H:166:GLU:HA	2.18	0.43
1:J:313:MET:HG3	1:J:313:MET:O	2.18	0.43
1:E:97:HIS:CE1	1:E:168:LEU:HD12	2.53	0.43
1:D:52:GLU:OE2	1:D:53:ILE:HA	2.18	0.43
1:A:123:GLY:HA2	1:A:170:ARG:CD	2.47	0.43
1:H:315:GLU:HG3	1:H:366:TYR:OH	2.19	0.43
1:E:301:LEU:HD23	1:E:301:LEU:HA	1.82	0.43
1:J:245:VAL:HA	1:J:246:GLY:HA3	1.53	0.43
1:C:110:TRP:CD1	1:C:110:TRP:N	2.87	0.43
1:G:41:GLN:HE21	1:G:41:GLN:CA	2.23	0.43
1:B:180:ASP:OD1	1:B:182:ARG:HD3	2.18	0.43
1:C:260:PRO:HG2	1:C:263:ILE:HD12	2.00	0.43
1:F:14:GLU:H	1:F:14:GLU:CD	2.21	0.43
1:J:288:GLU:O	1:J:291:GLU:HB2	2.19	0.43
1:J:289:LEU:HA	1:J:289:LEU:HD12	1.91	0.43
1:A:52:GLU:HG2	1:A:55:ARG:NH1	2.32	0.43
1:F:142:ILE:HD13	1:F:230:LEU:CD1	2.47	0.43
1:J:142:ILE:HD13	1:J:230:LEU:CD1	2.48	0.43
1:J:362:TYR:O	1:J:365:GLN:HG3	2.19	0.43
1:J:255:HIS:CD2	1:J:256:PRO:HD2	2.54	0.43
1:D:333:ASP:OD1	1:D:333:ASP:C	2.55	0.43
1:J:131:ARG:HD2	1:J:131:ARG:HA	1.84	0.43
1:E:259:VAL:CG2	1:E:360:TYR:CE1	2.97	0.43
1:I:142:ILE:HD13	1:I:230:LEU:HD12	2.01	0.43
1:G:270:ASP:C	1:G:270:ASP:OD2	2.57	0.43
1:J:333:ASP:C	1:J:333:ASP:OD1	2.56	0.43
1:C:244:VAL:C	1:C:245:VAL:HG12	2.39	0.43
1:H:180:ASP:OD1	1:H:182:ARG:HB2	2.19	0.43
1:H:177:LEU:HD23	1:H:198:VAL:HG22	2.00	0.43
1:C:140:TRP:CZ3	1:C:367:LEU:HB3	2.54	0.43
1:F:246:GLY:CA	1:F:247:GLN:CB	2.96	0.42
1:F:277:ARG:CZ	1:F:281:HIS:HD2	2.32	0.42
1:I:364:GLN:CB	5:I:2010:HOH:O	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:TYR:CD2	1:D:255:HIS:ND1	2.87	0.42
1:F:100:ASP:O	1:F:103:ILE:HD12	2.19	0.42
1:F:270:ASP:C	1:F:270:ASP:OD2	2.57	0.42
1:A:258:ARG:HH22	1:A:361:ASP:CG	2.22	0.42
1:C:262:HIS:CE1	5:C:2020:HOH:O	2.69	0.42
1:A:248:PRO:CG	1:D:252:ARG:HH12	2.32	0.42
1:H:177:LEU:CD2	1:H:198:VAL:HG22	2.48	0.42
1:E:224:ASP:HB3	1:E:341:PHE:CZ	2.55	0.42
1:I:362:TYR:O	1:I:365:GLN:HG3	2.19	0.42
1:F:109:ASP:HB3	1:F:110:TRP:H	1.60	0.42
1:D:218:ARG:HG2	1:D:218:ARG:HH11	1.83	0.42
1:F:177:LEU:HD23	1:F:198:VAL:HG22	2.01	0.42
1:G:381:GLU:HG2	1:G:382:ASN:N	2.34	0.42
1:J:140:TRP:CD2	1:J:367:LEU:HD13	2.54	0.42
1:F:110:TRP:N	1:F:110:TRP:CD1	2.87	0.42
1:B:110:TRP:O	1:B:127:HIS:HE1	2.02	0.42
1:A:255:HIS:ND1	1:D:368:TYR:CD2	2.88	0.42
1:C:330:GLN:HB2	1:C:336:TRP:CD1	2.54	0.42
1:G:64:ARG:HG2	5:G:2004:HOH:O	2.18	0.42
1:J:258:ARG:HH22	1:J:361:ASP:CG	2.23	0.42
1:G:72:LEU:HB3	1:G:73:ARG:H	1.62	0.42
1:D:52:GLU:OE2	1:D:53:ILE:CA	2.68	0.42
1:D:66:GLN:NE2	2:D:400:GDX:HN21	2.16	0.42
1:F:16:LEU:HD13	1:F:101:ALA:HB1	2.01	0.42
1:G:140:TRP:CD2	1:G:367:LEU:HD13	2.54	0.42
1:J:110:TRP:O	1:J:127:HIS:HE1	2.03	0.42
1:B:131:ARG:O	1:B:360:TYR:HE2	2.03	0.42
1:H:367:LEU:O	1:H:370:MET:HB3	2.20	0.42
1:H:218:ARG:HB3	1:H:218:ARG:NH1	2.34	0.42
1:A:248:PRO:CB	1:D:252:ARG:HH12	2.32	0.42
1:E:153:HIS:HE1	1:G:120:PHE:O	2.02	0.42
1:E:181:GLU:OE1	1:E:185:ARG:NH2	2.53	0.42
1:C:301:LEU:HA	1:C:301:LEU:HD23	1.84	0.42
1:E:203:GLY:HA2	1:E:249:ALA:HB2	2.00	0.42
1:D:14:GLU:CD	1:D:14:GLU:H	2.23	0.42
1:J:201:GLN:HA	1:J:245:VAL:CG1	2.50	0.42
1:A:131:ARG:HD2	1:A:131:ARG:HA	1.81	0.42
1:D:35:ILE:HG23	1:D:35:ILE:HD12	1.66	0.42
1:A:218:ARG:HG2	1:A:218:ARG:HH11	1.84	0.41
1:D:246:GLY:O	1:D:247:GLN:CG	2.66	0.41
1:F:218:ARG:HH11	1:F:218:ARG:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:10:HIS:CE1	1:J:38:GLU:OE2	2.71	0.41
1:J:181:GLU:OE1	1:J:185:ARG:NH2	2.53	0.41
1:D:132:ALA:CB	1:D:135:ASP:OD2	2.68	0.41
1:D:224:ASP:HB3	1:D:341:PHE:CZ	2.55	0.41
1:E:362:TYR:O	1:E:365:GLN:HG3	2.20	0.41
1:D:142:ILE:HD11	1:D:230:LEU:HD11	2.02	0.41
1:B:98:PHE:O	1:B:166:GLU:HA	2.21	0.41
1:I:224:ASP:HB3	1:I:341:PHE:CZ	2.55	0.41
1:C:224:ASP:HB3	1:C:341:PHE:CZ	2.55	0.41
1:E:14:GLU:CD	1:E:14:GLU:H	2.23	0.41
1:H:333:ASP:C	1:H:333:ASP:OD1	2.59	0.41
1:J:326:LEU:HD23	1:J:326:LEU:HA	1.91	0.41
1:G:176:MET:CE	1:G:202:GLN:HG3	2.50	0.41
1:G:315:GLU:HG3	1:G:366:TYR:OH	2.19	0.41
1:B:123:GLY:HA2	1:B:170:ARG:CD	2.46	0.41
1:G:191:ILE:HD11	1:G:195:TYR:CE1	2.56	0.41
1:H:362:TYR:O	1:H:365:GLN:HG3	2.19	0.41
1:J:366:TYR:C	1:J:366:TYR:CD1	2.93	0.41
1:B:330:GLN:HB2	1:B:336:TRP:CD1	2.54	0.41
1:A:364:GLN:O	1:A:365:GLN:C	2.59	0.41
1:A:218:ARG:CG	1:A:218:ARG:HH11	2.33	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.93	0.41
1:F:188:ASP:HB2	1:F:232:GLU:OE2	2.21	0.41
1:H:277:ARG:CZ	1:H:281:HIS:HD2	2.33	0.41
1:J:14:GLU:H	1:J:14:GLU:CD	2.23	0.41
1:H:224:ASP:HB3	1:H:341:PHE:CZ	2.56	0.41
1:I:259:VAL:HG23	1:I:259:VAL:H	1.56	0.41
1:G:247:GLN:OE1	1:G:247:GLN:O	2.38	0.41
1:H:330:GLN:HB2	1:H:336:TRP:CD1	2.56	0.41
1:A:35:ILE:HD12	1:A:35:ILE:HG23	1.65	0.41
1:C:14:GLU:H	1:C:14:GLU:CD	2.24	0.41
1:A:52:GLU:O	1:A:53:ILE:C	2.59	0.41
1:B:258:ARG:NH2	1:B:361:ASP:OD1	2.54	0.41
1:E:72:LEU:HB3	5:E:2021:HOH:O	2.21	0.41
1:G:142:ILE:CD1	1:G:230:LEU:HD12	2.50	0.41
1:I:136:ALA:HB1	1:I:139:THR:HB	2.02	0.41
1:C:131:ARG:HD2	1:C:131:ARG:HA	1.82	0.41
1:B:168:LEU:HD23	1:B:169:MET:N	2.35	0.41
1:D:362:TYR:O	1:D:365:GLN:CG	2.69	0.41
1:G:261:VAL:N	5:G:2016:HOH:O	2.29	0.41
1:B:277:ARG:CZ	1:B:281:HIS:HD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:O	1:B:226:LEU:HB2	2.21	0.41
1:D:223:LEU:HD22	1:D:274:THR:HG21	2.03	0.41
1:I:333:ASP:C	1:I:333:ASP:OD1	2.59	0.41
1:G:177:LEU:O	1:G:180:ASP:N	2.54	0.41
1:B:283:THR:HG22	1:B:286:GLN:N	2.16	0.41
1:F:244:VAL:CG1	1:F:245:VAL:H	2.33	0.41
1:A:283:THR:CG2	1:A:286:GLN:H	2.16	0.40
1:I:291:GLU:OE1	1:I:302:ARG:NH2	2.54	0.40
1:F:140:TRP:CD2	1:F:367:LEU:HD13	2.56	0.40
1:H:247:GLN:HA	1:H:248:PRO:HD2	1.63	0.40
1:J:35:ILE:HG23	1:J:35:ILE:HD12	1.79	0.40
1:E:289:LEU:HD12	1:E:289:LEU:HA	1.97	0.40
1:C:16:LEU:HD13	1:C:101:ALA:HB1	2.04	0.40
1:D:43:TYR:CE2	1:D:65:LEU:HD13	2.56	0.40
1:G:177:LEU:O	1:G:178:TYR:C	2.60	0.40
1:D:131:ARG:HA	1:D:131:ARG:HD2	1.82	0.40
1:D:247:GLN:HA	1:D:248:PRO:HD2	1.32	0.40
1:B:182:ARG:NH2	1:B:201:GLN:OE1	2.43	0.40
1:F:290:LEU:HB3	1:F:298:ARG:HG3	2.01	0.40
1:C:194:LEU:O	1:C:198:VAL:HG13	2.22	0.40
1:E:70:GLY:HA2	1:E:185:ARG:HA	2.02	0.40
1:I:177:LEU:CD2	1:I:198:VAL:HG22	2.52	0.40
1:J:110:TRP:CD1	1:J:110:TRP:N	2.88	0.40
1:F:110:TRP:H	1:F:110:TRP:HD1	1.68	0.40
1:G:362:TYR:CD2	1:G:362:TYR:C	2.95	0.40
1:H:315:GLU:HG2	1:H:370:MET:HG3	2.02	0.40
1:B:97:HIS:CE1	1:B:168:LEU:HD12	2.57	0.40
1:J:260:PRO:HG2	1:J:263:ILE:HD12	2.03	0.40
1:E:66:GLN:HE21	2:E:400:GDX:HN21	1.69	0.40
1:G:262:HIS:CD2	1:G:263:ILE:HG13	2.56	0.40
1:I:330:GLN:HB2	1:I:336:TRP:CD1	2.57	0.40
1:F:224:ASP:HB3	1:F:341:PHE:CZ	2.57	0.40
1:I:339:LEU:HA	1:I:339:LEU:HD12	1.89	0.40
1:B:214:GLY:CA	5:B:2016:HOH:O	2.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:O	1:G:179:GLU:OE2[1_554]	1.86	0.34
1:A:181:GLU:OE2	1:B:64:ARG:NH2[3_545]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/397 (96%)	357 (94%)	16 (4%)	6 (2%)	12	38
1	B	379/397 (96%)	363 (96%)	13 (3%)	3 (1%)	24	58
1	C	379/397 (96%)	363 (96%)	13 (3%)	3 (1%)	24	58
1	D	379/397 (96%)	360 (95%)	14 (4%)	5 (1%)	15	44
1	E	379/397 (96%)	363 (96%)	14 (4%)	2 (0%)	34	69
1	F	379/397 (96%)	364 (96%)	13 (3%)	2 (0%)	34	69
1	G	379/397 (96%)	359 (95%)	15 (4%)	5 (1%)	15	44
1	H	379/397 (96%)	365 (96%)	12 (3%)	2 (0%)	34	69
1	I	379/397 (96%)	366 (97%)	11 (3%)	2 (0%)	34	69
1	J	379/397 (96%)	353 (93%)	22 (6%)	4 (1%)	17	50
All	All	3790/3970 (96%)	3613 (95%)	143 (4%)	34 (1%)	21	55

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ASP
1	B	109	ASP
1	B	247	GLN
1	B	248	PRO
1	C	109	ASP
1	C	245	VAL
1	D	50	ALA
1	D	51	PRO
1	D	109	ASP
1	E	109	ASP
1	E	247	GLN
1	F	109	ASP
1	G	109	ASP
1	G	248	PRO

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Mol	Chain	Res	Type
1	H	109	ASP
1	H	250	ILE
1	I	109	ASP
1	I	247	GLN
1	J	109	ASP
1	J	284	PRO
1	J	286	GLN
1	J	287	VAL
1	A	52	GLU
1	A	53	ILE
1	A	223	LEU
1	D	54	SER
1	D	248	PRO
1	F	245	VAL
1	G	178	TYR
1	A	246	GLY
1	G	72	LEU
1	G	304	CYS
1	C	250	ILE
1	A	186	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	326/338 (96%)	290 (89%)	36 (11%)	8 23
1	B	326/338 (96%)	290 (89%)	36 (11%)	8 23
1	C	326/338 (96%)	292 (90%)	34 (10%)	9 25
1	D	326/338 (96%)	289 (89%)	37 (11%)	7 22
1	E	326/338 (96%)	294 (90%)	32 (10%)	10 28
1	F	326/338 (96%)	294 (90%)	32 (10%)	10 28
1	G	326/338 (96%)	297 (91%)	29 (9%)	12 34
1	H	326/338 (96%)	293 (90%)	33 (10%)	9 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	326/338 (96%)	295 (90%)	31 (10%)	11 30
1	J	326/338 (96%)	292 (90%)	34 (10%)	9 25
All	All	3260/3380 (96%)	2926 (90%)	334 (10%)	9 26

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	GLU
1	A	41	GLN
1	A	44	GLU
1	A	54	SER
1	A	55	ARG
1	A	63	VAL
1	A	65	LEU
1	A	68	ARG
1	A	72	LEU
1	A	84	LEU
1	A	91	THR
1	A	92	GLN
1	A	109	ASP
1	A	124	LEU
1	A	131	ARG
1	A	159	ILE
1	A	167	LEU
1	A	181	GLU
1	A	182	ARG
1	A	186	ARG
1	A	218	ARG
1	A	223	LEU
1	A	237	ILE
1	A	244	VAL
1	A	247	GLN
1	A	258	ARG
1	A	266	ARG
1	A	270	ASP
1	A	283	THR
1	A	289	LEU
1	A	301	LEU
1	A	343	LEU
1	A	357	LEU

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Mol	Chain	Res	Type
1	A	364	GLN
1	A	365	GLN
1	B	11	GLU
1	B	14	GLU
1	B	41	GLN
1	B	42	THR
1	B	44	GLU
1	B	48	ARG
1	B	54	SER
1	B	55	ARG
1	B	63	VAL
1	B	68	ARG
1	B	72	LEU
1	B	84	LEU
1	B	92	GLN
1	B	109	ASP
1	B	124	LEU
1	B	131	ARG
1	B	159	ILE
1	B	167	LEU
1	B	181	GLU
1	B	183	VAL
1	B	186	ARG
1	B	209	CYS
1	B	218	ARG
1	B	223	LEU
1	B	237	ILE
1	B	247	GLN
1	B	258	ARG
1	B	266	ARG
1	B	283	THR
1	B	289	LEU
1	B	291	GLU
1	B	301	LEU
1	B	316	MET
1	B	343	LEU
1	B	364	GLN
1	B	365	GLN
1	C	11	GLU
1	C	14	GLU
1	C	41	GLN
1	C	44	GLU

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Mol	Chain	Res	Type
1	C	48	ARG
1	C	54	SER
1	C	63	VAL
1	C	68	ARG
1	C	72	LEU
1	C	84	LEU
1	C	92	GLN
1	C	109	ASP
1	C	124	LEU
1	C	159	ILE
1	C	167	LEU
1	C	181	GLU
1	C	182	ARG
1	C	209	CYS
1	C	218	ARG
1	C	223	LEU
1	C	237	ILE
1	C	250	ILE
1	C	258	ARG
1	C	259	VAL
1	C	266	ARG
1	C	283	THR
1	C	289	LEU
1	C	291	GLU
1	C	301	LEU
1	C	316	MET
1	C	343	LEU
1	C	357	LEU
1	C	364	GLN
1	C	365	GLN
1	D	11	GLU
1	D	14	GLU
1	D	21	ARG
1	D	41	GLN
1	D	44	GLU
1	D	48	ARG
1	D	52	GLU
1	D	54	SER
1	D	55	ARG
1	D	65	LEU
1	D	68	ARG
1	D	72	LEU

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Mol	Chain	Res	Type
1	D	84	LEU
1	D	92	GLN
1	D	109	ASP
1	D	124	LEU
1	D	159	ILE
1	D	167	LEU
1	D	179	GLU
1	D	181	GLU
1	D	182	ARG
1	D	183	VAL
1	D	209	CYS
1	D	218	ARG
1	D	223	LEU
1	D	247	GLN
1	D	258	ARG
1	D	259	VAL
1	D	266	ARG
1	D	283	THR
1	D	289	LEU
1	D	291	GLU
1	D	301	LEU
1	D	316	MET
1	D	343	LEU
1	D	364	GLN
1	D	365	GLN
1	E	11	GLU
1	E	14	GLU
1	E	41	GLN
1	E	44	GLU
1	E	48	ARG
1	E	54	SER
1	E	65	LEU
1	E	68	ARG
1	E	72	LEU
1	E	84	LEU
1	E	92	GLN
1	E	109	ASP
1	E	124	LEU
1	E	167	LEU
1	E	179	GLU
1	E	181	GLU
1	E	186	ARG

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Mol	Chain	Res	Type
1	E	209	CYS
1	E	218	ARG
1	E	223	LEU
1	E	237	ILE
1	E	247	GLN
1	E	258	ARG
1	E	266	ARG
1	E	283	THR
1	E	289	LEU
1	E	291	GLU
1	E	301	LEU
1	E	343	LEU
1	E	357	LEU
1	E	364	GLN
1	E	365	GLN
1	F	11	GLU
1	F	14	GLU
1	F	21	ARG
1	F	41	GLN
1	F	44	GLU
1	F	48	ARG
1	F	54	SER
1	F	63	VAL
1	F	68	ARG
1	F	72	LEU
1	F	84	LEU
1	F	92	GLN
1	F	109	ASP
1	F	124	LEU
1	F	167	LEU
1	F	181	GLU
1	F	182	ARG
1	F	183	VAL
1	F	186	ARG
1	F	218	ARG
1	F	223	LEU
1	F	237	ILE
1	F	258	ARG
1	F	266	ARG
1	F	283	THR
1	F	289	LEU
1	F	291	GLU

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Mol	Chain	Res	Type
1	F	301	LEU
1	F	316	MET
1	F	343	LEU
1	F	364	GLN
1	F	365	GLN
1	G	11	GLU
1	G	14	GLU
1	G	41	GLN
1	G	44	GLU
1	G	48	ARG
1	G	54	SER
1	G	63	VAL
1	G	65	LEU
1	G	72	LEU
1	G	84	LEU
1	G	92	GLN
1	G	109	ASP
1	G	124	LEU
1	G	179	GLU
1	G	181	GLU
1	G	182	ARG
1	G	183	VAL
1	G	218	ARG
1	G	223	LEU
1	G	247	GLN
1	G	258	ARG
1	G	266	ARG
1	G	283	THR
1	G	289	LEU
1	G	291	GLU
1	G	301	LEU
1	G	343	LEU
1	G	364	GLN
1	G	365	GLN
1	H	11	GLU
1	H	14	GLU
1	H	41	GLN
1	H	44	GLU
1	H	54	SER
1	H	63	VAL
1	H	68	ARG
1	H	72	LEU

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Mol	Chain	Res	Type
1	H	84	LEU
1	H	92	GLN
1	H	109	ASP
1	H	124	LEU
1	H	167	LEU
1	H	179	GLU
1	H	181	GLU
1	H	182	ARG
1	H	183	VAL
1	H	209	CYS
1	H	218	ARG
1	H	223	LEU
1	H	237	ILE
1	H	250	ILE
1	H	257	HIS
1	H	258	ARG
1	H	266	ARG
1	H	283	THR
1	H	289	LEU
1	H	291	GLU
1	H	301	LEU
1	H	316	MET
1	H	343	LEU
1	H	364	GLN
1	H	365	GLN
1	I	11	GLU
1	I	14	GLU
1	I	21	ARG
1	I	41	GLN
1	I	44	GLU
1	I	54	SER
1	I	63	VAL
1	I	68	ARG
1	I	72	LEU
1	I	84	LEU
1	I	92	GLN
1	I	109	ASP
1	I	124	LEU
1	I	167	LEU
1	I	181	GLU
1	I	182	ARG
1	I	218	ARG

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Mol	Chain	Res	Type
1	I	223	LEU
1	I	237	ILE
1	I	247	GLN
1	I	250	ILE
1	I	258	ARG
1	I	266	ARG
1	I	283	THR
1	I	289	LEU
1	I	291	GLU
1	I	301	LEU
1	I	316	MET
1	I	343	LEU
1	I	364	GLN
1	I	365	GLN
1	J	11	GLU
1	J	14	GLU
1	J	41	GLN
1	J	44	GLU
1	J	48	ARG
1	J	54	SER
1	J	65	LEU
1	J	68	ARG
1	J	72	LEU
1	J	84	LEU
1	J	92	GLN
1	J	109	ASP
1	J	124	LEU
1	J	167	LEU
1	J	181	GLU
1	J	182	ARG
1	J	186	ARG
1	J	218	ARG
1	J	223	LEU
1	J	230	LEU
1	J	244	VAL
1	J	245	VAL
1	J	247	GLN
1	J	258	ARG
1	J	266	ARG
1	J	283	THR
1	J	285	ARG
1	J	289	LEU

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Mol	Chain	Res	Type
1	J	291	GLU
1	J	301	LEU
1	J	343	LEU
1	J	364	GLN
1	J	365	GLN
1	J	369	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	41	GLN
1	A	66	GLN
1	A	81	ASN
1	A	127	HIS
1	A	257	HIS
1	A	262	HIS
1	A	281	HIS
1	B	10	HIS
1	B	30	HIS
1	B	41	GLN
1	B	66	GLN
1	B	81	ASN
1	B	127	HIS
1	B	257	HIS
1	B	281	HIS
1	C	10	HIS
1	C	41	GLN
1	C	66	GLN
1	C	81	ASN
1	C	127	HIS
1	C	257	HIS
1	C	276	HIS
1	C	281	HIS
1	D	10	HIS
1	D	30	HIS
1	D	41	GLN
1	D	66	GLN
1	D	81	ASN
1	D	202	GLN
1	D	255	HIS
1	D	257	HIS

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Mol	Chain	Res	Type
1	D	276	HIS
1	D	281	HIS
1	E	10	HIS
1	E	30	HIS
1	E	41	GLN
1	E	66	GLN
1	E	81	ASN
1	E	153	HIS
1	E	255	HIS
1	E	257	HIS
1	E	276	HIS
1	E	281	HIS
1	F	10	HIS
1	F	41	GLN
1	F	66	GLN
1	F	81	ASN
1	F	153	HIS
1	F	257	HIS
1	F	276	HIS
1	F	281	HIS
1	G	10	HIS
1	G	41	GLN
1	G	66	GLN
1	G	81	ASN
1	G	257	HIS
1	G	281	HIS
1	H	10	HIS
1	H	41	GLN
1	H	66	GLN
1	H	81	ASN
1	H	127	HIS
1	H	257	HIS
1	H	262	HIS
1	H	276	HIS
1	H	281	HIS
1	I	10	HIS
1	I	30	HIS
1	I	41	GLN
1	I	66	GLN
1	I	81	ASN
1	I	127	HIS
1	I	255	HIS

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Mol	Chain	Res	Type
1	I	257	HIS
1	I	262	HIS
1	I	276	HIS
1	I	281	HIS
1	J	10	HIS
1	J	30	HIS
1	J	41	GLN
1	J	66	GLN
1	J	81	ASN
1	J	127	HIS
1	J	255	HIS
1	J	257	HIS
1	J	276	HIS
1	J	281	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GDX	A	400	3	33,42,43	1.51	5 (15%)	44,65,67	1.82	12 (27%)
2	GDX	B	400	3	33,42,43	1.57	8 (24%)	44,65,67	2.21	15 (34%)
2	GDX	C	400	3	33,42,43	1.23	4 (12%)	44,65,67	1.82	9 (20%)
2	GDX	D	400	3	33,42,43	1.52	5 (15%)	44,65,67	1.83	8 (18%)
2	GDX	E	400	3	33,42,43	1.63	6 (18%)	44,65,67	1.90	10 (22%)
2	GDX	F	400	3	33,42,43	1.45	5 (15%)	44,65,67	1.77	6 (13%)
2	GDX	G	400	3	33,42,43	1.69	7 (21%)	44,65,67	1.80	7 (15%)
2	GDX	H	400	3	33,42,43	1.23	3 (9%)	44,65,67	1.65	8 (18%)
2	GDX	I	400	3	33,42,43	1.25	4 (12%)	44,65,67	1.59	9 (20%)
2	GDX	J	400	3	33,42,43	1.22	3 (9%)	44,65,67	1.74	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDX	A	400	3	-	0/18/59/61	0/4/4/4
2	GDX	B	400	3	-	0/18/59/61	0/4/4/4
2	GDX	C	400	3	-	0/18/59/61	0/4/4/4
2	GDX	D	400	3	-	0/18/59/61	0/4/4/4
2	GDX	E	400	3	-	0/18/59/61	0/4/4/4
2	GDX	F	400	3	-	0/18/59/61	0/4/4/4
2	GDX	G	400	3	-	0/18/59/61	0/4/4/4
2	GDX	H	400	3	-	0/18/59/61	0/4/4/4
2	GDX	I	400	3	-	0/18/59/61	0/4/4/4
2	GDX	J	400	3	-	0/18/59/61	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	GDX	PB-O2B	-3.25	1.41	1.54
2	D	400	GDX	C6-C5	-2.90	1.35	1.41
2	B	400	GDX	C6-C5	-2.71	1.35	1.41
2	B	400	GDX	PA-O2A	-2.37	1.44	1.54
2	C	400	GDX	PA-O2A	-2.25	1.45	1.54
2	G	400	GDX	C6-C5	-2.02	1.37	1.41
2	J	400	GDX	C5'-C6'	2.06	1.53	1.50
2	B	400	GDX	O2'-C2'	2.11	1.48	1.43
2	A	400	GDX	O5'-C1'	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	GDX	C2-N1	2.24	1.39	1.35
2	G	400	GDX	O2'-C2'	2.24	1.48	1.43
2	B	400	GDX	C6-N1	2.25	1.37	1.33
2	I	400	GDX	O5'-C5'	2.26	1.47	1.43
2	G	400	GDX	O5'-C1'	2.30	1.47	1.41
2	C	400	GDX	C5'-C6'	2.40	1.54	1.50
2	F	400	GDX	C2-N1	2.40	1.39	1.35
2	F	400	GDX	O4D-C1D	2.40	1.44	1.41
2	C	400	GDX	O5'-C5'	2.43	1.48	1.43
2	G	400	GDX	PB-O1B	2.43	1.67	1.60
2	A	400	GDX	PB-O1B	2.45	1.67	1.60
2	G	400	GDX	C6-N1	2.53	1.37	1.33
2	A	400	GDX	C2-N1	2.56	1.39	1.35
2	H	400	GDX	C5'-C6'	2.56	1.54	1.50
2	F	400	GDX	C5'-C6'	2.60	1.54	1.50
2	D	400	GDX	O2'-C2'	2.64	1.49	1.43
2	A	400	GDX	C5'-C6'	2.66	1.54	1.50
2	E	400	GDX	O2'-C2'	2.68	1.49	1.43
2	B	400	GDX	PB-O1B	2.69	1.67	1.60
2	H	400	GDX	C2-N1	2.74	1.40	1.35
2	I	400	GDX	C2-N1	2.77	1.40	1.35
2	I	400	GDX	C5'-C6'	2.79	1.55	1.50
2	B	400	GDX	O5'-C5'	3.04	1.49	1.43
2	I	400	GDX	C6-N1	3.07	1.38	1.33
2	J	400	GDX	C2-N1	3.16	1.41	1.35
2	B	400	GDX	PA-O5D	3.20	1.73	1.59
2	C	400	GDX	C6-N1	3.24	1.39	1.33
2	H	400	GDX	C6-N1	3.25	1.39	1.33
2	D	400	GDX	C6-N1	3.30	1.39	1.33
2	E	400	GDX	O5'-C1'	3.32	1.50	1.41
2	E	400	GDX	O4D-C1D	3.33	1.45	1.41
2	B	400	GDX	C5'-C6'	3.35	1.56	1.50
2	J	400	GDX	C6-N1	3.37	1.39	1.33
2	G	400	GDX	C5'-C6'	3.42	1.56	1.50
2	D	400	GDX	O4D-C1D	3.53	1.45	1.41
2	D	400	GDX	O5'-C5'	3.85	1.50	1.43
2	F	400	GDX	C6-N1	3.98	1.40	1.33
2	F	400	GDX	O5'-C5'	4.03	1.51	1.43
2	E	400	GDX	O5'-C5'	4.71	1.52	1.43
2	G	400	GDX	O5'-C5'	5.34	1.53	1.43
2	A	400	GDX	O5'-C5'	5.52	1.53	1.43

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	GDX	C5-C6-N1	-5.97	115.42	123.59
2	F	400	GDX	O5'-C1'-O1B	-5.88	103.61	111.36
2	A	400	GDX	N3-C2-N1	-5.75	118.69	127.44
2	D	400	GDX	N3-C2-N1	-5.14	119.62	127.44
2	B	400	GDX	N3-C2-N1	-5.07	119.73	127.44
2	E	400	GDX	N3-C2-N1	-4.98	119.85	127.44
2	C	400	GDX	C5-C6-N1	-4.98	116.78	123.59
2	H	400	GDX	N3-C2-N1	-4.97	119.87	127.44
2	G	400	GDX	N3-C2-N1	-4.79	120.15	127.44
2	J	400	GDX	N3-C2-N1	-4.79	120.15	127.44
2	E	400	GDX	O5'-C1'-C2'	-4.43	101.19	110.28
2	G	400	GDX	C5-C6-N1	-4.42	117.54	123.59
2	D	400	GDX	C5-C6-N1	-4.39	117.58	123.59
2	C	400	GDX	N3-C2-N1	-4.38	120.77	127.44
2	I	400	GDX	O5'-C1'-C2'	-4.21	101.64	110.28
2	I	400	GDX	N3-C2-N1	-4.10	121.20	127.44
2	G	400	GDX	O5'-C1'-O1B	-4.06	106.00	111.36
2	F	400	GDX	N3-C2-N1	-4.04	121.29	127.44
2	F	400	GDX	C5-C6-N1	-3.99	118.13	123.59
2	J	400	GDX	C5-C6-N1	-3.90	118.26	123.59
2	I	400	GDX	C5-C6-N1	-3.82	118.36	123.59
2	D	400	GDX	O5'-C1'-C2'	-3.73	102.62	110.28
2	A	400	GDX	C5-C6-N1	-3.63	118.62	123.59
2	E	400	GDX	C5-C6-N1	-3.57	118.70	123.59
2	H	400	GDX	O5'-C1'-C2'	-3.37	103.36	110.28
2	J	400	GDX	O5'-C1'-C2'	-3.31	103.48	110.28
2	J	400	GDX	O5'-C5'-C4'	-3.21	106.01	109.13
2	B	400	GDX	O1B-PB-O3B	-3.17	96.99	109.46
2	C	400	GDX	O5'-C1'-C2'	-3.16	103.79	110.28
2	A	400	GDX	O4'-C4'-C3'	-3.10	103.36	110.34
2	H	400	GDX	C5-C6-N1	-3.00	119.48	123.59
2	G	400	GDX	PB-O3A-PA	-2.92	124.53	132.73
2	G	400	GDX	O5'-C1'-C2'	-2.92	104.29	110.28
2	D	400	GDX	O5'-C1'-O1B	-2.91	107.52	111.36
2	A	400	GDX	O6A-C6'-C5'	-2.91	115.80	124.30
2	D	400	GDX	PB-O3A-PA	-2.63	125.35	132.73
2	A	400	GDX	O5'-C1'-C2'	-2.55	105.04	110.28
2	B	400	GDX	O2A-PA-O5D	-2.55	95.62	108.46
2	E	400	GDX	O6A-C6'-C5'	-2.49	117.02	124.30
2	C	400	GDX	C4'-C5'-C6'	-2.49	108.70	112.54
2	A	400	GDX	C4-C5-N7	-2.48	107.20	109.48
2	B	400	GDX	O5'-C1'-O1B	-2.48	108.09	111.36
2	I	400	GDX	C4-C5-N7	-2.48	107.20	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	400	GDX	PB-O3A-PA	-2.43	125.90	132.73
2	A	400	GDX	O1B-PB-O3B	-2.42	99.94	109.46
2	I	400	GDX	PB-O3A-PA	-2.42	125.94	132.73
2	E	400	GDX	C4'-C5'-C6'	-2.41	108.82	112.54
2	H	400	GDX	O5'-C1'-O1B	-2.41	108.19	111.36
2	B	400	GDX	C4'-C3'-C2'	-2.40	106.32	110.79
2	A	400	GDX	C6-C5-C4	-2.36	118.07	120.90
2	A	400	GDX	C1D-N9-C4	-2.26	123.53	126.94
2	C	400	GDX	O5'-C1'-O1B	-2.25	108.40	111.36
2	E	400	GDX	C6-C5-C4	-2.23	118.23	120.90
2	J	400	GDX	O5'-C1'-O1B	-2.22	108.43	111.36
2	J	400	GDX	O4D-C1D-N9	-2.20	103.49	108.10
2	C	400	GDX	C4-C5-N7	-2.16	107.49	109.48
2	I	400	GDX	O4D-C1D-N9	-2.16	103.58	108.10
2	B	400	GDX	O6A-C6'-C5'	-2.15	118.00	124.30
2	I	400	GDX	O3A-PA-O5D	-2.09	97.40	102.94
2	G	400	GDX	O3A-PA-O5D	-2.07	97.44	102.94
2	H	400	GDX	C4'-C5'-C6'	-2.05	109.39	112.54
2	B	400	GDX	O5'-C1'-C2'	-2.01	106.16	110.28
2	B	400	GDX	C1D-N9-C4	-2.00	123.92	126.94
2	A	400	GDX	N2-C2-N3	2.02	121.67	117.80
2	D	400	GDX	O2B-PB-O3A	2.05	114.42	105.09
2	B	400	GDX	N2-C2-N3	2.08	121.78	117.80
2	A	400	GDX	O1B-C1'-C2'	2.15	112.41	108.39
2	H	400	GDX	N2-C2-N1	2.25	120.93	117.20
2	B	400	GDX	O2A-PA-O3A	2.27	115.40	105.09
2	H	400	GDX	C6-N1-C2	2.33	119.17	115.94
2	I	400	GDX	C6-N1-C2	2.36	119.22	115.94
2	E	400	GDX	N2-C2-N3	2.38	122.36	117.80
2	E	400	GDX	C2D-C1D-N9	2.43	118.00	114.29
2	C	400	GDX	N2-C2-N1	2.45	121.26	117.20
2	F	400	GDX	C6-N1-C2	2.60	119.55	115.94
2	B	400	GDX	O2B-PB-O3B	2.74	127.39	112.53
2	B	400	GDX	O5'-C5'-C4'	2.81	111.86	109.13
2	J	400	GDX	C6-N1-C2	3.23	120.43	115.94
2	F	400	GDX	O5'-C5'-C4'	3.24	112.28	109.13
2	I	400	GDX	O1B-C1'-C2'	3.36	114.67	108.39
2	J	400	GDX	O1B-C1'-C2'	3.55	115.01	108.39
2	C	400	GDX	C6-N1-C2	3.77	121.17	115.94
2	D	400	GDX	C6-N1-C2	3.79	121.19	115.94
2	G	400	GDX	C6-N1-C2	4.02	121.52	115.94
2	H	400	GDX	O1B-C1'-C2'	4.03	115.91	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	400	GDX	C6-N1-C2	4.15	121.69	115.94
2	F	400	GDX	O1B-C1'-C2'	4.43	116.66	108.39
2	A	400	GDX	C6-N1-C2	4.44	122.11	115.94
2	C	400	GDX	O1B-C1'-C2'	4.73	117.23	108.39
2	D	400	GDX	O1B-C1'-C2'	5.09	117.91	108.39
2	B	400	GDX	C6-N1-C2	5.39	123.42	115.94
2	B	400	GDX	O1B-C1'-C2'	5.44	118.55	108.39
2	E	400	GDX	O1B-C1'-C2'	5.52	118.69	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	GDX	4	0
2	B	400	GDX	4	0
2	C	400	GDX	3	0
2	D	400	GDX	4	0
2	E	400	GDX	3	0
2	F	400	GDX	3	0
2	G	400	GDX	3	0
2	H	400	GDX	3	0
2	I	400	GDX	3	0
2	J	400	GDX	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	381/397 (95%)	0.79	13 (3%) 49 36	50, 57, 67, 83	0
1	B	381/397 (95%)	0.69	5 (1%) 79 71	49, 57, 67, 83	0
1	C	381/397 (95%)	0.39	11 (2%) 55 43	50, 57, 67, 83	0
1	D	381/397 (95%)	0.43	9 (2%) 62 50	50, 57, 67, 83	0
1	E	381/397 (95%)	0.38	10 (2%) 59 47	50, 57, 67, 83	0
1	F	381/397 (95%)	0.96	74 (19%) 1 1	50, 57, 67, 83	0
1	G	381/397 (95%)	0.83	58 (15%) 3 1	50, 57, 67, 83	0
1	H	381/397 (95%)	0.47	14 (3%) 45 33	50, 57, 67, 83	0
1	I	381/397 (95%)	0.33	14 (3%) 45 33	50, 57, 67, 83	0
1	J	381/397 (95%)	0.75	49 (12%) 5 2	50, 57, 67, 83	0
All	All	3810/3970 (95%)	0.60	257 (6%) 21 12	49, 57, 68, 83	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	382	ASN	19.0
1	J	2	SER	6.0
1	G	10	HIS	5.5
1	F	2	SER	5.3
1	J	246	GLY	5.2
1	F	101	ALA	5.1
1	G	42	THR	5.0
1	B	382	ASN	5.0
1	F	32	VAL	5.0
1	F	8	PHE	4.9
1	F	92	GLN	4.8
1	F	61	VAL	4.7
1	F	93	TRP	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	86	TYR	4.6
1	G	218	ARG	4.4
1	F	60	PRO	4.3
1	F	36	GLY	4.2
1	G	24	ALA	4.2
1	J	91	THR	4.2
1	J	24	ALA	4.2
1	G	46	VAL	4.0
1	J	13	PRO	4.0
1	F	46	VAL	4.0
1	F	84	LEU	4.0
1	G	53	ILE	4.0
1	E	2	SER	3.9
1	F	94	GLU	3.8
1	F	30	HIS	3.8
1	G	13	PRO	3.8
1	G	216	ALA	3.8
1	F	44	GLU	3.8
1	J	87	PHE	3.7
1	H	2	SER	3.7
1	F	58	GLY	3.7
1	J	250	ILE	3.7
1	F	62	SER	3.7
1	J	81	ASN	3.6
1	J	38	GLU	3.6
1	G	78	ASP	3.6
1	F	88	LEU	3.6
1	G	380	LEU	3.6
1	J	53	ILE	3.6
1	H	30	HIS	3.6
1	J	25	ALA	3.5
1	D	2	SER	3.5
1	F	218	ARG	3.5
1	H	55	ARG	3.5
1	G	16	LEU	3.5
1	F	65	LEU	3.5
1	J	42	THR	3.4
1	J	93	TRP	3.4
1	G	103	ILE	3.4
1	F	33	LEU	3.4
1	G	15	VAL	3.4
1	G	226	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	88	LEU	3.4
1	G	39	ARG	3.4
1	H	301	LEU	3.4
1	G	43	TYR	3.3
1	J	55	ARG	3.3
1	G	65	LEU	3.3
1	G	41	GLN	3.3
1	F	37	TYR	3.3
1	E	381	GLU	3.2
1	C	42	THR	3.2
1	G	187	SER	3.2
1	F	7	PRO	3.2
1	J	92	GLN	3.2
1	F	69	LEU	3.2
1	F	246	GLY	3.1
1	G	19	ASN	3.1
1	E	57	THR	3.1
1	F	35	ILE	3.1
1	G	162	PRO	3.1
1	F	48	ARG	3.1
1	F	381	GLU	3.1
1	F	21	ARG	3.1
1	J	247	GLN	3.1
1	J	32	VAL	3.1
1	G	51	PRO	3.1
1	D	8	PHE	3.0
1	G	7	PRO	3.0
1	F	42	THR	3.0
1	G	219	LEU	3.0
1	J	51	PRO	3.0
1	G	336	TRP	3.0
1	F	82	THR	3.0
1	F	247	GLN	3.0
1	H	92	GLN	3.0
1	G	98	PHE	3.0
1	B	58	GLY	2.9
1	G	335	ASP	2.9
1	G	12	HIS	2.9
1	G	120	PHE	2.9
1	F	45	ALA	2.9
1	J	41	GLN	2.9
1	F	57	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	81	ASN	2.9
1	J	33	LEU	2.9
1	F	59	THR	2.9
1	F	55	ARG	2.8
1	I	2	SER	2.8
1	J	120	PHE	2.8
1	C	52	GLU	2.8
1	F	79	GLY	2.8
1	G	44	GLU	2.8
1	F	87	PHE	2.8
1	F	11	GLU	2.8
1	J	334	PRO	2.8
1	D	282	TRP	2.8
1	I	92	GLN	2.8
1	J	63	VAL	2.8
1	G	76	LYS	2.8
1	G	48	ARG	2.8
1	I	29	VAL	2.8
1	J	194	LEU	2.7
1	G	215	LYS	2.7
1	G	62	SER	2.7
1	I	32	VAL	2.7
1	J	3	LEU	2.7
1	E	54	SER	2.7
1	I	57	THR	2.7
1	F	15	VAL	2.7
1	F	178	TYR	2.6
1	J	185	ARG	2.6
1	F	66	GLN	2.6
1	G	22	VAL	2.6
1	F	123	GLY	2.6
1	J	15	VAL	2.6
1	H	249	ALA	2.6
1	I	53	ILE	2.5
1	I	56	ALA	2.5
1	J	61	VAL	2.5
1	D	41	GLN	2.5
1	A	376	TYR	2.5
1	I	27	PRO	2.5
1	J	57	THR	2.5
1	J	90	GLU	2.5
1	F	111	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	31	GLU	2.5
1	F	19	ASN	2.5
1	H	60	PRO	2.5
1	B	220	TYR	2.5
1	G	220	TYR	2.5
1	F	97	HIS	2.5
1	G	231	VAL	2.5
1	J	70	GLY	2.5
1	G	223	LEU	2.5
1	H	376	TYR	2.5
1	G	237	ILE	2.5
1	J	179	GLU	2.5
1	F	10	HIS	2.5
1	G	163	LEU	2.4
1	F	43	TYR	2.4
1	G	5	VAL	2.4
1	C	289	LEU	2.4
1	F	63	VAL	2.4
1	F	110	TRP	2.4
1	H	25	ALA	2.4
1	G	106	PHE	2.4
1	C	57	THR	2.4
1	I	46	VAL	2.4
1	C	56	ALA	2.4
1	G	290	LEU	2.4
1	J	218	ARG	2.4
1	H	53	ILE	2.4
1	C	17	LEU	2.4
1	F	78	ASP	2.4
1	F	189	TRP	2.3
1	G	228	THR	2.3
1	G	221	GLY	2.3
1	F	106	PHE	2.3
1	F	220	TYR	2.3
1	F	99	TYR	2.3
1	G	217	HIS	2.3
1	F	39	ARG	2.3
1	J	6	PHE	2.3
1	F	70	GLY	2.3
1	G	40	ASP	2.3
1	G	55	ARG	2.3
1	J	86	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	381	GLU	2.3
1	H	94	GLU	2.3
1	C	55	ARG	2.3
1	J	48	ARG	2.3
1	J	152	PRO	2.3
1	F	83	ALA	2.2
1	G	37	TYR	2.2
1	G	127	HIS	2.2
1	F	74	PRO	2.2
1	F	181	GLU	2.2
1	J	59	THR	2.2
1	A	236	ALA	2.2
1	C	184	ARG	2.2
1	J	7	PRO	2.2
1	B	86	TYR	2.2
1	F	31	GLU	2.2
1	F	80	MET	2.2
1	J	178	TYR	2.2
1	J	62	SER	2.2
1	G	33	LEU	2.2
1	E	215	LYS	2.2
1	A	134	THR	2.2
1	J	37	TYR	2.2
1	A	133	SER	2.2
1	G	2	SER	2.2
1	H	29	VAL	2.2
1	G	211	ILE	2.2
1	C	381	GLU	2.2
1	I	30	HIS	2.2
1	F	38	GLU	2.2
1	D	78	ASP	2.2
1	A	140	TRP	2.2
1	A	365	GLN	2.2
1	E	29	VAL	2.2
1	J	29	VAL	2.1
1	F	23	ALA	2.1
1	F	213	GLU	2.1
1	F	223	LEU	2.1
1	F	67	GLU	2.1
1	F	53	ILE	2.1
1	F	165	GLY	2.1
1	D	217	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	319	ALA	2.1
1	G	123	GLY	2.1
1	C	53	ILE	2.1
1	F	184	ARG	2.1
1	J	170	ARG	2.1
1	G	189	TRP	2.1
1	F	41	GLN	2.1
1	E	120	PHE	2.1
1	J	30	HIS	2.1
1	A	139	THR	2.1
1	F	102	ASP	2.1
1	E	94	GLU	2.1
1	A	229	MET	2.1
1	A	233	CYS	2.1
1	D	185	ARG	2.1
1	D	286	GLN	2.1
1	A	137	MET	2.0
1	I	58	GLY	2.0
1	A	304	CYS	2.0
1	B	233	CYS	2.0
1	I	94	GLU	2.0
1	A	148	ALA	2.0
1	J	248	PRO	2.0
1	G	61	VAL	2.0
1	H	20	VAL	2.0
1	F	9	LYS	2.0
1	D	92	GLN	2.0
1	H	377	GLN	2.0
1	A	326	LEU	2.0
1	C	51	PRO	2.0
1	I	55	ARG	2.0
1	J	80	MET	2.0
1	E	376	TYR	2.0
1	I	36	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GDX	I	400	39/40	0.93	0.21	-0.19	59,63,65,67	0
2	GDX	A	400	39/40	0.96	0.27	-0.24	60,63,65,67	0
2	GDX	B	400	39/40	0.97	0.25	-0.45	59,63,65,66	0
2	GDX	E	400	39/40	0.96	0.20	-0.50	59,63,65,67	0
2	GDX	G	400	39/40	0.86	0.26	-0.59	60,63,65,66	0
2	GDX	J	400	39/40	0.94	0.22	-0.63	60,63,64,66	0
2	GDX	H	400	39/40	0.92	0.19	-0.64	60,63,64,66	0
2	GDX	D	400	39/40	0.96	0.20	-0.76	59,63,65,66	0
2	GDX	C	400	39/40	0.95	0.18	-1.11	59,63,65,66	0
3	MN	E	500	1/1	0.94	0.14	-1.23	79,79,79,79	0
3	MN	I	500	1/1	0.94	0.14	-1.28	80,80,80,80	0
2	GDX	F	400	39/40	0.92	0.20	-1.30	59,63,64,66	0
3	MN	G	500	1/1	0.90	0.13	-1.46	79,79,79,79	0
3	MN	D	500	1/1	0.95	0.12	-2.15	80,80,80,80	0
3	MN	F	500	1/1	0.87	0.12	-2.16	80,80,80,80	0
3	MN	H	500	1/1	0.89	0.15	-2.63	80,80,80,80	0
3	MN	J	500	1/1	0.84	0.07	-2.64	80,80,80,80	0
3	MN	C	500	1/1	0.92	0.07	-5.58	80,80,80,80	0
4	CL	E	1382	1/1	0.97	0.20	-	65,65,65,65	0
4	CL	F	1382	1/1	0.71	0.25	-	102,102,102,102	0
4	CL	G	1382	1/1	0.82	0.18	-	79,79,79,79	0
3	MN	A	500	1/1	0.90	0.18	-	80,80,80,80	0
4	CL	J	1382	1/1	0.88	0.12	-	82,82,82,82	0
4	CL	B	1382	1/1	0.92	0.14	-	38,38,38,38	0
4	CL	D	1382	1/1	0.86	0.12	-	55,55,55,55	0
4	CL	I	1382	1/1	0.87	0.19	-	70,70,70,70	0
4	CL	H	1382	1/1	0.91	0.23	-	77,77,77,77	0
4	CL	C	1382	1/1	0.96	0.18	-	58,58,58,58	0
3	MN	B	500	1/1	0.92	0.20	-	82,82,82,82	0
4	CL	A	1382	1/1	0.94	0.15	-	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.