Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:48 AM GMT

PDB ID	:	2BO7
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	:	2.95 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:

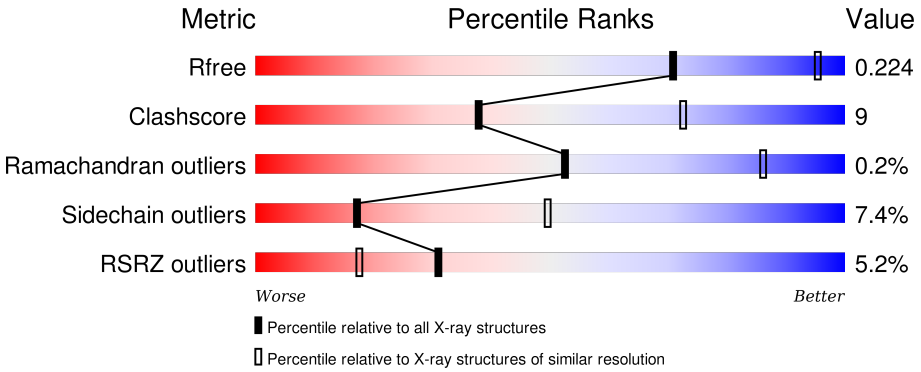
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	75% 15% • 5%
1	B	397	72% 19% • 5%
1	C	397	4% 75% 17% • • 5%
1	D	397	3% 75% 16% • 5%
1	E	397	3% 76% 16% • 5%

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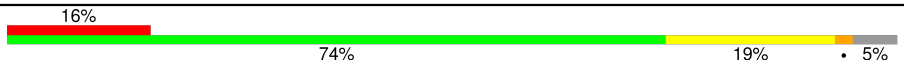
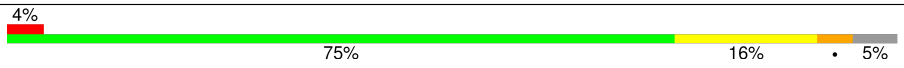
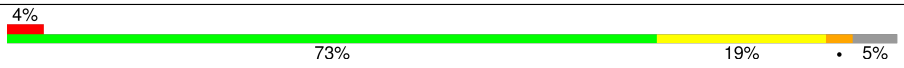
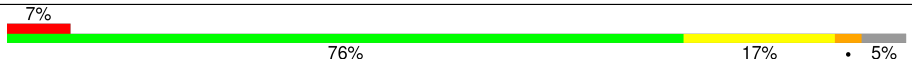
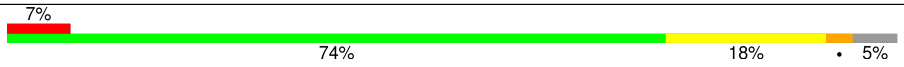
Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	
1	I	397	
1	J	397	

2 Entry composition

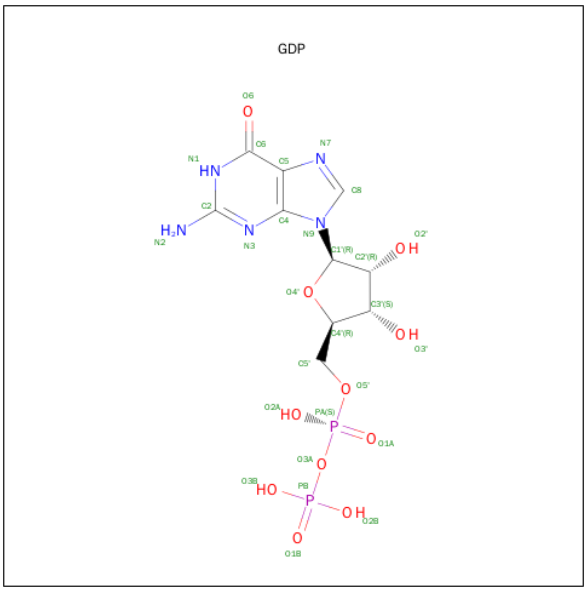
There are 4 unique types of molecules in this entry. The entry contains 31437 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	B	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	C	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	D	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	E	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	F	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	G	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	H	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	I	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	J	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	G	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	H	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	J	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

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

- Molecule 4 is water.

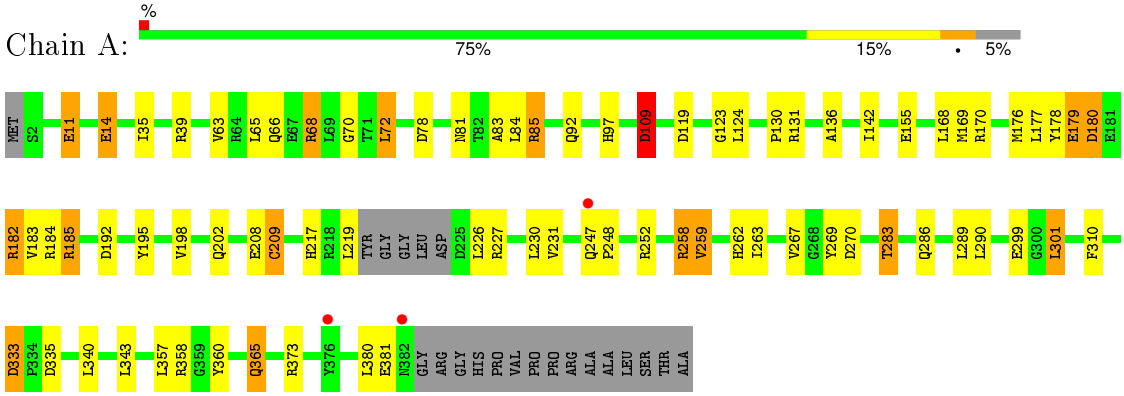
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	24	Total O 24 24	0	0
4	B	27	Total O 27 27	0	0
4	C	18	Total O 18 18	0	0
4	D	10	Total O 10 10	0	0
4	E	10	Total O 10 10	0	0
4	F	9	Total O 9 9	0	0
4	G	14	Total O 14 14	0	0
4	H	2	Total O 2 2	0	0
4	I	8	Total O 8 8	0	0
4	J	5	Total O 5 5	0	0

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.

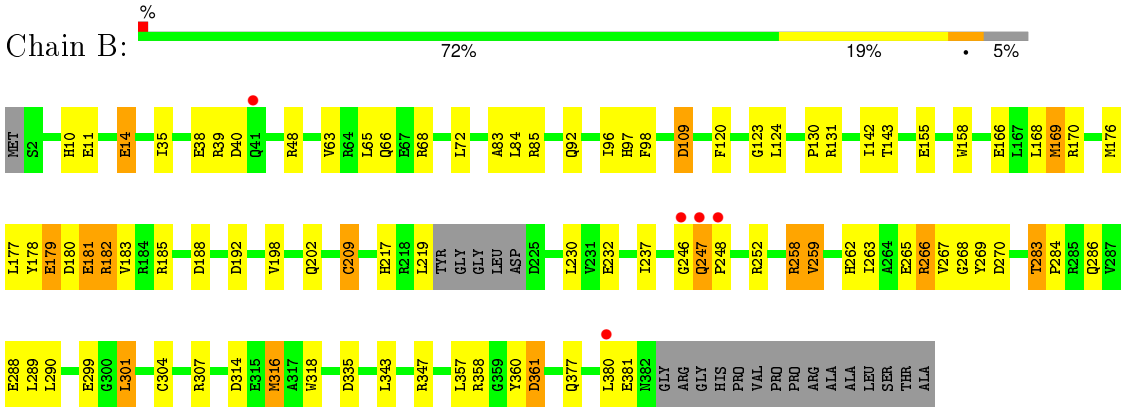
- Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain A:



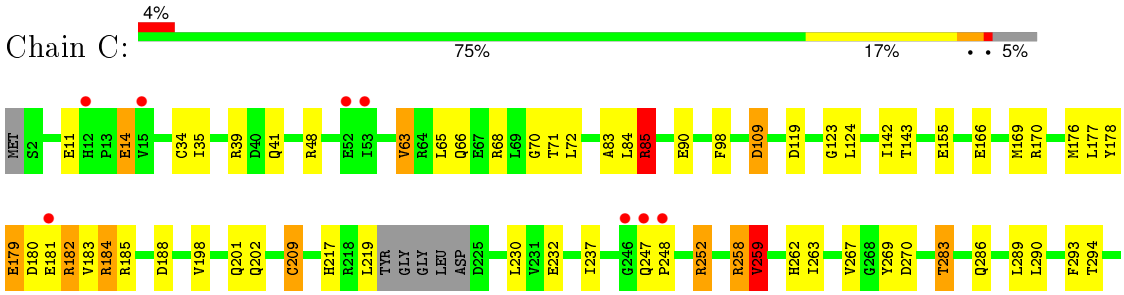
- Molecule 1: MANNOSYLGLYCERATE SYNTHASE

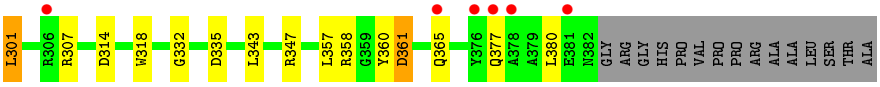
Chain B:



- Molecule 1: MANNOSYLGLYCERATE SYNTHASE

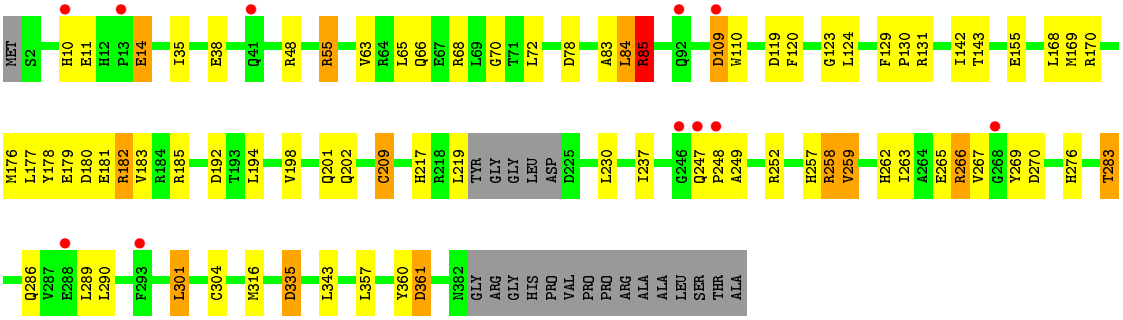
Chain C:





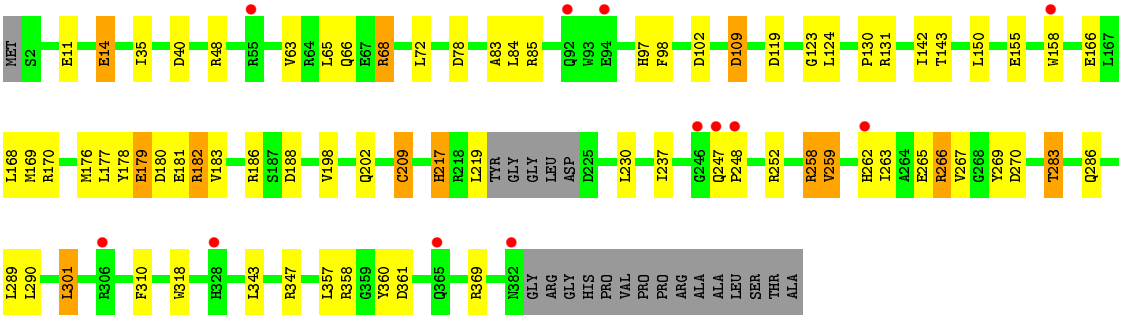
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain D:



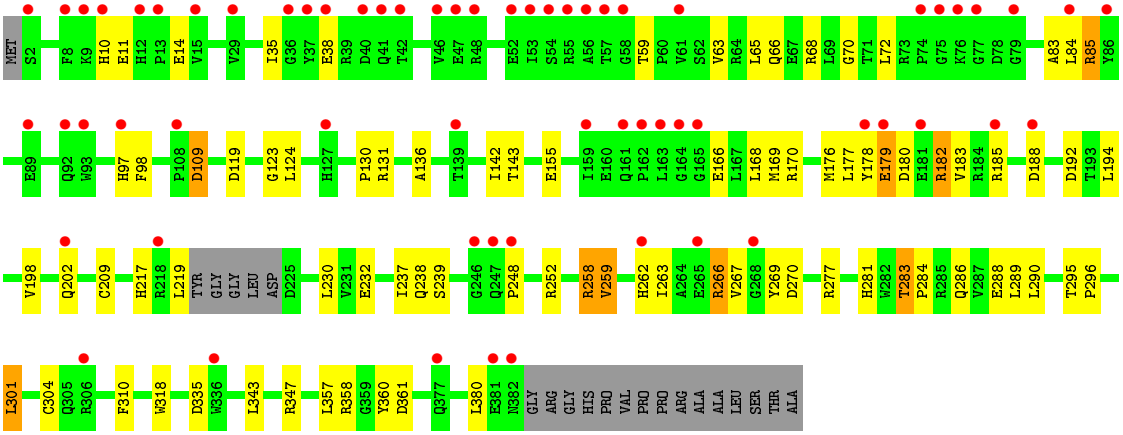
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain E:



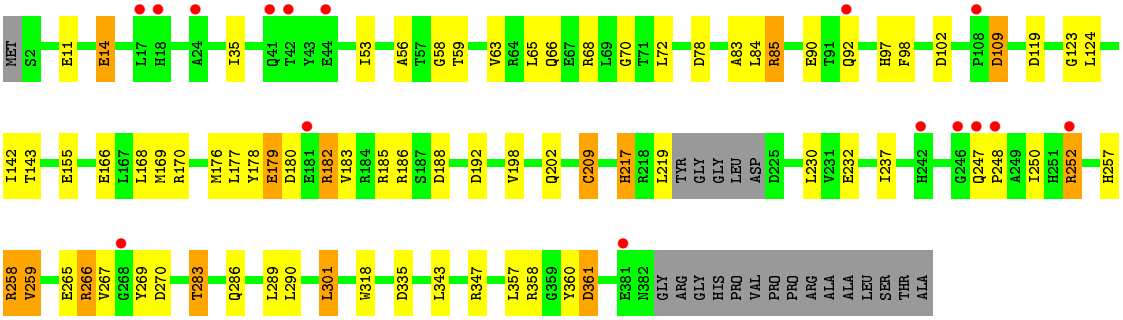
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain F:



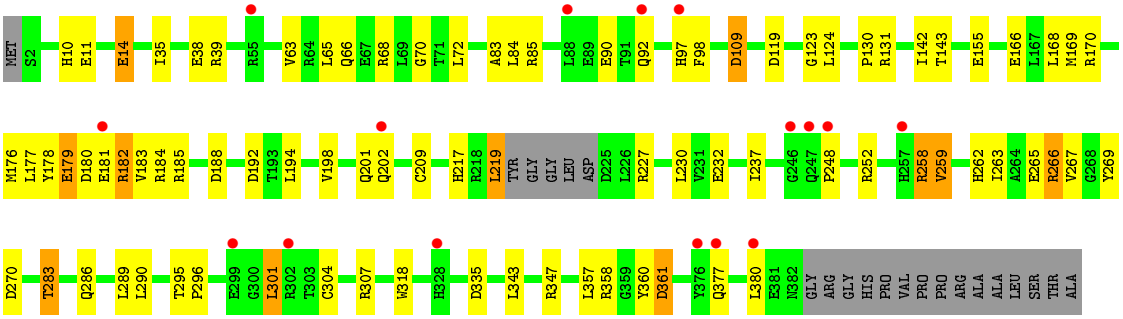
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain G:



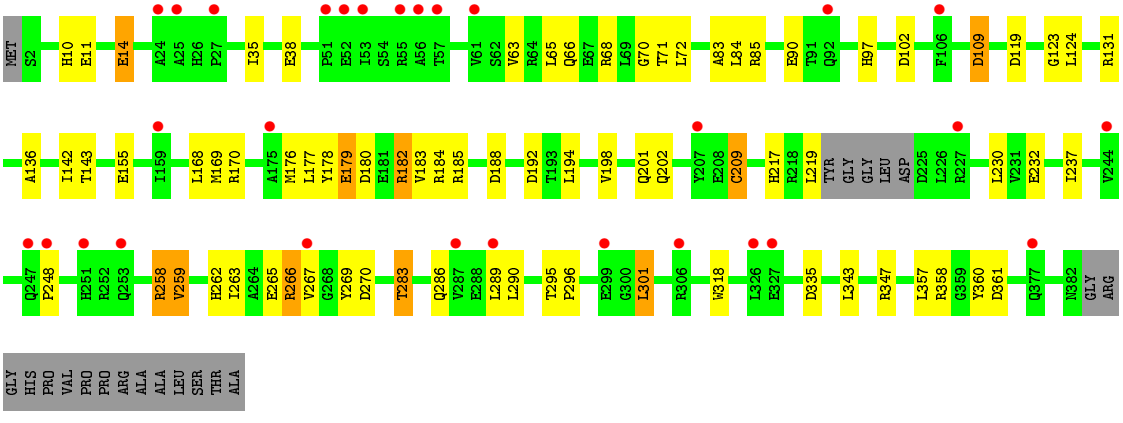
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain H:



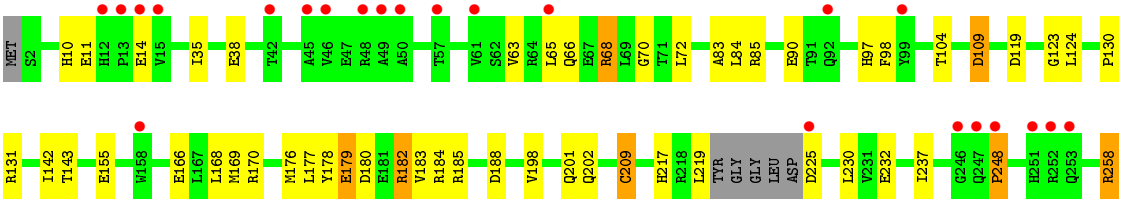
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain I:



• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

Chain J:




V259
H262
I263
R266
V267
G268
Y269
D270
R277
H281
W282
T283
Q286
L289
L290
L301
C304
R307
F310
W318
G332
D335
L343
R347
L357
R358
G359
Y360
D361
Q365
Q377
L380
E381
N382
GLY
ARG
GLY
HIS
PRO
VAL
PRO
PRO
ARG
ALA
ALA
LEU
SER
THR
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	406.70Å 162.14Å 108.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	223.61 – 2.95 40.03 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (223.61-2.95) 97.8 (40.03-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.207 , 0.224 0.208 , 0.224	Depositor DCC
R_{free} test set	7443 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 148068 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31437	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: GDP, CO

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	0.93	5/3191 (0.2%)	0.92	12/4341 (0.3%)
1	B	0.99	9/3191 (0.3%)	0.93	9/4341 (0.2%)
1	C	0.76	2/3191 (0.1%)	0.85	10/4341 (0.2%)
1	D	0.79	3/3191 (0.1%)	0.84	9/4341 (0.2%)
1	E	0.81	4/3191 (0.1%)	0.86	8/4341 (0.2%)
1	F	0.50	0/3191	0.74	4/4341 (0.1%)
1	G	0.62	0/3191	0.80	7/4341 (0.2%)
1	H	0.53	0/3191	0.76	5/4341 (0.1%)
1	I	0.56	1/3191 (0.0%)	0.78	7/4341 (0.2%)
1	J	0.61	0/3191	0.77	5/4341 (0.1%)
All	All	0.73	24/31910 (0.1%)	0.83	76/43410 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	GLU	CD-OE2	8.03	1.34	1.25
1	B	181	GLU	CD-OE1	7.68	1.34	1.25
1	B	247	GLN	C-O	7.66	1.38	1.23
1	D	209	CYS	CB-SG	-7.22	1.70	1.82
1	E	209	CYS	CB-SG	-7.19	1.70	1.82
1	D	120	PHE	CE1-CZ	7.09	1.50	1.37
1	A	209	CYS	CB-SG	-7.06	1.70	1.82
1	A	373	ARG	NE-CZ	6.72	1.41	1.33
1	B	316	MET	CG-SD	6.72	1.98	1.81
1	B	299	GLU	CD-OE2	6.51	1.32	1.25
1	B	209	CYS	CB-SG	-6.40	1.71	1.82
1	A	365	GLN	CG-CD	6.27	1.65	1.51
1	C	209	CYS	CB-SG	-6.08	1.72	1.82
1	A	299	GLU	CD-OE2	5.83	1.32	1.25
1	A	208	GLU	CD-OE1	5.69	1.31	1.25
1	E	181	GLU	CD-OE2	5.61	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	GLU	CD-OE1	5.55	1.31	1.25
1	E	181	GLU	CD-OE1	5.50	1.31	1.25
1	E	181	GLU	CG-CD	5.47	1.60	1.51
1	D	129	PHE	CE2-CZ	5.45	1.47	1.37
1	B	181	GLU	CG-CD	5.42	1.60	1.51
1	I	209	CYS	CB-SG	-5.31	1.73	1.81
1	B	120	PHE	CE1-CZ	5.29	1.47	1.37
1	C	365	GLN	CG-CD	5.07	1.62	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	270	ASP	CB-CG-OD2	8.79	126.21	118.30
1	B	192	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	270	ASP	CB-CG-OD2	7.78	125.30	118.30
1	C	270	ASP	CB-CG-OD2	7.57	125.12	118.30
1	B	109	ASP	CB-CG-OD2	7.49	125.04	118.30
1	D	209	CYS	CB-CA-C	-7.40	95.60	110.40
1	D	361	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	109	ASP	CB-CG-OD2	7.23	124.81	118.30
1	B	270	ASP	CB-CG-OD2	7.20	124.78	118.30
1	C	109	ASP	CB-CG-OD2	7.00	124.60	118.30
1	H	270	ASP	CB-CG-OD2	6.98	124.58	118.30
1	D	270	ASP	CB-CG-OD2	6.95	124.56	118.30
1	E	78	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	119	ASP	CB-CG-OD2	6.79	124.41	118.30
1	F	270	ASP	CB-CG-OD2	6.79	124.41	118.30
1	D	192	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	209	CYS	CB-CA-C	-6.72	96.97	110.40
1	I	109	ASP	CB-CG-OD2	6.68	124.31	118.30
1	J	109	ASP	CB-CG-OD2	6.63	124.27	118.30
1	G	270	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	78	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	358	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	E	40	ASP	CB-CG-OD2	6.46	124.12	118.30
1	E	270	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	209	CYS	CB-CA-C	-6.29	97.82	110.40
1	J	361	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	182	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	314	ASP	CB-CG-OD2	6.23	123.91	118.30
1	G	119	ASP	CB-CG-OD2	6.17	123.85	118.30
1	F	192	ASP	CB-CG-OD2	6.04	123.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	182	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	J	270	ASP	CB-CG-OD2	5.98	123.68	118.30
1	F	109	ASP	CB-CG-OD2	5.97	123.67	118.30
1	H	109	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	361	ASP	CB-CG-OD2	5.90	123.61	118.30
1	I	361	ASP	CB-CG-OD2	5.87	123.58	118.30
1	E	68	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	209	CYS	CB-CA-C	-5.82	98.77	110.40
1	G	109	ASP	CB-CG-OD2	5.77	123.50	118.30
1	F	119	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	184	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	G	361	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	361	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	192	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	119	ASP	CB-CG-OD2	5.59	123.33	118.30
1	E	119	ASP	CB-CG-OD2	5.58	123.33	118.30
1	C	85	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	185	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	78	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	314	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	333	ASP	CB-CG-OD2	5.52	123.27	118.30
1	I	192	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	226	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	C	119	ASP	CB-CG-OD2	5.50	123.25	118.30
1	I	102	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	119	ASP	CB-CG-OD2	5.46	123.22	118.30
1	G	209	CYS	CB-CA-C	-5.42	99.55	110.40
1	E	109	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	209	CYS	CB-CA-C	-5.37	99.66	110.40
1	H	361	ASP	CB-CG-OD2	5.36	123.13	118.30
1	G	192	ASP	CB-CG-OD2	5.34	123.10	118.30
1	J	209	CYS	CB-CA-C	-5.34	99.73	110.40
1	C	184	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	259	VAL	CB-CA-C	-5.27	101.39	111.40
1	A	39	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	I	119	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	335	ASP	CB-CG-OD2	5.24	123.01	118.30
1	H	192	ASP	CB-CG-OD2	5.22	123.00	118.30
1	J	119	ASP	CB-CG-OD2	5.19	122.97	118.30
1	G	78	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	109	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	85	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	209	CYS	CB-CA-C	-5.05	100.29	110.40
1	E	188	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	180	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	182	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3102	0	3006	70	1
1	B	3102	0	3006	67	0
1	C	3102	0	3006	67	2
1	D	3102	0	3006	74	2
1	E	3102	0	3006	55	2
1	F	3102	0	3006	67	0
1	G	3102	0	3006	65	1
1	H	3102	0	3006	67	0
1	I	3102	0	3006	53	0
1	J	3102	0	3006	56	2
2	A	28	0	12	4	0
2	B	28	0	12	4	0
2	C	28	0	12	4	0
2	D	28	0	12	4	0
2	E	28	0	12	4	0
2	F	28	0	12	4	0
2	G	28	0	12	4	0
2	H	28	0	12	4	0
2	I	28	0	12	5	0
2	J	28	0	12	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	24	0	0	5	0
4	B	27	0	0	0	0
4	C	18	0	0	5	0
4	D	10	0	0	5	0
4	E	10	0	0	1	0
4	F	9	0	0	5	0
4	G	14	0	0	9	0
4	H	2	0	0	1	0
4	I	8	0	0	1	0
4	J	5	0	0	3	0
All	All	31437	0	30180	565	5

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 9.

All (565) 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:F:180:ASP:HA	4:F:2006:HOH:O	1.57	1.04
1:A:109:ASP:HB2	4:A:2008:HOH:O	1.56	1.04
1:B:258:ARG:HH11	1:B:258:ARG:HG2	1.21	1.02
1:F:238:GLN:HB3	4:F:2007:HOH:O	1.60	1.01
1:A:176:MET:SD	1:A:202:GLN:HG3	2.00	1.01
1:H:258:ARG:HG2	1:H:258:ARG:HH11	1.22	1.01
1:A:258:ARG:HH11	1:A:258:ARG:HG2	1.27	0.99
1:J:258:ARG:HG2	1:J:258:ARG:HH11	1.26	0.99
1:E:258:ARG:HG2	1:E:258:ARG:HH11	1.28	0.97
1:D:258:ARG:HG2	1:D:258:ARG:HH11	1.29	0.97
1:G:258:ARG:HG2	1:G:258:ARG:HH11	1.26	0.97
1:I:258:ARG:HG2	1:I:258:ARG:HH11	1.29	0.96
1:G:66:GLN:HE22	2:G:1383:GDP:HN1	1.16	0.94
1:F:66:GLN:HE22	2:F:1383:GDP:HN1	1.14	0.94
1:A:66:GLN:HE22	2:A:1383:GDP:HN1	1.13	0.93
1:F:258:ARG:HH11	1:F:258:ARG:HG2	1.29	0.93
1:E:66:GLN:HE22	2:E:1383:GDP:HN1	1.09	0.92
1:B:85:ARG:HG3	1:B:178:TYR:OH	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:GLN:HE22	2:H:1383:GDP:HN1	1.15	0.91
1:I:66:GLN:HE22	2:I:1383:GDP:HN1	1.10	0.91
1:E:252:ARG:HH12	1:G:248:PRO:HG3	1.34	0.91
1:D:66:GLN:HE22	2:D:1383:GDP:HN1	1.12	0.91
1:B:66:GLN:HE22	2:B:1383:GDP:HN1	1.15	0.90
1:C:258:ARG:HG2	1:C:258:ARG:HH11	1.34	0.90
1:D:249:ALA:HB3	4:D:2004:HOH:O	1.71	0.89
1:B:252:ARG:HH12	1:C:248:PRO:CG	1.86	0.89
1:J:66:GLN:HE22	2:J:1383:GDP:HN1	1.14	0.89
1:C:66:GLN:HE22	2:C:1383:GDP:HN1	1.10	0.88
1:I:85:ARG:HG3	1:I:178:TYR:OH	1.75	0.86
1:H:85:ARG:HG3	1:H:178:TYR:OH	1.77	0.85
1:G:85:ARG:HG3	1:G:178:TYR:OH	1.74	0.84
1:F:85:ARG:HG3	1:F:178:TYR:OH	1.75	0.84
1:D:85:ARG:HG3	1:D:178:TYR:OH	1.79	0.83
1:E:252:ARG:HH12	1:G:248:PRO:CG	1.92	0.82
1:J:85:ARG:HG3	1:J:178:TYR:OH	1.78	0.82
1:A:252:ARG:NH1	1:D:155:GLU:OE1	2.12	0.82
1:C:85:ARG:HG3	1:C:178:TYR:OH	1.79	0.82
1:D:55:ARG:HG2	1:D:55:ARG:HH21	1.44	0.81
1:G:56:ALA:HB3	4:G:2002:HOH:O	1.80	0.80
1:A:85:ARG:HG3	1:A:178:TYR:OH	1.81	0.80
1:H:258:ARG:NH1	1:H:258:ARG:HG2	1.95	0.78
1:B:142:ILE:CD1	1:B:230:LEU:HD11	2.13	0.78
1:J:258:ARG:NH1	1:J:258:ARG:HG2	1.98	0.78
1:F:259:VAL:HG21	1:F:360:TYR:CE1	2.19	0.78
1:C:66:GLN:NE2	2:C:1383:GDP:HN1	1.84	0.76
1:I:259:VAL:HG21	1:I:360:TYR:CE1	2.20	0.76
1:A:248:PRO:CG	1:D:252:ARG:HH12	1.96	0.76
1:B:252:ARG:HH12	1:C:248:PRO:HG3	1.49	0.76
1:G:259:VAL:HG21	1:G:360:TYR:CE1	2.21	0.76
1:E:258:ARG:NH1	1:E:258:ARG:HG2	2.00	0.75
1:F:252:ARG:HH12	1:H:248:PRO:CG	2.01	0.73
1:E:85:ARG:HG3	1:E:178:TYR:OH	1.89	0.73
1:J:259:VAL:HG21	1:J:360:TYR:CE1	2.23	0.73
1:J:283:THR:HG22	1:J:286:GLN:H	1.53	0.72
1:H:259:VAL:HG21	1:H:360:TYR:CE1	2.25	0.72
1:F:258:ARG:HG2	1:F:258:ARG:NH1	2.02	0.71
1:G:56:ALA:CB	4:G:2002:HOH:O	2.35	0.71
1:J:142:ILE:CD1	1:J:230:LEU:HD11	2.21	0.71
1:A:11:GLU:HG3	4:A:2001:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:MET:SD	1:H:202:GLN:HG3	2.31	0.70
1:C:142:ILE:CD1	1:C:230:LEU:HD11	2.21	0.70
1:B:361:ASP:OD1	1:C:258:ARG:HD2	1.90	0.70
1:F:248:PRO:CG	1:H:252:ARG:HH12	2.05	0.70
1:F:252:ARG:HH12	1:H:248:PRO:HG3	1.55	0.70
1:C:176:MET:SD	1:C:202:GLN:HG3	2.32	0.70
1:B:258:ARG:NH1	1:B:258:ARG:HG2	1.94	0.69
1:J:142:ILE:HD12	1:J:230:LEU:CD1	2.23	0.69
1:F:142:ILE:CD1	1:F:230:LEU:HD11	2.23	0.69
1:B:155:GLU:OE1	1:C:252:ARG:NH1	2.25	0.69
1:B:248:PRO:CG	1:C:252:ARG:HH12	2.05	0.69
1:B:283:THR:HG22	1:B:286:GLN:H	1.58	0.69
1:B:248:PRO:HG3	1:C:252:ARG:HH12	1.57	0.69
1:A:259:VAL:HG21	1:A:360:TYR:CE1	2.28	0.68
1:A:123:GLY:HA2	1:A:170:ARG:HD3	1.75	0.68
1:G:358:ARG:HH21	1:H:266:ARG:HA	1.58	0.68
1:I:283:THR:HG22	1:I:286:GLN:H	1.59	0.68
1:F:258:ARG:HD2	1:H:361:ASP:OD1	1.93	0.68
1:F:283:THR:HG22	1:F:286:GLN:H	1.57	0.68
1:E:259:VAL:HG21	1:E:360:TYR:CE1	2.28	0.68
1:A:66:GLN:NE2	2:A:1383:GDP:HN1	1.91	0.68
1:I:66:GLN:NE2	2:I:1383:GDP:HN1	1.89	0.68
1:F:176:MET:SD	1:F:202:GLN:HG3	2.34	0.68
1:I:258:ARG:HG2	1:I:258:ARG:NH1	2.01	0.67
1:H:180:ASP:HB3	1:H:183:VAL:HG13	1.77	0.67
1:I:176:MET:SD	1:I:202:GLN:HG3	2.34	0.67
1:F:361:ASP:OD1	1:H:258:ARG:HD2	1.94	0.67
1:E:66:GLN:NE2	2:E:1383:GDP:HN1	1.88	0.67
1:D:259:VAL:HG21	1:D:360:TYR:CE1	2.29	0.67
1:F:248:PRO:HG3	1:H:252:ARG:HH12	1.59	0.67
1:I:357:LEU:HD13	1:J:357:LEU:HD13	1.77	0.67
1:B:85:ARG:HG3	1:B:178:TYR:CZ	2.31	0.66
1:G:258:ARG:HG2	1:G:258:ARG:NH1	2.00	0.66
1:J:66:GLN:NE2	2:J:1383:GDP:HN1	1.91	0.66
1:C:184:ARG:NH1	1:C:184:ARG:HG2	2.10	0.66
1:G:142:ILE:CD1	1:G:230:LEU:HD11	2.26	0.66
1:A:248:PRO:HG2	1:D:252:ARG:HH22	1.60	0.66
1:G:66:GLN:NE2	2:G:1383:GDP:HN1	1.89	0.66
1:C:259:VAL:HG21	1:C:360:TYR:CE1	2.30	0.66
1:D:176:MET:SD	1:D:202:GLN:HG3	2.36	0.66
1:A:248:PRO:HG2	1:D:252:ARG:NH2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:CG	1:B:258:ARG:HH11	2.02	0.65
1:E:123:GLY:HA2	1:E:170:ARG:HD3	1.78	0.65
1:B:267:VAL:HG12	1:B:269:TYR:H	1.62	0.65
1:F:180:ASP:HB3	1:F:183:VAL:HG13	1.78	0.65
1:D:249:ALA:CA	4:D:2004:HOH:O	2.44	0.65
1:E:248:PRO:HG3	1:G:252:ARG:HH12	1.61	0.65
1:H:142:ILE:CD1	1:H:230:LEU:HD11	2.27	0.64
1:E:361:ASP:OD1	1:G:258:ARG:HD2	1.97	0.64
1:B:180:ASP:HB3	1:B:183:VAL:HG13	1.79	0.64
1:C:293:PHE:C	4:C:2012:HOH:O	2.35	0.64
1:G:85:ARG:HG3	1:G:178:TYR:CZ	2.32	0.64
1:A:358:ARG:HH21	1:B:266:ARG:HA	1.61	0.64
1:D:142:ILE:CD1	1:D:230:LEU:HD11	2.28	0.64
1:E:283:THR:HG22	1:E:286:GLN:H	1.63	0.64
1:B:123:GLY:HA2	1:B:170:ARG:HD3	1.80	0.64
1:I:123:GLY:HA2	1:I:170:ARG:HD3	1.78	0.63
1:A:248:PRO:CG	1:D:252:ARG:HH22	2.10	0.63
1:J:142:ILE:HD12	1:J:230:LEU:HD11	1.79	0.63
1:F:123:GLY:HA2	1:F:170:ARG:HD3	1.80	0.63
1:G:123:GLY:HA2	1:G:170:ARG:HD3	1.79	0.63
1:C:41:GLN:HG3	4:C:2001:HOH:O	1.96	0.63
1:H:123:GLY:HA2	1:H:170:ARG:HD3	1.79	0.63
1:E:266:ARG:HA	1:F:358:ARG:NH2	2.14	0.63
1:F:85:ARG:HG3	1:F:178:TYR:CZ	2.33	0.63
1:A:283:THR:HG22	1:A:286:GLN:H	1.62	0.63
1:C:358:ARG:HH21	1:D:266:ARG:HA	1.63	0.63
1:J:176:MET:SD	1:J:202:GLN:HG3	2.39	0.62
1:C:123:GLY:HA2	1:C:170:ARG:HD3	1.81	0.62
1:B:288:GLU:HG3	1:F:284:PRO:HG2	1.81	0.62
1:H:142:ILE:HD12	1:H:230:LEU:CD1	2.29	0.62
1:G:176:MET:SD	1:G:202:GLN:HG3	2.39	0.62
1:G:59:THR:CG2	4:G:2003:HOH:O	2.46	0.62
1:I:85:ARG:HG3	1:I:178:TYR:CZ	2.33	0.62
1:J:85:ARG:HG3	1:J:178:TYR:CZ	2.34	0.62
1:C:258:ARG:HG2	1:C:258:ARG:NH1	2.04	0.62
1:H:219:LEU:C	4:H:2002:HOH:O	2.38	0.62
1:D:283:THR:HG22	1:D:286:GLN:H	1.63	0.62
1:E:258:ARG:CG	1:E:258:ARG:HH11	2.09	0.62
1:H:258:ARG:CG	1:H:258:ARG:HH11	2.06	0.61
1:H:142:ILE:HD12	1:H:230:LEU:HD11	1.82	0.61
1:A:358:ARG:CD	4:A:2020:HOH:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:THR:HG22	1:G:286:GLN:H	1.64	0.61
1:D:249:ALA:CB	4:D:2004:HOH:O	2.40	0.61
1:H:85:ARG:HG3	1:H:178:TYR:CZ	2.36	0.61
1:D:85:ARG:HG3	1:D:178:TYR:CZ	2.35	0.61
1:C:358:ARG:CD	4:C:2016:HOH:O	2.48	0.61
1:B:259:VAL:HG21	1:B:360:TYR:CE1	2.34	0.61
1:C:142:ILE:HD12	1:C:230:LEU:HD11	1.81	0.61
1:B:142:ILE:CD1	1:B:230:LEU:CD1	2.78	0.61
1:A:155:GLU:OE1	1:D:252:ARG:NH1	2.34	0.61
1:C:142:ILE:HD12	1:C:230:LEU:CD1	2.30	0.61
1:B:142:ILE:HD12	1:B:230:LEU:CD1	2.31	0.61
1:H:283:THR:HG22	1:H:286:GLN:H	1.65	0.60
1:J:180:ASP:HB3	1:J:183:VAL:HG13	1.81	0.60
1:B:179:GLU:HA	1:B:179:GLU:OE2	2.00	0.60
1:C:179:GLU:OE2	1:C:179:GLU:HA	2.00	0.60
1:C:180:ASP:HB3	1:C:183:VAL:HG13	1.83	0.60
1:F:66:GLN:NE2	2:F:1383:GDP:HN1	1.94	0.60
1:B:66:GLN:HE21	2:B:1383:GDP:HN21	1.50	0.60
1:A:258:ARG:HH11	1:A:258:ARG:CG	2.09	0.60
1:B:66:GLN:NE2	2:B:1383:GDP:HN1	1.92	0.60
1:D:66:GLN:NE2	2:D:1383:GDP:HN1	1.92	0.60
1:C:85:ARG:HG3	1:C:178:TYR:CZ	2.37	0.60
1:A:180:ASP:HB3	1:A:183:VAL:HG13	1.84	0.60
1:A:176:MET:SD	1:A:202:GLN:CG	2.84	0.59
1:F:142:ILE:HD12	1:F:230:LEU:CD1	2.32	0.59
1:C:358:ARG:HD3	4:C:2016:HOH:O	2.03	0.59
1:J:123:GLY:HA2	1:J:170:ARG:HD3	1.84	0.59
1:J:258:ARG:CG	1:J:258:ARG:HH11	2.08	0.59
1:B:142:ILE:HD12	1:B:230:LEU:HD11	1.84	0.59
1:E:248:PRO:CG	1:G:252:ARG:HH12	2.15	0.59
1:E:142:ILE:HD12	1:E:230:LEU:CD1	2.33	0.59
1:E:176:MET:SD	1:E:202:GLN:HG3	2.43	0.59
1:I:180:ASP:HB3	1:I:183:VAL:HG13	1.85	0.59
1:H:39:ARG:HB3	1:I:71:THR:HB	1.84	0.59
1:H:66:GLN:NE2	2:H:1383:GDP:HN1	1.93	0.59
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.68	0.59
1:C:283:THR:HG22	1:C:286:GLN:H	1.66	0.59
1:I:142:ILE:CD1	1:I:230:LEU:HD11	2.33	0.58
1:G:142:ILE:HD12	1:G:230:LEU:CD1	2.33	0.58
1:B:181:GLU:OE1	1:B:185:ARG:NH2	2.31	0.58
1:A:258:ARG:NH1	1:A:258:ARG:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:HG2	1:D:252:ARG:NH1	2.18	0.58
1:E:155:GLU:OE1	1:E:248:PRO:HB3	2.04	0.58
1:E:142:ILE:CD1	1:E:230:LEU:HD11	2.32	0.58
1:D:180:ASP:HB3	1:D:183:VAL:HG13	1.84	0.58
1:B:252:ARG:HH12	1:C:248:PRO:HG2	1.65	0.58
1:B:177:LEU:HD23	1:B:198:VAL:HG22	1.86	0.57
1:E:142:ILE:HD12	1:E:230:LEU:HD11	1.86	0.57
1:I:142:ILE:HD12	1:I:230:LEU:CD1	2.34	0.57
1:B:177:LEU:CD2	1:B:198:VAL:HG22	2.35	0.57
1:E:266:ARG:HA	1:F:358:ARG:HH21	1.69	0.57
1:I:142:ILE:HD12	1:I:230:LEU:HD11	1.86	0.57
1:G:180:ASP:HB3	1:G:183:VAL:HG13	1.84	0.57
2:I:1383:GDP:PB	4:I:2008:HOH:O	2.61	0.57
1:E:85:ARG:HG3	1:E:178:TYR:CZ	2.40	0.57
1:J:382:ASN:N	4:J:2005:HOH:O	2.37	0.57
1:D:155:GLU:OE1	1:D:248:PRO:HB3	2.04	0.57
1:G:66:GLN:HE21	2:G:1383:GDP:HN21	1.53	0.57
1:A:248:PRO:HG2	1:D:252:ARG:HH12	1.69	0.57
1:A:258:ARG:HD2	1:D:361:ASP:OD1	2.06	0.56
1:D:123:GLY:HA2	1:D:170:ARG:HD3	1.87	0.56
1:G:290:LEU:HD21	1:G:301:LEU:HD12	1.87	0.56
1:F:258:ARG:CG	1:F:258:ARG:HH11	2.13	0.56
1:J:66:GLN:HE21	2:J:1383:GDP:HN21	1.53	0.56
1:D:55:ARG:NH2	1:D:55:ARG:HG2	2.19	0.56
1:A:357:LEU:HD13	1:B:357:LEU:HD13	1.86	0.56
1:C:66:GLN:HE21	2:C:1383:GDP:HN21	1.54	0.56
1:F:142:ILE:HD12	1:F:230:LEU:HD11	1.87	0.56
1:E:358:ARG:HH21	1:F:266:ARG:HA	1.70	0.56
1:A:85:ARG:HG3	1:A:178:TYR:CZ	2.40	0.56
1:A:267:VAL:HG12	1:A:269:TYR:H	1.71	0.55
1:G:258:ARG:HH11	1:G:258:ARG:CG	2.10	0.55
1:C:358:ARG:NH2	1:D:266:ARG:HA	2.22	0.55
1:H:177:LEU:CD2	1:H:198:VAL:HG22	2.37	0.55
1:I:266:ARG:HA	1:J:358:ARG:NH2	2.21	0.55
1:B:284:PRO:HG2	1:F:288:GLU:OE1	2.07	0.55
1:H:177:LEU:HD23	1:H:198:VAL:HG22	1.88	0.54
1:A:290:LEU:HD21	1:A:301:LEU:HD12	1.89	0.54
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.22	0.54
1:E:267:VAL:HG12	1:E:269:TYR:H	1.73	0.54
1:G:58:GLY:C	4:G:2003:HOH:O	2.44	0.54
1:B:176:MET:SD	1:B:202:GLN:HG3	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:GLU:OE1	1:B:248:PRO:HB3	2.06	0.54
1:G:358:ARG:HD3	1:H:265:GLU:O	2.06	0.54
1:C:358:ARG:HD3	1:D:265:GLU:O	2.08	0.54
1:A:248:PRO:CG	1:D:252:ARG:NH1	2.70	0.54
1:F:142:ILE:CD1	1:F:230:LEU:CD1	2.85	0.54
1:E:290:LEU:HD21	1:E:301:LEU:HD12	1.89	0.54
1:G:142:ILE:HD12	1:G:230:LEU:HD11	1.87	0.54
1:D:142:ILE:HD12	1:D:230:LEU:HD11	1.90	0.54
1:F:290:LEU:HD21	1:F:301:LEU:HD12	1.89	0.54
1:I:177:LEU:CD2	1:I:198:VAL:HG22	2.37	0.54
1:D:258:ARG:HG2	1:D:258:ARG:NH1	2.05	0.54
1:C:290:LEU:HD21	1:C:301:LEU:HD12	1.90	0.54
1:H:290:LEU:HD21	1:H:301:LEU:HD12	1.89	0.54
1:E:180:ASP:HB3	1:E:183:VAL:HG13	1.90	0.54
1:G:35:ILE:HD12	1:G:83:ALA:HB2	1.90	0.54
1:A:142:ILE:CD1	1:A:230:LEU:HD11	2.38	0.54
1:J:182:ARG:NH2	1:J:201:GLN:OE1	2.39	0.53
1:B:66:GLN:NE2	2:B:1383:GDP:HN21	2.05	0.53
1:G:59:THR:HG22	4:G:2003:HOH:O	2.06	0.53
1:A:248:PRO:HG3	1:D:252:ARG:HH12	1.74	0.53
1:A:252:ARG:HH22	1:D:248:PRO:CG	2.22	0.53
1:G:358:ARG:NH2	1:H:266:ARG:HA	2.22	0.53
1:H:188:ASP:HB2	1:H:232:GLU:OE2	2.09	0.53
1:G:59:THR:HG23	4:G:2003:HOH:O	2.08	0.53
1:G:266:ARG:HA	1:H:358:ARG:HH21	1.74	0.53
1:D:290:LEU:HD21	1:D:301:LEU:HD12	1.91	0.53
1:D:249:ALA:C	4:D:2004:HOH:O	2.47	0.53
1:D:55:ARG:CG	1:D:55:ARG:HH21	2.13	0.53
1:A:168:LEU:C	1:A:168:LEU:HD23	2.29	0.53
1:J:66:GLN:NE2	2:J:1383:GDP:HN21	2.07	0.53
1:H:85:ARG:HG3	1:H:178:TYR:HH	1.72	0.53
1:D:142:ILE:HD12	1:D:230:LEU:CD1	2.39	0.53
1:I:155:GLU:OE1	1:I:248:PRO:HB3	2.09	0.53
1:A:14:GLU:CD	1:A:14:GLU:H	2.11	0.53
1:E:358:ARG:NH2	1:F:266:ARG:HA	2.24	0.52
1:F:177:LEU:HD23	1:F:198:VAL:HG22	1.91	0.52
1:D:249:ALA:N	4:D:2004:HOH:O	2.42	0.52
1:C:177:LEU:HD23	1:C:198:VAL:HG22	1.90	0.52
1:E:252:ARG:NH1	1:G:248:PRO:CG	2.67	0.52
1:J:177:LEU:CD2	1:J:198:VAL:HG22	2.40	0.52
1:A:248:PRO:HG2	1:D:252:ARG:CZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:GLU:OE1	1:F:248:PRO:HB3	2.09	0.52
1:A:179:GLU:OE2	1:A:179:GLU:HA	2.08	0.52
1:D:267:VAL:HG12	1:D:269:TYR:H	1.74	0.52
1:G:267:VAL:HG12	1:G:269:TYR:H	1.75	0.52
1:F:177:LEU:CD2	1:F:198:VAL:HG22	2.39	0.52
1:B:188:ASP:HB2	1:B:232:GLU:OE2	2.10	0.52
1:J:225:ASP:N	4:J:2002:HOH:O	2.43	0.52
1:C:155:GLU:OE1	1:C:248:PRO:HB3	2.08	0.52
1:G:97:HIS:CE1	1:G:168:LEU:HD12	2.45	0.51
1:B:252:ARG:NH1	1:C:248:PRO:HG2	2.24	0.51
1:C:357:LEU:HD13	1:D:357:LEU:HD13	1.91	0.51
1:H:267:VAL:HG12	1:H:269:TYR:H	1.75	0.51
1:J:290:LEU:HD21	1:J:301:LEU:HD12	1.92	0.51
1:I:266:ARG:HA	1:J:358:ARG:HH21	1.76	0.51
1:I:258:ARG:CG	1:I:258:ARG:HH11	2.13	0.51
1:F:238:GLN:CB	4:F:2007:HOH:O	2.35	0.51
1:E:265:GLU:O	1:F:358:ARG:HD3	2.10	0.51
1:B:92:GLN:OE1	1:B:92:GLN:HA	2.11	0.51
1:E:357:LEU:HD13	1:F:357:LEU:HD13	1.93	0.51
1:F:180:ASP:OD2	1:F:182:ARG:NH1	2.44	0.51
1:I:290:LEU:HD21	1:I:301:LEU:HD12	1.92	0.51
1:I:66:GLN:HE21	2:I:1383:GDP:HN21	1.59	0.50
1:F:283:THR:HG21	1:F:335:ASP:OD2	2.11	0.50
1:G:177:LEU:HD23	1:G:198:VAL:HG22	1.94	0.50
1:J:35:ILE:HD12	1:J:83:ALA:HB2	1.93	0.50
1:I:143:THR:HA	1:I:237:ILE:CD1	2.41	0.50
1:A:252:ARG:HH12	1:D:248:PRO:CG	2.24	0.50
1:I:177:LEU:HD23	1:I:198:VAL:HG22	1.93	0.50
1:J:180:ASP:OD2	1:J:182:ARG:NH1	2.44	0.50
1:E:66:GLN:HE21	2:E:1383:GDP:HN21	1.58	0.50
1:C:258:ARG:CG	1:C:258:ARG:HH11	2.13	0.50
1:H:155:GLU:OE1	1:H:248:PRO:HB3	2.12	0.50
1:J:142:ILE:CD1	1:J:230:LEU:CD1	2.84	0.50
1:D:177:LEU:HD23	1:D:198:VAL:HG22	1.93	0.50
1:B:10:HIS:HE1	1:B:38:GLU:OE2	1.94	0.50
1:A:66:GLN:HE21	2:A:1383:GDP:HN21	1.60	0.50
1:J:177:LEU:HD23	1:J:198:VAL:HG22	1.93	0.50
1:I:188:ASP:HB2	1:I:232:GLU:OE2	2.12	0.50
1:G:142:ILE:CD1	1:G:230:LEU:CD1	2.89	0.50
1:H:35:ILE:HD12	1:H:83:ALA:HB2	1.94	0.50
1:A:184:ARG:NH1	1:A:184:ARG:HG2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:HD21	1:B:301:LEU:HD12	1.94	0.50
1:E:258:ARG:HD2	1:G:361:ASP:OD1	2.12	0.49
1:H:142:ILE:CD1	1:H:230:LEU:CD1	2.90	0.49
1:A:262:HIS:CD2	1:A:263:ILE:HG13	2.47	0.49
1:H:143:THR:HA	1:H:237:ILE:CD1	2.40	0.49
1:D:66:GLN:NE2	2:D:1383:GDP:HN21	2.10	0.49
1:I:182:ARG:NH2	1:I:201:GLN:OE1	2.43	0.49
1:J:97:HIS:CE1	1:J:168:LEU:HD12	2.48	0.49
1:B:252:ARG:NH1	1:C:248:PRO:CG	2.66	0.49
1:C:142:ILE:CD1	1:C:230:LEU:CD1	2.87	0.49
1:E:369:ARG:HH11	1:G:257:HIS:HE1	1.60	0.49
1:H:180:ASP:OD2	1:H:182:ARG:NH1	2.45	0.49
1:E:158:TRP:CE2	1:G:252:ARG:HD2	2.47	0.49
1:A:358:ARG:HD3	1:B:265:GLU:O	2.12	0.49
1:D:85:ARG:HG3	1:D:178:TYR:HH	1.77	0.49
1:I:265:GLU:O	1:J:358:ARG:HD3	2.11	0.49
1:F:59:THR:HG21	4:F:2002:HOH:O	2.11	0.49
1:B:283:THR:HG21	1:B:335:ASP:OD2	2.12	0.49
1:A:358:ARG:HD3	4:A:2020:HOH:O	2.12	0.49
1:H:97:HIS:CE1	1:H:168:LEU:HD12	2.48	0.49
1:A:142:ILE:HD12	1:A:230:LEU:HD11	1.95	0.48
1:G:177:LEU:CD2	1:G:198:VAL:HG22	2.43	0.48
1:E:177:LEU:HD23	1:E:198:VAL:HG22	1.95	0.48
1:J:104:THR:C	4:J:2001:HOH:O	2.51	0.48
1:H:143:THR:HA	1:H:237:ILE:HD11	1.95	0.48
1:I:97:HIS:CE1	1:I:168:LEU:HD12	2.48	0.48
1:C:247:GLN:HB2	1:C:248:PRO:HD2	1.95	0.48
1:J:283:THR:HG21	1:J:335:ASP:OD2	2.13	0.48
1:A:358:ARG:NH2	1:B:266:ARG:HA	2.28	0.48
1:B:143:THR:HA	1:B:237:ILE:CD1	2.43	0.48
1:I:267:VAL:HG12	1:I:269:TYR:H	1.77	0.48
1:E:66:GLN:NE2	2:E:1383:GDP:HN21	2.11	0.48
1:A:358:ARG:NE	4:A:2020:HOH:O	2.47	0.48
1:D:180:ASP:OD2	1:D:182:ARG:NH1	2.47	0.48
1:D:181:GLU:OE1	1:D:185:ARG:NH2	2.43	0.48
1:E:247:GLN:HB2	1:G:250:ILE:HD11	1.96	0.48
1:E:179:GLU:OE2	1:E:179:GLU:HA	2.12	0.48
1:C:177:LEU:CD2	1:C:198:VAL:HG22	2.43	0.48
1:A:142:ILE:HD12	1:A:230:LEU:CD1	2.44	0.48
1:J:267:VAL:HG12	1:J:269:TYR:H	1.77	0.48
1:D:194:LEU:O	1:D:198:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:VAL:HG12	1:F:269:TYR:H	1.79	0.47
1:H:66:GLN:NE2	2:H:1383:GDP:HN21	2.13	0.47
1:I:66:GLN:NE2	2:I:1383:GDP:HN21	2.12	0.47
1:C:267:VAL:HG12	1:C:269:TYR:H	1.78	0.47
1:C:66:GLN:NE2	2:C:1383:GDP:HN21	2.11	0.47
1:J:143:THR:HA	1:J:237:ILE:CD1	2.43	0.47
1:D:66:GLN:HE21	2:D:1383:GDP:HN21	1.62	0.47
1:I:262:HIS:CD2	1:I:263:ILE:HG13	2.50	0.47
1:F:35:ILE:HD12	1:F:83:ALA:HB2	1.97	0.47
1:A:177:LEU:HD23	1:A:198:VAL:HG22	1.96	0.47
1:D:258:ARG:HH11	1:D:258:ARG:CG	2.13	0.47
1:G:66:GLN:NE2	2:G:1383:GDP:HN21	2.11	0.47
1:D:55:ARG:NH2	1:D:55:ARG:CG	2.70	0.47
1:C:180:ASP:OD2	1:C:182:ARG:NH1	2.47	0.47
1:G:180:ASP:OD2	1:G:182:ARG:NH1	2.47	0.47
1:C:35:ILE:HD12	1:C:83:ALA:HB2	1.95	0.47
1:G:265:GLU:O	1:H:358:ARG:HD3	2.14	0.47
1:I:283:THR:HG21	1:I:335:ASP:OD2	2.14	0.47
1:A:81:ASN:ND2	1:A:195:TYR:OH	2.48	0.47
1:H:304:CYS:HA	1:H:307:ARG:O	2.15	0.47
1:H:66:GLN:HE21	2:H:1383:GDP:HN21	1.62	0.47
1:D:142:ILE:CD1	1:D:230:LEU:CD1	2.93	0.47
1:F:194:LEU:O	1:F:198:VAL:HG13	2.15	0.47
1:F:262:HIS:CD2	1:F:263:ILE:HG13	2.50	0.47
1:A:155:GLU:OE1	1:A:248:PRO:HB3	2.15	0.46
1:D:130:PRO:O	1:D:131:ARG:HG2	2.15	0.46
1:C:181:GLU:OE1	1:C:185:ARG:NH2	2.47	0.46
1:H:70:GLY:HA2	1:H:185:ARG:HA	1.97	0.46
1:F:143:THR:HA	1:F:237:ILE:CD1	2.46	0.46
1:E:143:THR:HA	1:E:237:ILE:CD1	2.45	0.46
1:D:262:HIS:CD2	1:D:263:ILE:HG13	2.50	0.46
1:D:257:HIS:CD2	1:D:257:HIS:N	2.83	0.46
1:E:180:ASP:OD2	1:E:182:ARG:NH1	2.48	0.46
1:J:304:CYS:HA	1:J:307:ARG:O	2.16	0.46
1:G:357:LEU:HD13	1:H:357:LEU:HD13	1.97	0.46
1:E:318:TRP:HB2	1:E:347:ARG:HD3	1.97	0.46
1:F:66:GLN:HE21	2:F:1383:GDP:HN21	1.63	0.46
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.80	0.46
1:B:130:PRO:C	1:B:131:ARG:HG2	2.36	0.46
1:I:70:GLY:HA2	1:I:185:ARG:HA	1.98	0.46
1:F:66:GLN:NE2	2:F:1383:GDP:HN21	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:ARG:NH2	1:I:90:GLU:OE1	2.50	0.45
1:J:70:GLY:HA2	1:J:185:ARG:HA	1.98	0.45
1:I:14:GLU:CD	1:I:14:GLU:H	2.19	0.45
1:C:294:THR:N	4:C:2012:HOH:O	2.47	0.45
1:J:377:GLN:O	1:J:380:LEU:HB2	2.17	0.45
1:D:247:GLN:HB2	1:D:248:PRO:HD2	1.99	0.45
1:I:35:ILE:HD12	1:I:83:ALA:HB2	1.98	0.45
1:B:168:LEU:C	1:B:168:LEU:HD23	2.37	0.45
1:G:56:ALA:HB2	4:G:2002:HOH:O	2.12	0.45
1:B:177:LEU:HD23	1:B:198:VAL:CG2	2.47	0.45
1:G:267:VAL:N	4:G:2009:HOH:O	2.35	0.45
1:G:14:GLU:H	1:G:14:GLU:CD	2.20	0.45
1:A:177:LEU:CD2	1:A:198:VAL:HG22	2.46	0.45
1:B:198:VAL:O	1:B:202:GLN:HG2	2.17	0.45
1:I:318:TRP:HB2	1:I:347:ARG:HD3	1.99	0.45
1:J:318:TRP:HB2	1:J:347:ARG:HD3	1.99	0.45
1:C:307:ARG:HD2	1:D:276:HIS:CD2	2.51	0.45
1:I:179:GLU:HA	1:I:179:GLU:OE2	2.16	0.45
1:E:177:LEU:CD2	1:E:198:VAL:HG22	2.47	0.45
1:B:97:HIS:CE1	1:B:168:LEU:HD12	2.52	0.45
1:E:168:LEU:HD23	1:E:168:LEU:C	2.38	0.45
1:E:97:HIS:CE1	1:E:168:LEU:HD12	2.52	0.45
1:H:177:LEU:HD23	1:H:198:VAL:CG2	2.46	0.45
1:D:110:TRP:N	1:D:110:TRP:CD1	2.84	0.45
1:C:143:THR:HA	1:C:237:ILE:CD1	2.47	0.44
1:D:130:PRO:C	1:D:131:ARG:HG2	2.38	0.44
1:B:248:PRO:CG	1:C:252:ARG:NH1	2.78	0.44
1:I:177:LEU:HD23	1:I:198:VAL:CG2	2.47	0.44
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.83	0.44
1:C:98:PHE:O	1:C:166:GLU:HA	2.17	0.44
1:H:179:GLU:OE2	1:H:179:GLU:HA	2.17	0.44
1:B:304:CYS:HA	1:B:307:ARG:O	2.18	0.44
1:A:198:VAL:O	1:A:202:GLN:HG2	2.17	0.44
1:F:239:SER:N	4:F:2007:HOH:O	2.50	0.44
1:D:177:LEU:CD2	1:D:198:VAL:HG22	2.47	0.44
1:F:301:LEU:HD23	1:F:301:LEU:HA	1.88	0.44
1:F:70:GLY:HA2	1:F:185:ARG:HA	2.00	0.44
1:I:358:ARG:HH21	1:J:266:ARG:HA	1.83	0.44
1:B:98:PHE:O	1:B:166:GLU:HA	2.18	0.44
1:G:155:GLU:OE1	1:G:248:PRO:HB3	2.18	0.44
1:C:198:VAL:O	1:C:202:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:O	1:B:131:ARG:HG2	2.17	0.44
1:J:155:GLU:OE1	1:J:248:PRO:HB3	2.17	0.44
1:B:14:GLU:H	1:B:14:GLU:CD	2.20	0.44
1:A:68:ARG:NH1	1:A:72:LEU:O	2.49	0.44
1:B:262:HIS:CD2	1:B:263:ILE:HG13	2.52	0.43
1:F:177:LEU:HD23	1:F:198:VAL:CG2	2.48	0.43
1:I:143:THR:HA	1:I:237:ILE:HD11	1.99	0.43
1:J:143:THR:HA	1:J:237:ILE:HD11	2.00	0.43
1:G:179:GLU:HA	1:G:179:GLU:OE2	2.18	0.43
1:A:35:ILE:HD12	1:A:83:ALA:HB2	2.01	0.43
1:F:179:GLU:OE2	1:F:179:GLU:HA	2.18	0.43
1:A:66:GLN:NE2	2:A:1383:GDP:HN21	2.15	0.43
1:B:96:ILE:CG2	1:B:169:MET:HG3	2.48	0.43
1:D:168:LEU:C	1:D:168:LEU:HD23	2.39	0.43
1:C:377:GLN:O	1:C:380:LEU:HB2	2.18	0.43
1:C:182:ARG:NH2	1:C:201:GLN:OE1	2.46	0.43
1:H:194:LEU:O	1:H:198:VAL:HG13	2.18	0.43
1:D:70:GLY:HA2	1:D:185:ARG:HA	2.01	0.43
1:G:143:THR:HA	1:G:237:ILE:CD1	2.48	0.43
1:C:34:CYS:HB2	1:C:63:VAL:HG13	1.99	0.43
1:E:361:ASP:HB2	4:E:2010:HOH:O	2.17	0.43
1:A:252:ARG:HH12	1:D:248:PRO:HG3	1.83	0.43
1:H:318:TRP:HB2	1:H:347:ARG:HD3	1.99	0.43
1:G:247:GLN:HB2	1:G:248:PRO:HD2	2.01	0.43
1:H:283:THR:HG21	1:H:335:ASP:OD2	2.18	0.43
1:J:179:GLU:OE2	1:J:179:GLU:HA	2.19	0.43
1:F:98:PHE:O	1:F:166:GLU:HA	2.19	0.43
1:A:283:THR:HG21	1:A:335:ASP:OD2	2.18	0.43
1:I:142:ILE:CD1	1:I:230:LEU:CD1	2.95	0.43
1:G:70:GLY:HA2	1:G:185:ARG:HA	2.00	0.43
1:J:277:ARG:CZ	1:J:281:HIS:HD2	2.31	0.43
1:C:85:ARG:NH2	1:C:90:GLU:OE1	2.52	0.43
1:E:14:GLU:H	1:E:14:GLU:CD	2.21	0.43
1:J:177:LEU:HD23	1:J:198:VAL:CG2	2.49	0.43
1:C:262:HIS:CD2	1:C:263:ILE:HG13	2.53	0.43
1:G:188:ASP:HB2	1:G:232:GLU:OE2	2.19	0.43
1:F:97:HIS:CE1	1:F:168:LEU:HD12	2.54	0.43
1:B:247:GLN:HB2	1:B:248:PRO:HD2	1.99	0.42
1:I:180:ASP:OD2	1:I:182:ARG:NH1	2.51	0.42
1:C:70:GLY:HA2	1:C:185:ARG:HA	2.01	0.42
1:B:35:ILE:HD12	1:B:83:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:VAL:O	1:I:202:GLN:HG2	2.18	0.42
1:D:143:THR:HA	1:D:237:ILE:CD1	2.48	0.42
1:F:130:PRO:O	1:F:131:ARG:HG2	2.18	0.42
1:G:318:TRP:HB2	1:G:347:ARG:HD3	2.01	0.42
1:D:35:ILE:HD12	1:D:83:ALA:HB2	2.01	0.42
1:J:85:ARG:NH2	1:J:90:GLU:OE1	2.52	0.42
1:H:262:HIS:CD2	1:H:263:ILE:HG13	2.54	0.42
1:H:98:PHE:O	1:H:166:GLU:HA	2.19	0.42
1:H:182:ARG:NH2	1:H:201:GLN:OE1	2.46	0.42
1:J:262:HIS:CD2	1:J:263:ILE:HG13	2.54	0.42
1:G:53:ILE:HA	4:G:2002:HOH:O	2.20	0.42
1:B:143:THR:HA	1:B:237:ILE:HD11	2.00	0.42
1:B:377:GLN:O	1:B:380:LEU:HB2	2.20	0.42
1:H:227:ARG:HG2	1:H:227:ARG:NH1	2.35	0.42
1:D:14:GLU:H	1:D:14:GLU:CD	2.22	0.42
1:B:258:ARG:HD2	1:C:361:ASP:OD1	2.19	0.42
1:C:170:ARG:H	1:C:170:ARG:HG2	1.69	0.42
1:D:301:LEU:O	1:D:304:CYS:HB2	2.20	0.42
1:C:307:ARG:CD	1:D:276:HIS:CD2	3.03	0.42
1:F:188:ASP:HB2	1:F:232:GLU:OE2	2.20	0.42
1:E:262:HIS:CD2	1:E:263:ILE:HG13	2.55	0.42
1:J:10:HIS:HE1	1:J:38:GLU:OE2	2.02	0.42
1:C:188:ASP:HB2	1:C:232:GLU:OE2	2.20	0.42
1:H:377:GLN:O	1:H:380:LEU:HB2	2.20	0.42
1:H:39:ARG:CB	1:I:71:THR:HB	2.49	0.41
1:C:283:THR:HG21	1:C:335:ASP:OD2	2.20	0.41
1:C:318:TRP:HB2	1:C:347:ARG:HD3	2.01	0.41
1:E:35:ILE:HD12	1:E:83:ALA:HB2	2.02	0.41
1:A:92:GLN:OE1	1:A:92:GLN:HA	2.20	0.41
1:B:85:ARG:HE	1:B:85:ARG:HB3	1.67	0.41
1:H:85:ARG:NH2	1:H:90:GLU:OE1	2.53	0.41
1:D:198:VAL:O	1:D:202:GLN:HG2	2.19	0.41
1:J:168:LEU:HD23	1:J:168:LEU:C	2.40	0.41
1:B:40:ASP:C	1:B:40:ASP:OD1	2.59	0.41
1:G:85:ARG:NH2	1:G:90:GLU:OE1	2.53	0.41
1:F:130:PRO:C	1:F:131:ARG:HG2	2.40	0.41
1:A:70:GLY:HA2	1:A:185:ARG:HA	2.03	0.41
1:A:333:ASP:C	1:A:333:ASP:OD1	2.58	0.41
1:H:92:GLN:HA	1:H:92:GLN:OE1	2.20	0.41
1:I:295:THR:HB	1:I:296:PRO:HD3	2.02	0.41
1:F:143:THR:HA	1:F:237:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:HIS:HE1	1:H:38:GLU:OE2	2.03	0.41
1:G:283:THR:HG21	1:G:335:ASP:OD2	2.20	0.41
1:F:131:ARG:CZ	1:F:136:ALA:HB2	2.50	0.41
1:G:102:ASP:OD2	1:G:217:HIS:HB2	2.21	0.41
1:E:102:ASP:OD2	1:E:217:HIS:HB2	2.21	0.41
1:J:184:ARG:HG2	1:J:184:ARG:NH1	2.35	0.41
1:H:184:ARG:NH1	1:H:184:ARG:HG2	2.35	0.41
1:A:170:ARG:H	1:A:170:ARG:HG2	1.74	0.41
1:E:130:PRO:C	1:E:131:ARG:HG2	2.41	0.41
1:J:188:ASP:HB2	1:J:232:GLU:OE2	2.21	0.41
1:J:98:PHE:O	1:J:166:GLU:HA	2.20	0.41
1:F:301:LEU:O	1:F:304:CYS:HB2	2.21	0.41
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.76	0.41
1:J:130:PRO:C	1:J:131:ARG:HG2	2.41	0.41
1:H:295:THR:HB	1:H:296:PRO:HD3	2.02	0.41
1:F:318:TRP:HB2	1:F:347:ARG:HD3	2.03	0.41
1:B:158:TRP:CE2	1:C:252:ARG:HD2	2.56	0.41
1:D:283:THR:HG21	1:D:335:ASP:OD2	2.19	0.41
1:H:181:GLU:OE1	1:H:185:ARG:NH2	2.50	0.41
1:I:170:ARG:HG2	1:I:170:ARG:H	1.76	0.41
1:E:143:THR:HA	1:E:237:ILE:HD11	2.02	0.41
1:E:98:PHE:O	1:E:166:GLU:HA	2.21	0.41
1:F:380:LEU:HD23	1:F:380:LEU:HA	1.96	0.41
1:A:130:PRO:O	1:A:131:ARG:HG2	2.21	0.41
1:F:10:HIS:HE1	1:F:38:GLU:OE2	2.04	0.41
1:I:85:ARG:HB3	1:I:85:ARG:HE	1.68	0.41
1:J:142:ILE:HD12	1:J:230:LEU:HD12	1.98	0.41
1:J:142:ILE:HD11	1:J:230:LEU:HD11	2.01	0.41
1:H:168:LEU:HD23	1:H:168:LEU:C	2.42	0.41
1:F:168:LEU:HD23	1:F:168:LEU:C	2.41	0.41
1:A:131:ARG:CZ	1:A:136:ALA:HB2	2.51	0.41
1:G:98:PHE:O	1:G:166:GLU:HA	2.21	0.41
1:C:14:GLU:H	1:C:14:GLU:CD	2.23	0.41
1:F:252:ARG:HH12	1:H:248:PRO:HG2	1.82	0.40
1:I:194:LEU:O	1:I:198:VAL:HG13	2.21	0.40
1:I:131:ARG:CZ	1:I:136:ALA:HB2	2.52	0.40
1:A:247:GLN:HB2	1:A:248:PRO:HD2	2.03	0.40
1:B:318:TRP:HB2	1:B:347:ARG:HD3	2.02	0.40
1:F:295:THR:HB	1:F:296:PRO:HD3	2.04	0.40
1:D:84:LEU:HD12	1:D:84:LEU:HA	1.85	0.40
1:D:10:HIS:HE1	1:D:38:GLU:OE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ARG:NH1	1:G:248:PRO:HG2	2.35	0.40
1:J:198:VAL:O	1:J:202:GLN:HG2	2.21	0.40
1:A:97:HIS:CE1	1:A:168:LEU:HD12	2.57	0.40
1:E:102:ASP:CG	1:E:217:HIS:HB2	2.42	0.40
1:A:130:PRO:C	1:A:131:ARG:HG2	2.42	0.40
1:I:10:HIS:HE1	1:I:38:GLU:OE2	2.04	0.40
1:H:130:PRO:C	1:H:131:ARG:HG2	2.42	0.40
1:D:182:ARG:NH2	1:D:201:GLN:OE1	2.46	0.40
1:F:277:ARG:CZ	1:F:281:HIS:HD2	2.35	0.40
1:G:92:GLN:HA	1:G:92:GLN:OE1	2.21	0.40
1:E:252:ARG:NH1	1:G:248:PRO:HG3	2.17	0.40
1:H:14:GLU:H	1:H:14:GLU:CD	2.24	0.40
1:I:184:ARG:NH1	1:I:184:ARG:HG2	2.36	0.40
1:A:231:VAL:HG12	1:A:340:LEU:HD23	2.03	0.40

All (5) 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:D:55:ARG:CD	1:E:150:LEU:O[1_554]	1.25	0.95
1:A:380:LEU:O	1:G:179:GLU:OE2[1_554]	2.09	0.11
1:C:71:THR:OG1	1:J:332:GLY:O[3_556]	2.09	0.11
1:D:55:ARG:CD	1:E:150:LEU:C[1_554]	2.15	0.05
1:C:332:GLY:O	1:J:68:ARG:NH2[3_556]	2.19	0.01

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	372/397 (94%)	362 (97%)	9 (2%)	1 (0%)	46 81
1	B	372/397 (94%)	361 (97%)	9 (2%)	2 (0%)	34 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	372/397 (94%)	362 (97%)	10 (3%)	0	100	100
1	D	372/397 (94%)	361 (97%)	11 (3%)	0	100	100
1	E	372/397 (94%)	361 (97%)	10 (3%)	1 (0%)	46	81
1	F	372/397 (94%)	362 (97%)	9 (2%)	1 (0%)	46	81
1	G	372/397 (94%)	359 (96%)	13 (4%)	0	100	100
1	H	372/397 (94%)	361 (97%)	11 (3%)	0	100	100
1	I	372/397 (94%)	361 (97%)	11 (3%)	0	100	100
1	J	372/397 (94%)	363 (98%)	7 (2%)	2 (0%)	34	74
All	All	3720/3970 (94%)	3613 (97%)	100 (3%)	7 (0%)	52	86

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	A	310	PHE
1	B	246	GLY
1	E	310	PHE
1	F	310	PHE
1	J	310	PHE
1	J	248	PRO

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	323/338 (96%)	299 (93%)	24 (7%)	17	49
1	B	323/338 (96%)	298 (92%)	25 (8%)	16	47
1	C	323/338 (96%)	298 (92%)	25 (8%)	16	47
1	D	323/338 (96%)	297 (92%)	26 (8%)	15	45
1	E	323/338 (96%)	299 (93%)	24 (7%)	17	49
1	F	323/338 (96%)	300 (93%)	23 (7%)	18	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	323/338 (96%)	298 (92%)	25 (8%)	16 47
1	H	323/338 (96%)	301 (93%)	22 (7%)	20 54
1	I	323/338 (96%)	301 (93%)	22 (7%)	20 54
1	J	323/338 (96%)	301 (93%)	22 (7%)	20 54
All	All	3230/3380 (96%)	2992 (93%)	238 (7%)	17 49

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	GLU
1	A	63	VAL
1	A	65	LEU
1	A	68	ARG
1	A	72	LEU
1	A	84	LEU
1	A	85	ARG
1	A	109	ASP
1	A	124	LEU
1	A	169	MET
1	A	179	GLU
1	A	182	ARG
1	A	209	CYS
1	A	217	HIS
1	A	219	LEU
1	A	258	ARG
1	A	259	VAL
1	A	283	THR
1	A	289	LEU
1	A	301	LEU
1	A	343	LEU
1	A	365	GLN
1	A	381	GLU
1	B	11	GLU
1	B	14	GLU
1	B	39	ARG
1	B	48	ARG
1	B	63	VAL
1	B	65	LEU
1	B	68	ARG
1	B	72	LEU

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Mol	Chain	Res	Type
1	B	84	LEU
1	B	109	ASP
1	B	124	LEU
1	B	169	MET
1	B	179	GLU
1	B	182	ARG
1	B	209	CYS
1	B	217	HIS
1	B	219	LEU
1	B	258	ARG
1	B	259	VAL
1	B	266	ARG
1	B	283	THR
1	B	289	LEU
1	B	301	LEU
1	B	316	MET
1	B	343	LEU
1	C	11	GLU
1	C	14	GLU
1	C	39	ARG
1	C	48	ARG
1	C	63	VAL
1	C	65	LEU
1	C	68	ARG
1	C	72	LEU
1	C	84	LEU
1	C	85	ARG
1	C	109	ASP
1	C	124	LEU
1	C	169	MET
1	C	179	GLU
1	C	182	ARG
1	C	209	CYS
1	C	217	HIS
1	C	219	LEU
1	C	252	ARG
1	C	258	ARG
1	C	259	VAL
1	C	283	THR
1	C	289	LEU
1	C	301	LEU
1	C	343	LEU

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Mol	Chain	Res	Type
1	D	11	GLU
1	D	14	GLU
1	D	48	ARG
1	D	55	ARG
1	D	63	VAL
1	D	65	LEU
1	D	68	ARG
1	D	72	LEU
1	D	84	LEU
1	D	85	ARG
1	D	109	ASP
1	D	124	LEU
1	D	169	MET
1	D	179	GLU
1	D	182	ARG
1	D	209	CYS
1	D	217	HIS
1	D	219	LEU
1	D	258	ARG
1	D	259	VAL
1	D	266	ARG
1	D	283	THR
1	D	289	LEU
1	D	301	LEU
1	D	316	MET
1	D	343	LEU
1	E	11	GLU
1	E	14	GLU
1	E	48	ARG
1	E	63	VAL
1	E	65	LEU
1	E	68	ARG
1	E	72	LEU
1	E	84	LEU
1	E	109	ASP
1	E	124	LEU
1	E	169	MET
1	E	179	GLU
1	E	182	ARG
1	E	186	ARG
1	E	209	CYS
1	E	217	HIS

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Mol	Chain	Res	Type
1	E	219	LEU
1	E	258	ARG
1	E	259	VAL
1	E	266	ARG
1	E	283	THR
1	E	289	LEU
1	E	301	LEU
1	E	343	LEU
1	F	11	GLU
1	F	14	GLU
1	F	63	VAL
1	F	65	LEU
1	F	68	ARG
1	F	72	LEU
1	F	84	LEU
1	F	85	ARG
1	F	109	ASP
1	F	124	LEU
1	F	169	MET
1	F	179	GLU
1	F	182	ARG
1	F	209	CYS
1	F	217	HIS
1	F	219	LEU
1	F	258	ARG
1	F	259	VAL
1	F	266	ARG
1	F	283	THR
1	F	289	LEU
1	F	301	LEU
1	F	343	LEU
1	G	11	GLU
1	G	14	GLU
1	G	63	VAL
1	G	65	LEU
1	G	68	ARG
1	G	72	LEU
1	G	84	LEU
1	G	85	ARG
1	G	109	ASP
1	G	124	LEU
1	G	169	MET

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Mol	Chain	Res	Type
1	G	179	GLU
1	G	182	ARG
1	G	186	ARG
1	G	209	CYS
1	G	217	HIS
1	G	219	LEU
1	G	252	ARG
1	G	258	ARG
1	G	259	VAL
1	G	266	ARG
1	G	283	THR
1	G	289	LEU
1	G	301	LEU
1	G	343	LEU
1	H	11	GLU
1	H	14	GLU
1	H	63	VAL
1	H	65	LEU
1	H	68	ARG
1	H	72	LEU
1	H	84	LEU
1	H	109	ASP
1	H	124	LEU
1	H	169	MET
1	H	179	GLU
1	H	182	ARG
1	H	209	CYS
1	H	217	HIS
1	H	219	LEU
1	H	258	ARG
1	H	259	VAL
1	H	266	ARG
1	H	283	THR
1	H	289	LEU
1	H	301	LEU
1	H	343	LEU
1	I	11	GLU
1	I	14	GLU
1	I	63	VAL
1	I	65	LEU
1	I	68	ARG
1	I	72	LEU

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Mol	Chain	Res	Type
1	I	84	LEU
1	I	109	ASP
1	I	124	LEU
1	I	169	MET
1	I	179	GLU
1	I	182	ARG
1	I	209	CYS
1	I	217	HIS
1	I	219	LEU
1	I	258	ARG
1	I	259	VAL
1	I	266	ARG
1	I	283	THR
1	I	289	LEU
1	I	301	LEU
1	I	343	LEU
1	J	11	GLU
1	J	14	GLU
1	J	63	VAL
1	J	65	LEU
1	J	68	ARG
1	J	72	LEU
1	J	84	LEU
1	J	109	ASP
1	J	124	LEU
1	J	169	MET
1	J	179	GLU
1	J	182	ARG
1	J	209	CYS
1	J	217	HIS
1	J	219	LEU
1	J	258	ARG
1	J	259	VAL
1	J	266	ARG
1	J	283	THR
1	J	289	LEU
1	J	301	LEU
1	J	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	30	HIS
1	A	66	GLN
1	A	81	ASN
1	A	253	GLN
1	A	257	HIS
1	A	281	HIS
1	B	10	HIS
1	B	30	HIS
1	B	66	GLN
1	B	81	ASN
1	B	153	HIS
1	B	257	HIS
1	B	276	HIS
1	B	281	HIS
1	C	10	HIS
1	C	66	GLN
1	C	81	ASN
1	C	257	HIS
1	C	276	HIS
1	C	281	HIS
1	D	10	HIS
1	D	30	HIS
1	D	66	GLN
1	D	81	ASN
1	D	253	GLN
1	D	257	HIS
1	D	276	HIS
1	D	281	HIS
1	E	10	HIS
1	E	30	HIS
1	E	66	GLN
1	E	81	ASN
1	E	153	HIS
1	E	253	GLN
1	E	257	HIS
1	E	281	HIS
1	F	10	HIS
1	F	30	HIS
1	F	66	GLN
1	F	81	ASN
1	F	253	GLN
1	F	257	HIS

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Mol	Chain	Res	Type
1	F	281	HIS
1	G	10	HIS
1	G	30	HIS
1	G	66	GLN
1	G	81	ASN
1	G	253	GLN
1	G	257	HIS
1	G	281	HIS
1	H	10	HIS
1	H	30	HIS
1	H	66	GLN
1	H	81	ASN
1	H	253	GLN
1	H	257	HIS
1	H	262	HIS
1	H	281	HIS
1	I	10	HIS
1	I	30	HIS
1	I	66	GLN
1	I	81	ASN
1	I	257	HIS
1	I	281	HIS
1	J	10	HIS
1	J	30	HIS
1	J	66	GLN
1	J	81	ASN
1	J	253	GLN
1	J	257	HIS
1	J	281	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 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	GDP	A	1383	3	23,30,30	1.19	3 (13%)	30,47,47	2.01	9 (30%)
2	GDP	B	1383	3	23,30,30	1.05	2 (8%)	30,47,47	1.87	8 (26%)
2	GDP	C	1383	3	23,30,30	1.25	2 (8%)	30,47,47	1.92	8 (26%)
2	GDP	D	1383	3	23,30,30	1.13	2 (8%)	30,47,47	1.99	8 (26%)
2	GDP	E	1383	3	23,30,30	1.16	2 (8%)	30,47,47	1.97	7 (23%)
2	GDP	F	1383	3	23,30,30	1.11	2 (8%)	30,47,47	1.89	8 (26%)
2	GDP	G	1383	3	23,30,30	1.16	2 (8%)	30,47,47	1.86	7 (23%)
2	GDP	H	1383	3	23,30,30	1.14	2 (8%)	30,47,47	1.86	7 (23%)
2	GDP	I	1383	3	23,30,30	1.10	2 (8%)	30,47,47	1.98	7 (23%)
2	GDP	J	1383	3	23,30,30	1.12	2 (8%)	30,47,47	1.85	6 (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	GDP	A	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	B	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	C	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	D	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	E	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	F	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	G	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	H	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	I	1383	3	-	0/12/32/32	0/3/3/3
2	GDP	J	1383	3	-	0/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1383	GDP	C6-C5	2.38	1.46	1.41
2	G	1383	GDP	C5-C4	2.75	1.46	1.40
2	A	1383	GDP	C6-C5	2.77	1.46	1.41
2	I	1383	GDP	C5-C4	2.78	1.46	1.40
2	B	1383	GDP	C5-C4	2.86	1.46	1.40
2	A	1383	GDP	C5-C4	2.88	1.47	1.40
2	F	1383	GDP	C5-C4	2.88	1.47	1.40
2	J	1383	GDP	C5-C4	2.91	1.47	1.40
2	D	1383	GDP	C6-C5	2.93	1.47	1.41
2	D	1383	GDP	C5-C4	2.94	1.47	1.40
2	A	1383	GDP	O4'-C1'	2.97	1.45	1.41
2	H	1383	GDP	C5-C4	3.00	1.47	1.40
2	C	1383	GDP	C5-C4	3.13	1.47	1.40
2	F	1383	GDP	C6-C5	3.15	1.47	1.41
2	E	1383	GDP	C5-C4	3.23	1.47	1.40
2	E	1383	GDP	C6-C5	3.29	1.47	1.41
2	I	1383	GDP	C6-C5	3.37	1.48	1.41
2	J	1383	GDP	C6-C5	3.41	1.48	1.41
2	H	1383	GDP	C6-C5	3.76	1.48	1.41
2	C	1383	GDP	C6-C5	3.92	1.49	1.41
2	G	1383	GDP	C6-C5	3.93	1.49	1.41

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1383	GDP	C5-C6-N1	-4.87	116.92	123.59
2	A	1383	GDP	C5-C6-N1	-4.85	116.96	123.59
2	D	1383	GDP	C5-C6-N1	-4.73	117.12	123.59
2	B	1383	GDP	C5-C6-N1	-4.70	117.17	123.59
2	H	1383	GDP	C5-C6-N1	-4.62	117.27	123.59
2	C	1383	GDP	C5-C6-N1	-4.40	117.57	123.59
2	I	1383	GDP	C5-C6-N1	-4.38	117.60	123.59
2	J	1383	GDP	C5-C6-N1	-4.09	118.00	123.59
2	F	1383	GDP	C5-C6-N1	-3.96	118.17	123.59
2	I	1383	GDP	N3-C2-N1	-3.94	121.44	127.44
2	E	1383	GDP	C4-C5-N7	-3.91	105.88	109.48
2	J	1383	GDP	C6-C5-C4	-3.88	116.25	120.90
2	C	1383	GDP	C1'-N9-C4	-3.76	121.26	126.94
2	G	1383	GDP	C5-C6-N1	-3.72	118.50	123.59
2	F	1383	GDP	C6-C5-C4	-3.71	116.47	120.90
2	C	1383	GDP	C6-C5-C4	-3.60	116.60	120.90
2	G	1383	GDP	C6-C5-C4	-3.58	116.62	120.90
2	H	1383	GDP	C4-C5-N7	-3.56	106.21	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1383	GDP	C4-C5-N7	-3.54	106.22	109.48
2	A	1383	GDP	N3-C2-N1	-3.47	122.16	127.44
2	G	1383	GDP	N3-C2-N1	-3.40	122.27	127.44
2	J	1383	GDP	N3-C2-N1	-3.33	122.36	127.44
2	I	1383	GDP	C6-C5-C4	-3.32	116.93	120.90
2	F	1383	GDP	N3-C2-N1	-3.31	122.40	127.44
2	D	1383	GDP	N3-C2-N1	-3.30	122.42	127.44
2	I	1383	GDP	C4-C5-N7	-3.29	106.45	109.48
2	A	1383	GDP	C4-C5-N7	-3.26	106.48	109.48
2	F	1383	GDP	C1'-N9-C4	-3.19	122.13	126.94
2	D	1383	GDP	C6-C5-C4	-3.18	117.10	120.90
2	D	1383	GDP	C4-C5-N7	-3.05	106.67	109.48
2	C	1383	GDP	C4-C5-N7	-3.04	106.68	109.48
2	B	1383	GDP	N3-C2-N1	-3.02	122.84	127.44
2	H	1383	GDP	N3-C2-N1	-3.01	122.86	127.44
2	H	1383	GDP	C6-C5-C4	-3.00	117.31	120.90
2	J	1383	GDP	C1'-N9-C4	-2.99	122.42	126.94
2	E	1383	GDP	C6-C5-C4	-2.89	117.44	120.90
2	B	1383	GDP	PA-O3A-PB	-2.79	123.30	132.67
2	H	1383	GDP	C1'-N9-C4	-2.77	122.76	126.94
2	B	1383	GDP	C6-C5-C4	-2.76	117.60	120.90
2	D	1383	GDP	C1'-N9-C4	-2.74	122.81	126.94
2	G	1383	GDP	C1'-N9-C4	-2.71	122.85	126.94
2	F	1383	GDP	C4-C5-N7	-2.69	107.01	109.48
2	A	1383	GDP	C6-C5-C4	-2.68	117.70	120.90
2	B	1383	GDP	C4-C5-N7	-2.67	107.03	109.48
2	E	1383	GDP	C1'-N9-C4	-2.65	122.94	126.94
2	A	1383	GDP	C1'-N9-C4	-2.63	122.97	126.94
2	C	1383	GDP	PA-O3A-PB	-2.62	123.87	132.67
2	E	1383	GDP	N3-C2-N1	-2.56	123.54	127.44
2	D	1383	GDP	PA-O3A-PB	-2.49	124.31	132.67
2	G	1383	GDP	PA-O3A-PB	-2.44	124.48	132.67
2	A	1383	GDP	PA-O3A-PB	-2.40	124.62	132.67
2	I	1383	GDP	PA-O3A-PB	-2.39	124.64	132.67
2	F	1383	GDP	PA-O3A-PB	-2.37	124.73	132.67
2	I	1383	GDP	C1'-N9-C4	-2.33	123.43	126.94
2	C	1383	GDP	N3-C2-N1	-2.26	124.00	127.44
2	B	1383	GDP	C1'-N9-C4	-2.21	123.61	126.94
2	A	1383	GDP	O3A-PA-O5'	-2.14	97.27	102.94
2	E	1383	GDP	O3A-PA-O5'	-2.13	97.29	102.94
2	H	1383	GDP	PA-O3A-PB	-2.05	125.79	132.67
2	D	1383	GDP	O3B-PB-O3A	2.08	114.54	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1383	GDP	O3B-PB-O3A	2.09	114.55	105.09
2	J	1383	GDP	O3B-PB-O3A	2.24	115.25	105.09
2	C	1383	GDP	O3B-PB-O3A	2.49	116.39	105.09
2	A	1383	GDP	O3B-PB-O3A	2.52	116.52	105.09
2	B	1383	GDP	O3B-PB-O3A	2.86	118.08	105.09
2	G	1383	GDP	C6-N1-C2	4.66	122.40	115.94
2	C	1383	GDP	C6-N1-C2	4.74	122.52	115.94
2	F	1383	GDP	C6-N1-C2	4.88	122.72	115.94
2	H	1383	GDP	C6-N1-C2	5.04	122.93	115.94
2	J	1383	GDP	C6-N1-C2	5.06	122.96	115.94
2	B	1383	GDP	C6-N1-C2	5.07	122.98	115.94
2	A	1383	GDP	C6-N1-C2	5.19	123.14	115.94
2	E	1383	GDP	C6-N1-C2	5.33	123.34	115.94
2	D	1383	GDP	C6-N1-C2	5.48	123.54	115.94
2	I	1383	GDP	C6-N1-C2	5.63	123.75	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1383	GDP	4	0
2	B	1383	GDP	4	0
2	C	1383	GDP	4	0
2	D	1383	GDP	4	0
2	E	1383	GDP	4	0
2	F	1383	GDP	4	0
2	G	1383	GDP	4	0
2	H	1383	GDP	4	0
2	I	1383	GDP	5	0
2	J	1383	GDP	4	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	376/397 (94%)	0.18	3 (0%) 87 73	62, 63, 65, 67	0
1	B	376/397 (94%)	0.22	5 (1%) 79 61	62, 63, 65, 67	0
1	C	376/397 (94%)	0.34	14 (3%) 45 27	62, 63, 65, 67	0
1	D	376/397 (94%)	0.32	11 (2%) 55 35	62, 63, 65, 67	0
1	E	376/397 (94%)	0.39	12 (3%) 51 32	62, 63, 65, 67	0
1	F	376/397 (94%)	0.90	63 (16%) 2 1	62, 63, 65, 67	0
1	G	376/397 (94%)	0.35	16 (4%) 39 23	62, 63, 65, 67	0
1	H	376/397 (94%)	0.40	16 (4%) 39 23	62, 63, 65, 67	0
1	I	376/397 (94%)	0.56	29 (7%) 16 8	62, 63, 65, 67	0
1	J	376/397 (94%)	0.52	28 (7%) 17 9	62, 63, 65, 67	0
All	All	3760/3970 (94%)	0.42	197 (5%) 31 17	62, 63, 65, 67	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	248	PRO	12.6
1	E	382	ASN	11.0
1	B	247	GLN	9.2
1	F	247	GLN	8.6
1	D	248	PRO	7.1
1	G	247	GLN	6.7
1	D	247	GLN	6.0
1	J	247	GLN	5.9
1	C	247	GLN	5.7
1	I	248	PRO	5.6
1	G	248	PRO	5.5
1	F	53	ILE	5.4
1	B	248	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	248	PRO	5.2
1	H	247	GLN	5.2
1	F	92	GLN	5.1
1	E	247	GLN	5.1
1	F	178	TYR	4.9
1	F	377	GLN	4.7
1	A	247	GLN	4.5
1	I	247	GLN	4.5
1	E	246	GLY	4.4
1	F	74	PRO	4.4
1	F	42	THR	4.4
1	F	37	TYR	4.2
1	H	248	PRO	4.1
1	J	248	PRO	4.1
1	D	268	GLY	4.1
1	F	179	GLU	4.0
1	J	13	PRO	3.8
1	I	253	GLN	3.8
1	F	2	SER	3.8
1	F	75	GLY	3.8
1	J	268	GLY	3.7
1	F	79	GLY	3.7
1	I	327	GLU	3.6
1	J	45	ALA	3.6
1	F	246	GLY	3.6
1	I	306	ARG	3.6
1	J	48	ARG	3.5
1	F	10	HIS	3.5
1	F	56	ALA	3.5
1	J	50	ALA	3.5
1	F	61	VAL	3.4
1	F	77	GLY	3.4
1	J	246	GLY	3.4
1	C	181	GLU	3.4
1	D	41	GLN	3.3
1	D	246	GLY	3.3
1	F	162	PRO	3.2
1	F	57	THR	3.2
1	F	139	THR	3.2
1	C	53	ILE	3.2
1	I	289	LEU	3.2
1	F	15	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	257	HIS	3.1
1	J	61	VAL	3.1
1	C	15	VAL	3.1
1	J	42	THR	3.0
1	G	41	GLN	3.0
1	H	202	GLN	3.0
1	E	248	PRO	3.0
1	H	328	HIS	3.0
1	F	55	ARG	3.0
1	J	253	GLN	3.0
1	I	227	ARG	3.0
1	F	58	GLY	3.0
1	C	52	GLU	2.9
1	F	38	GLU	2.9
1	I	52	GLU	2.9
1	G	381	GLU	2.9
1	B	246	GLY	2.9
1	I	175	ALA	2.9
1	H	88	LEU	2.9
1	F	185	ARG	2.9
1	F	161	GLN	2.9
1	F	165	GLY	2.9
1	F	306	ARG	2.9
1	I	56	ALA	2.9
1	J	46	VAL	2.9
1	I	92	GLN	2.8
1	I	53	ILE	2.8
1	H	92	GLN	2.8
1	H	380	LEU	2.8
1	F	93	TRP	2.8
1	I	55	ARG	2.8
1	F	76	LYS	2.8
1	I	251	HIS	2.8
1	G	42	THR	2.7
1	J	15	VAL	2.7
1	F	164	GLY	2.7
1	F	336	TRP	2.7
1	E	262	HIS	2.7
1	E	92	GLN	2.7
1	C	377	GLN	2.7
1	I	25	ALA	2.7
1	F	163	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	265	GLU	2.7
1	C	306	ARG	2.7
1	I	27	PRO	2.6
1	J	380	LEU	2.6
1	F	40	ASP	2.6
1	J	225	ASP	2.6
1	C	246	GLY	2.6
1	B	41	GLN	2.6
1	F	8	PHE	2.6
1	G	44	GLU	2.6
1	J	14	GLU	2.6
1	J	251	HIS	2.6
1	C	381	GLU	2.6
1	F	41	GLN	2.6
1	I	24	ALA	2.6
1	I	287	VAL	2.5
1	I	244	VAL	2.5
1	F	268	GLY	2.5
1	J	252	ARG	2.5
1	D	288	GLU	2.5
1	F	13	PRO	2.5
1	J	12	HIS	2.5
1	E	365	GLN	2.5
1	G	181	GLU	2.5
1	F	36	GLY	2.5
1	H	246	GLY	2.5
1	H	302	ARG	2.4
1	F	12	HIS	2.4
1	F	52	GLU	2.4
1	F	89	GLU	2.4
1	F	48	ARG	2.4
1	F	97	HIS	2.4
1	I	106	PHE	2.4
1	F	54	SER	2.4
1	F	108	PRO	2.4
1	F	86	TYR	2.4
1	G	246	GLY	2.4
1	H	55	ARG	2.4
1	H	376	TYR	2.4
1	I	377	GLN	2.4
1	F	29	VAL	2.4
1	F	159	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	218	ARG	2.4
1	J	267	VAL	2.4
1	F	84	LEU	2.3
1	F	127	HIS	2.3
1	G	17	LEU	2.3
1	B	380	LEU	2.3
1	I	207	TYR	2.3
1	I	159	ILE	2.3
1	J	49	ALA	2.3
1	G	242	HIS	2.3
1	E	328	HIS	2.3
1	C	376	TYR	2.2
1	J	158	TRP	2.2
1	F	188	ASP	2.2
1	G	108	PRO	2.2
1	J	266	ARG	2.2
1	J	92	GLN	2.2
1	E	55	ARG	2.2
1	C	365	GLN	2.2
1	I	299	GLU	2.2
1	F	262	HIS	2.2
1	J	365	GLN	2.2
1	J	57	THR	2.2
1	F	46	VAL	2.2
1	G	24	ALA	2.2
1	E	158	TRP	2.2
1	E	306	ARG	2.2
1	I	51	PRO	2.2
1	F	181	GLU	2.2
1	H	377	GLN	2.2
1	J	65	LEU	2.2
1	F	382	ASN	2.2
1	H	299	GLU	2.1
1	I	267	VAL	2.1
1	J	99	TYR	2.1
1	H	181	GLU	2.1
1	I	57	THR	2.1
1	A	376	TYR	2.1
1	F	202	GLN	2.1
1	G	92	GLN	2.1
1	C	378	ALA	2.1
1	F	381	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	9	LYS	2.1
1	D	293	PHE	2.1
1	E	94	GLU	2.1
1	I	326	LEU	2.1
1	G	18	HIS	2.1
1	D	92	GLN	2.1
1	F	47	GLU	2.1
1	G	268	GLY	2.1
1	I	61	VAL	2.1
1	D	109	ASP	2.0
1	A	382	ASN	2.0
1	C	12	HIS	2.0
1	D	10	HIS	2.0
1	H	97	HIS	2.0
1	D	13	PRO	2.0
1	G	252	ARG	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	GDP	F	1383	28/28	0.82	0.35	0.01	63,63,64,65	0
2	GDP	G	1383	28/28	0.95	0.19	-0.18	63,63,64,65	0
2	GDP	I	1383	28/28	0.96	0.19	-0.53	63,63,64,66	0
2	GDP	J	1383	28/28	0.94	0.18	-0.89	62,63,64,66	0
2	GDP	D	1383	28/28	0.95	0.16	-0.95	62,63,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GDP	H	1383	28/28	0.96	0.17	-1.43	63,63,64,65	0
2	GDP	A	1383	28/28	0.95	0.15	-1.56	62,63,64,66	0
2	GDP	C	1383	28/28	0.97	0.14	-2.10	62,63,64,66	0
2	GDP	B	1383	28/28	0.97	0.14	-2.14	62,63,64,66	0
2	GDP	E	1383	28/28	0.95	0.14	-2.20	62,63,64,66	0
3	CO	B	1384	1/1	0.90	0.10	-	67,67,67,67	0
3	CO	I	1384	1/1	0.97	0.06	-	67,67,67,67	0
3	CO	D	1384	1/1	0.95	0.05	-	68,68,68,68	0
3	CO	G	1384	1/1	0.97	0.04	-	66,66,66,66	0
3	CO	J	1384	1/1	0.95	0.06	-	67,67,67,67	0
3	CO	E	1384	1/1	0.91	0.09	-	67,67,67,67	0
3	CO	H	1384	1/1	0.96	0.03	-	67,67,67,67	0
3	CO	C	1384	1/1	0.96	0.05	-	67,67,67,67	0
3	CO	A	1384	1/1	0.95	0.08	-	67,67,67,67	0
3	CO	F	1384	1/1	0.92	0.14	-	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.