Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:12 PM GMT

PDB ID	:	1SJD
Title	:	x-ray structure of o-succinylbenzoate synthase complexed with n-succinyl phenylglycine
Authors	:	Thoden, J.B.; Taylor-Ringia, E.A.; Garrett, J.B.; Gerlt, J.A.; Holden, H.M.; Rayment, I.
Deposited on	:	2004-03-03
Resolution	:	1.87 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:

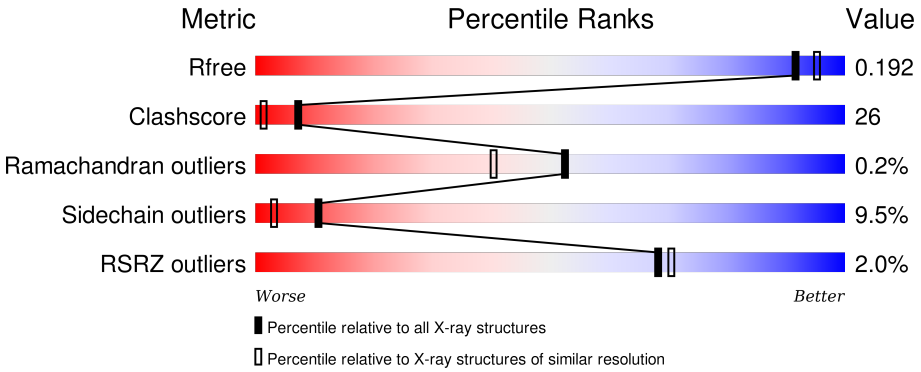
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.87 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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	368	57% 32% 10%
1	B	368	% 67% 23% 9%
1	C	368	% 61% 32% 6%
1	D	368	7% 47% 38% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NPG	B	1163	-	-	-	X
2	NPG	D	1500	-	-	X	X

2 Entry composition

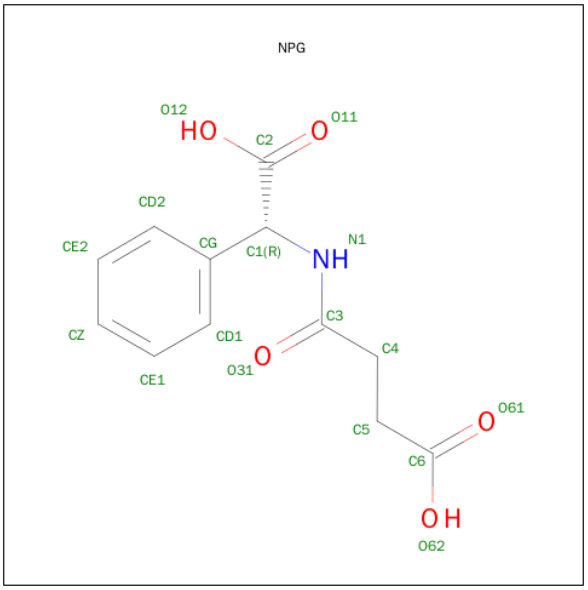
There are 3 unique types of molecules in this entry. The entry contains 12337 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2765	1758	480	515	12			
1	B	368	Total	C	N	O	S	0	0	0
			2772	1761	481	518	12			
1	C	367	Total	C	N	O	S	0	0	0
			2765	1758	480	515	12			
1	D	367	Total	C	N	O	S	0	0	0
			2765	1758	480	515	12			

- Molecule 2 is N-SUCCINYL PHENYLGLYCINE (three-letter code: NPG) (formula: $C_{12}H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	12	1	5		
2	B	1	Total	C	N	O	0	0
			18	12	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			18	12	1	5		
2	D	1	Total	C	N	O	0	0
			18	12	1	5		
2	B	1	Total	C	N	O	0	0
			18	12	1	5		
2	C	1	Total	C	N	O	0	0
			18	12	1	5		

- Molecule 3 is water.

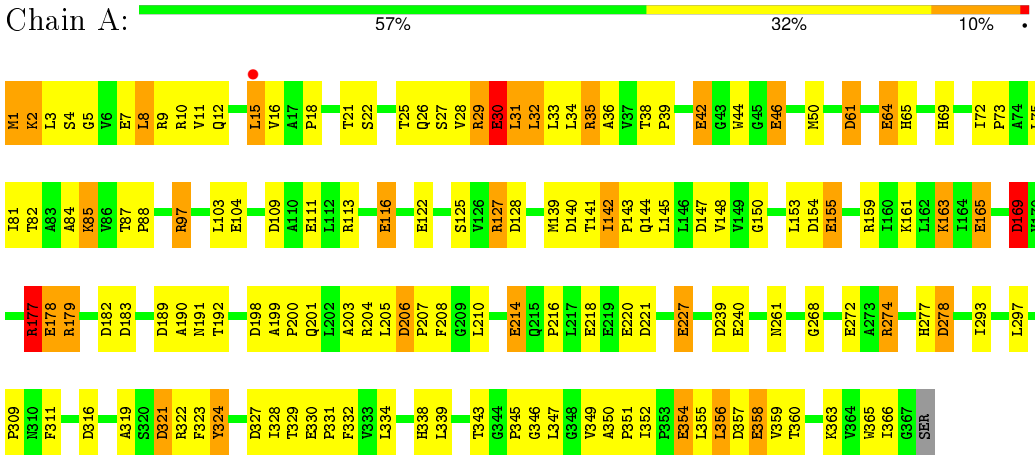
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	261	Total	O	0	0
			261	261		
3	B	375	Total	O	0	0
			375	375		
3	C	336	Total	O	0	0
			336	336		
3	D	190	Total	O	0	0
			190	190		

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.

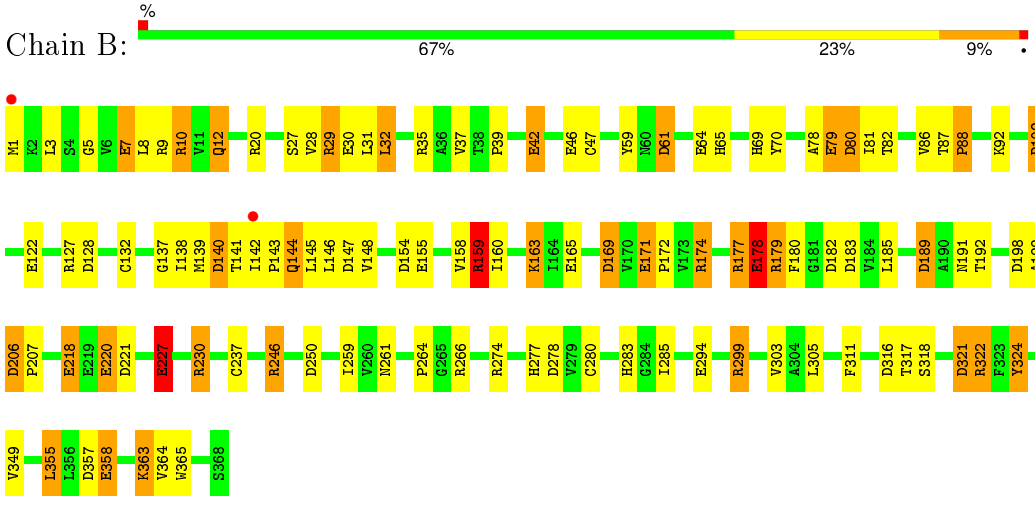
- Molecule 1: N-acylamino acid racemase

Chain A:



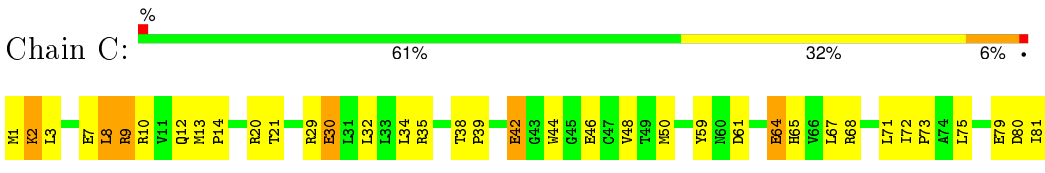
- Molecule 1: N-acylamino acid racemase

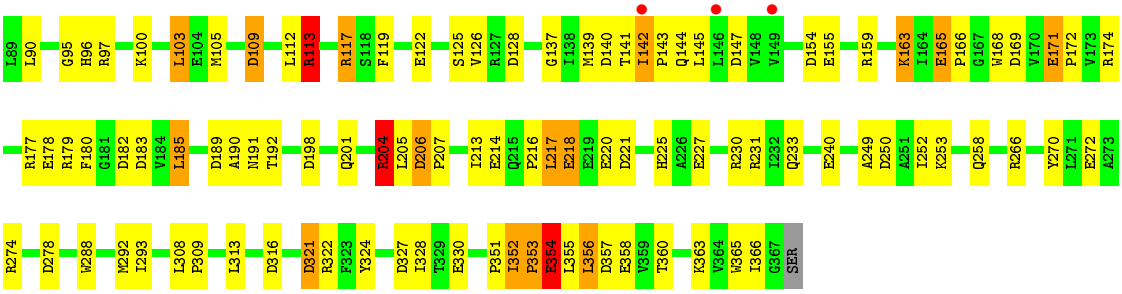
Chain B:



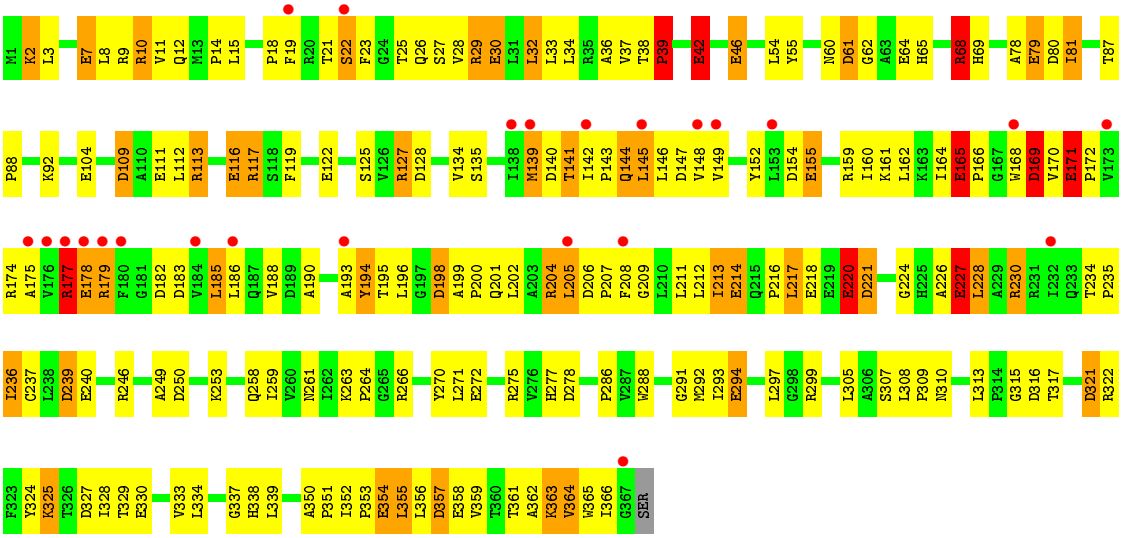
- Molecule 1: N-acylamino acid racemase

Chain C:





- Molecule 1: N-acylamino acid racemase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	215.20Å 215.20Å 257.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.87 49.66 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-1.87) 99.7 (49.66-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.87 (at 1.87Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.196 , 0.241 0.193 , 0.192	Depositor DCC
R_{free} test set	18681 reflections (11.11%)	DCC
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 115.9	EDS
Estimated twinning fraction	0.017 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.014 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.011 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 186821 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12337	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: NPG

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	0.98	20/2821 (0.7%)	1.36	43/3842 (1.1%)
1	B	0.96	18/2828 (0.6%)	1.41	51/3850 (1.3%)
1	C	0.98	18/2821 (0.6%)	1.46	51/3842 (1.3%)
1	D	1.04	23/2821 (0.8%)	1.45	46/3842 (1.2%)
All	All	0.99	79/11291 (0.7%)	1.42	191/15376 (1.2%)

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	220	GLU	CD-OE2	9.11	1.35	1.25
1	D	358	GLU	CD-OE2	7.63	1.34	1.25
1	D	178	GLU	CD-OE2	7.59	1.33	1.25
1	A	178	GLU	CD-OE2	7.56	1.33	1.25
1	A	358	GLU	CD-OE2	7.54	1.33	1.25
1	C	30	GLU	CD-OE2	7.51	1.33	1.25
1	C	214	GLU	CD-OE2	7.51	1.33	1.25
1	A	155	GLU	CD-OE2	7.48	1.33	1.25
1	D	171	GLU	CD-OE2	7.45	1.33	1.25
1	A	116	GLU	CD-OE2	7.19	1.33	1.25
1	A	171	GLU	CD-OE2	7.14	1.33	1.25
1	C	227	GLU	CD-OE2	7.06	1.33	1.25
1	D	165	GLU	CD-OE2	7.00	1.33	1.25
1	B	79	GLU	CD-OE2	6.96	1.33	1.25
1	A	354	GLU	CD-OE2	6.95	1.33	1.25
1	C	178	GLU	CD-OE2	6.94	1.33	1.25
1	D	155	GLU	CD-OE2	6.94	1.33	1.25
1	B	171	GLU	CD-OE2	6.84	1.33	1.25
1	D	218	GLU	CD-OE2	6.83	1.33	1.25
1	D	79	GLU	CD-OE2	6.83	1.33	1.25
1	D	227	GLU	CD-OE2	6.79	1.33	1.25
1	B	178	GLU	CD-OE2	6.77	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	354	GLU	CD-OE2	6.73	1.33	1.25
1	D	330	GLU	CD-OE2	6.68	1.33	1.25
1	B	155	GLU	CD-OE2	6.65	1.32	1.25
1	A	30	GLU	CD-OE2	6.63	1.32	1.25
1	D	104	GLU	CD-OE2	6.59	1.32	1.25
1	D	240	GLU	CD-OE2	6.57	1.32	1.25
1	D	214	GLU	CD-OE2	6.56	1.32	1.25
1	C	171	GLU	CD-OE2	6.55	1.32	1.25
1	A	79	GLU	CD-OE2	6.51	1.32	1.25
1	B	42	GLU	CD-OE2	6.41	1.32	1.25
1	D	30	GLU	CD-OE2	6.40	1.32	1.25
1	D	46	GLU	CD-OE2	6.38	1.32	1.25
1	B	46	GLU	CD-OE2	6.35	1.32	1.25
1	C	46	GLU	CD-OE2	6.30	1.32	1.25
1	A	104	GLU	CD-OE2	6.25	1.32	1.25
1	C	330	GLU	CD-OE2	6.22	1.32	1.25
1	C	354	GLU	CD-OE2	6.16	1.32	1.25
1	B	122	GLU	CD-OE2	6.14	1.32	1.25
1	D	42	GLU	CD-OE2	6.14	1.32	1.25
1	C	218	GLU	CD-OE2	6.11	1.32	1.25
1	C	42	GLU	CD-OE2	6.11	1.32	1.25
1	A	227	GLU	CD-OE2	6.09	1.32	1.25
1	B	165	GLU	CD-OE2	6.03	1.32	1.25
1	C	358	GLU	CD-OE2	6.02	1.32	1.25
1	C	79	GLU	CD-OE2	6.00	1.32	1.25
1	A	7	GLU	CD-OE2	5.92	1.32	1.25
1	B	30	GLU	CD-OE2	5.89	1.32	1.25
1	C	272	GLU	CD-OE2	5.88	1.32	1.25
1	B	218	GLU	CD-OE2	5.82	1.32	1.25
1	A	122	GLU	CD-OE2	5.82	1.32	1.25
1	C	122	GLU	CD-OE2	5.77	1.31	1.25
1	C	155	GLU	CD-OE2	5.71	1.31	1.25
1	B	294	GLU	CD-OE2	5.71	1.31	1.25
1	A	272	GLU	CD-OE2	5.55	1.31	1.25
1	A	330	GLU	CD-OE2	5.54	1.31	1.25
1	B	116	GLU	CD-OE2	5.54	1.31	1.25
1	C	165	GLU	CD-OE2	5.52	1.31	1.25
1	A	220	GLU	CD-OE2	5.50	1.31	1.25
1	D	122	GLU	CD-OE2	5.49	1.31	1.25
1	A	64	GLU	CD-OE2	5.42	1.31	1.25
1	B	358	GLU	CD-OE2	5.33	1.31	1.25
1	D	111	GLU	CD-OE2	5.32	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLU	CD-OE2	5.31	1.31	1.25
1	B	7	GLU	CD-OE2	5.26	1.31	1.25
1	B	227	GLU	CD-OE2	5.22	1.31	1.25
1	A	46	GLU	CD-OE2	5.19	1.31	1.25
1	A	42	GLU	CD-OE2	5.17	1.31	1.25
1	D	116	GLU	CD-OE2	5.17	1.31	1.25
1	D	272	GLU	CD-OE2	5.16	1.31	1.25
1	A	240	GLU	CD-OE2	5.14	1.31	1.25
1	B	220	GLU	CD-OE2	5.09	1.31	1.25
1	B	330	GLU	CD-OE2	5.05	1.31	1.25
1	D	294	GLU	CD-OE2	5.05	1.31	1.25
1	C	64	GLU	CD-OE2	5.05	1.31	1.25
1	D	64	GLU	CD-OE2	5.05	1.31	1.25
1	C	240	GLU	CD-OE2	5.03	1.31	1.25
1	A	214	GLU	CD-OE2	5.02	1.31	1.25

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	230	ARG	NE-CZ-NH1	13.27	126.94	120.30
1	C	140	ASP	CB-CG-OD2	-10.82	108.56	118.30
1	B	159	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	D	299	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	154	ASP	CB-CG-OD1	9.42	126.77	118.30
1	D	68	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	321	ASP	CB-CG-OD2	-8.94	110.25	118.30
1	C	321	ASP	CB-CG-OD1	8.83	126.25	118.30
1	C	321	ASP	CB-CG-OD2	-8.77	110.40	118.30
1	C	109	ASP	CB-CG-OD1	8.67	126.10	118.30
1	B	154	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	C	97	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	B	299	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	C	221	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	A	177	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	140	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	A	128	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	B	183	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	B	322	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	140	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	299	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	113	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	221	ASP	CB-CG-OD2	-7.62	111.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	61	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	109	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	D	357	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	C	274	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	C	230	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	183	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	206	ASP	CB-CG-OD2	-7.47	111.57	118.30
1	D	68	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	109	ASP	CB-CG-OD1	7.47	125.02	118.30
1	B	10	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	C	117	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	266	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	198	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	357	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	316	ASP	CB-CG-OD2	-7.30	111.72	118.30
1	A	198	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	177	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	C	147	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	A	154	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	183	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	D	275	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	230	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	D	61	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	206	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	D	246	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	147	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	154	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	C	109	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	B	246	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	316	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	97	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	140	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	324	TYR	CB-CG-CD1	-7.01	116.79	121.00
1	C	352	ILE	C-N-CD	-6.97	105.25	120.60
1	C	327	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	C	169	ASP	CB-CG-OD1	6.95	124.56	118.30
1	B	316	ASP	CB-CG-OD1	6.95	124.56	118.30
1	C	231	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	154	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	D	327	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	80	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	D	221	ASP	CB-CG-OD2	-6.90	112.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	182	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	357	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	D	128	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	169	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	128	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	321	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	198	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	169	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	189	ASP	CB-CG-OD1	6.64	124.28	118.30
1	D	39	PRO	C-N-CA	6.63	138.27	121.70
1	C	20	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	159	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	189	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	239	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	128	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	278	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	128	ASP	CB-CG-OD1	6.50	124.14	118.30
1	D	278	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	316	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	B	266	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	221	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	80	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	327	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	C	183	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	357	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	147	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	117	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	147	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	C	230	ARG	CD-NE-CZ	6.37	132.52	123.60
1	D	321	ASP	CB-CG-OD1	6.36	124.02	118.30
1	C	182	ASP	CB-CG-OD1	6.35	124.02	118.30
1	D	230	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	147	ASP	CB-CG-OD1	6.33	123.99	118.30
1	D	113	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	182	ASP	CB-CG-OD1	6.32	123.98	118.30
1	C	128	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	357	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	182	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	D	10	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	206	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	61	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	206	ASP	CB-CG-OD1	6.14	123.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	147	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	D	80	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	206	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	C	154	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	D	140	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	357	ASP	CB-CG-OD1	6.06	123.75	118.30
1	C	221	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	61	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	D	29	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	109	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	198	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	109	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	182	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	9	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	D	61	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	324	TYR	CB-CG-CD2	5.93	124.56	121.00
1	A	327	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	127	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	198	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	165	GLU	CB-CA-C	-5.89	98.62	110.40
1	C	113	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	266	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	274	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	169	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	70	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	D	177	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	321	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	C	270	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	D	128	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	183	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	278	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	D	127	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	D	154	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	182	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	169	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	D	230	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	204	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	80	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	D	327	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	204	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	140	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	316	ASP	CB-CG-OD2	-5.58	113.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	D	140	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	80	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	127	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	239	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	169	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	324	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	C	204	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	198	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	D	183	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	C	250	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	174	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	61	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	221	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	204	ARG	CD-NE-CZ	5.45	131.23	123.60
1	B	183	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	239	ASP	CB-CG-OD1	5.41	123.16	118.30
1	A	278	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	D	179	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	316	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	180	PHE	CB-CG-CD1	5.31	124.52	120.80
1	B	10	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	C	250	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	169	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	278	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	322	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	70	TYR	CB-CG-CD1	5.22	124.14	121.00
1	D	117	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	97	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	321	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	189	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	250	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	179	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	250	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	206	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	117	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	105	MET	CG-SD-CE	5.09	108.34	100.20
1	B	204	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	C	169	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	357	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	266	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	D	316	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2765	0	2805	130	1
1	B	2772	0	2810	85	0
1	C	2765	0	2805	111	0
1	D	2765	0	2805	260	1
2	A	18	0	11	1	0
2	B	36	0	21	1	0
2	C	36	0	21	7	0
2	D	18	0	11	12	0
3	A	261	0	0	10	1
3	B	375	0	0	8	0
3	C	336	0	0	11	0
3	D	190	0	0	7	1
All	All	12337	0	11289	585	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 26.

All (585) 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:D:38:THR:HB	1:D:39:PRO:HD2	1.20	1.17
1:C:10:ARG:HD2	1:C:32:LEU:CD1	1.74	1.14
1:D:141:THR:HG23	1:D:143:PRO:HD2	1.16	1.12
1:A:1:MET:CE	1:A:38:THR:HG21	1.83	1.09
1:A:1:MET:HE3	1:A:38:THR:HG21	1.06	1.03
1:A:1:MET:HE3	1:A:38:THR:CG2	1.88	1.02
1:B:12:GLN:NE2	1:B:28:VAL:HG11	1.74	1.01
1:D:139:MET:HB2	1:D:168:TRP:CZ2	1.99	0.98
1:D:206:ASP:HB2	1:D:207:PRO:HD3	1.46	0.98
1:D:221:ASP:OD2	1:D:224:GLY:HA3	1.64	0.96
1:D:206:ASP:N	1:D:207:PRO:HD2	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:HB	1:A:39:PRO:HD2	1.51	0.93
1:D:328:ILE:O	1:D:351:PRO:HA	1.70	0.92
1:D:236:ILE:N	1:D:236:ILE:HD13	1.84	0.91
1:C:141:THR:HG22	1:C:144:GLN:H	1.35	0.91
1:D:205:LEU:C	1:D:207:PRO:HD2	1.91	0.91
1:C:10:ARG:HD2	1:C:32:LEU:HD12	1.53	0.90
1:D:141:THR:CG2	1:D:143:PRO:HD2	1.99	0.90
1:A:29:ARG:HD2	1:A:31:LEU:HD23	1.53	0.90
1:D:213:ILE:HG22	1:D:234:THR:HG22	1.56	0.88
1:D:182:ASP:O	3:D:1681:HOH:O	1.91	0.88
1:A:206:ASP:N	1:A:207:PRO:HD2	1.86	0.88
1:D:293:ILE:HD12	2:D:1500:NPG:HE2	1.55	0.88
1:D:206:ASP:N	1:D:207:PRO:CD	2.37	0.87
1:D:18:PRO:HA	1:D:26:GLN:O	1.74	0.87
1:D:109:ASP:O	1:D:113:ARG:HG3	1.74	0.87
1:D:201:GLN:O	1:D:204:ARG:HB2	1.76	0.86
1:A:144:GLN:O	1:A:148:VAL:HG23	1.74	0.85
1:D:213:ILE:HG22	1:D:234:THR:CG2	2.07	0.85
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.58	0.85
1:D:217:LEU:HD21	1:D:228:LEU:HD23	1.59	0.84
1:B:139:MET:HB3	1:B:144:GLN:HG2	1.59	0.84
1:A:8:LEU:HD12	1:A:366:ILE:HD13	1.59	0.83
1:D:139:MET:HB2	1:D:168:TRP:CH2	2.12	0.83
1:C:141:THR:HG23	1:C:143:PRO:HD2	1.60	0.83
1:D:171:GLU:OE1	1:D:174:ARG:NH1	2.11	0.83
1:C:220:GLU:HG2	3:C:1656:HOH:O	1.79	0.82
1:C:204:ARG:HH11	1:C:204:ARG:HG2	1.43	0.82
1:D:227:GLU:O	1:D:230:ARG:HB2	1.80	0.82
1:D:162:LEU:CD1	1:D:186:LEU:HD11	2.11	0.81
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.61	0.81
1:D:32:LEU:HD23	1:D:33:LEU:N	1.96	0.80
1:D:293:ILE:HG13	2:D:1500:NPG:HD2	1.63	0.80
1:D:228:LEU:HD12	1:D:228:LEU:O	1.81	0.80
1:C:109:ASP:O	1:C:113:ARG:HG3	1.80	0.80
1:D:363:LYS:HG2	1:D:364:VAL:N	1.97	0.80
1:A:201:GLN:O	1:A:204:ARG:HB2	1.82	0.79
1:B:199:ALA:HB3	1:B:200:PRO:HD3	1.63	0.79
1:C:8:LEU:CD2	1:C:64:GLU:HG3	2.11	0.79
1:B:78:ALA:HB3	1:B:81:ILE:HD11	1.64	0.79
1:D:162:LEU:HD11	1:D:186:LEU:HD11	1.65	0.79
1:C:12:GLN:HG2	1:C:30:GLU:HG2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:HG22	1:A:84:ALA:H	1.48	0.78
1:D:139:MET:CG	1:D:145:LEU:HB2	2.13	0.78
1:A:12:GLN:HG2	1:A:30:GLU:HG3	1.66	0.78
1:D:353:PRO:O	1:D:357:ASP:N	2.12	0.77
1:D:78:ALA:HB3	1:D:81:ILE:CD1	2.14	0.77
1:D:38:THR:HB	1:D:39:PRO:CD	2.10	0.77
1:D:216:PRO:C	1:D:217:LEU:HD23	2.03	0.77
1:C:220:GLU:OE2	3:C:1656:HOH:O	2.00	0.77
1:A:82:THR:HG22	1:A:84:ALA:N	1.98	0.77
1:C:10:ARG:HD2	1:C:32:LEU:HD11	1.66	0.77
1:D:148:VAL:HG12	1:D:152:TYR:CE1	2.21	0.76
1:D:21:THR:HG22	1:D:22:SER:N	2.01	0.76
1:D:293:ILE:HD12	2:D:1500:NPG:CE2	2.15	0.76
1:D:21:THR:HG22	1:D:23:PHE:H	1.50	0.76
1:D:32:LEU:HD23	1:D:32:LEU:C	2.07	0.75
1:A:113:ARG:HA	1:A:345:PRO:HB2	1.68	0.75
1:D:21:THR:HG21	1:D:23:PHE:CE1	2.21	0.75
1:C:87:THR:HB	1:C:88:PRO:HD3	1.69	0.74
1:D:226:ALA:O	3:D:1660:HOH:O	2.03	0.74
1:D:334:LEU:HD12	1:D:339:LEU:CD1	2.16	0.74
1:D:38:THR:CB	1:D:39:PRO:HD2	1.99	0.74
1:D:169:ASP:HB2	1:D:170:VAL:HG23	1.70	0.74
1:D:141:THR:HG22	1:D:144:GLN:HB2	1.70	0.74
1:D:55:TYR:OH	1:D:266:ARG:HD3	1.87	0.73
1:D:194:TYR:N	1:D:194:TYR:CD1	2.56	0.73
1:A:21:THR:HG22	1:A:163:LYS:HE2	1.71	0.72
1:B:142:ILE:N	1:B:143:PRO:CD	2.53	0.72
1:C:50:MET:HE2	3:C:1475:HOH:O	1.90	0.72
1:B:206:ASP:HB2	1:B:207:PRO:HD3	1.72	0.72
1:A:203:ALA:HB3	3:A:1414:HOH:O	1.89	0.72
1:D:146:LEU:HD22	1:D:179:ARG:HG2	1.72	0.71
1:A:206:ASP:N	1:A:207:PRO:CD	2.53	0.71
1:C:10:ARG:CD	1:C:32:LEU:CD1	2.61	0.71
1:A:8:LEU:HD12	1:A:366:ILE:CD1	2.19	0.71
1:C:68:ARG:HD3	3:C:1709:HOH:O	1.91	0.71
1:B:10:ARG:NH2	1:B:61:ASP:OD1	2.21	0.71
1:D:363:LYS:NZ	1:D:363:LYS:CB	2.53	0.71
1:C:39:PRO:HG2	3:C:1623:HOH:O	1.89	0.71
1:D:194:TYR:CE2	1:D:202:LEU:HD21	2.26	0.71
1:C:38:THR:HB	1:C:39:PRO:HD2	1.72	0.71
1:A:64:GLU:OE2	3:A:1429:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:LEU:C	1:D:228:LEU:HD12	2.11	0.70
1:D:334:LEU:HD12	1:D:339:LEU:HD13	1.71	0.70
1:A:33:LEU:HD13	1:A:297:LEU:HD12	1.73	0.70
1:B:1:MET:HB2	3:B:1339:HOH:O	1.92	0.70
1:D:171:GLU:HA	1:D:171:GLU:OE1	1.89	0.70
1:B:141:THR:CB	1:B:143:PRO:HD2	2.21	0.70
1:C:141:THR:HG23	1:C:143:PRO:CD	2.21	0.70
1:D:213:ILE:CG1	1:D:216:PRO:HG3	2.23	0.69
1:D:21:THR:CG2	1:D:22:SER:N	2.55	0.69
1:D:2:LYS:HD2	1:D:3:LEU:N	2.07	0.69
1:D:236:ILE:N	1:D:236:ILE:CD1	2.54	0.69
1:A:8:LEU:HD23	1:A:32:LEU:CD2	2.22	0.68
1:D:291:GLY:O	2:D:1500:NPG:N1	2.27	0.68
1:B:12:GLN:NE2	1:B:28:VAL:CG1	2.52	0.68
1:B:141:THR:OG1	1:B:143:PRO:HD2	1.94	0.67
1:A:1:MET:CE	1:A:38:THR:CG2	2.59	0.67
1:D:363:LYS:HZ3	1:D:363:LYS:HB3	1.60	0.67
1:C:206:ASP:N	1:C:207:PRO:CD	2.57	0.67
1:C:8:LEU:CD2	1:C:64:GLU:CG	2.73	0.66
1:D:352:ILE:O	1:D:355:LEU:HB2	1.95	0.65
1:D:21:THR:CG2	1:D:22:SER:H	2.10	0.65
1:A:329:THR:HG21	1:A:349:VAL:CG1	2.27	0.65
1:D:353:PRO:HA	1:D:356:LEU:HB3	1.76	0.65
1:B:185:LEU:N	1:B:185:LEU:CD1	2.59	0.65
1:A:163:LYS:HE3	1:A:191:ASN:OD1	1.97	0.65
1:C:8:LEU:HD23	1:C:64:GLU:HG3	1.79	0.65
1:A:65:HIS:HD2	1:B:59:TYR:OH	1.79	0.65
1:D:141:THR:HG22	1:D:144:GLN:H	1.62	0.64
1:C:64:GLU:O	1:C:68:ARG:HG3	1.97	0.64
1:D:33:LEU:O	1:D:34:LEU:HD23	1.97	0.64
1:D:8:LEU:HD13	1:D:366:ILE:CD1	2.27	0.64
1:D:352:ILE:HB	1:D:355:LEU:HD22	1.79	0.64
1:D:12:GLN:O	1:D:14:PRO:HD3	1.97	0.64
1:C:252:ILE:HA	3:C:1573:HOH:O	1.96	0.64
1:A:78:ALA:HB3	1:A:81:ILE:HD11	1.79	0.64
1:A:206:ASP:HB2	1:A:207:PRO:HD3	1.79	0.64
1:B:159:ARG:HG2	1:B:160:ILE:N	2.12	0.64
1:A:35:ARG:HG3	1:A:44:TRP:CE2	2.33	0.64
1:A:10:ARG:NH2	1:A:61:ASP:OD1	2.24	0.64
1:D:32:LEU:CD2	1:D:32:LEU:C	2.66	0.63
1:D:15:LEU:HD23	1:D:324:TYR:HE2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ALA:O	1:D:42:GLU:HB3	1.98	0.63
1:D:217:LEU:HD21	1:D:228:LEU:CD2	2.28	0.63
1:C:48:VAL:HB	1:C:292:MET:HG3	1.81	0.63
1:D:171:GLU:HB2	3:D:1513:HOH:O	1.98	0.63
1:D:338:HIS:O	1:D:339:LEU:HD12	1.99	0.63
1:C:201:GLN:O	1:C:204:ARG:HB2	1.99	0.63
1:D:217:LEU:N	1:D:217:LEU:HD23	2.14	0.62
1:A:8:LEU:CD2	1:A:32:LEU:HD21	2.29	0.62
1:A:8:LEU:HD23	1:A:32:LEU:HD21	1.81	0.62
1:C:366:ILE:HD12	1:C:366:ILE:N	2.14	0.62
1:B:227:GLU:OE1	1:B:230:ARG:NH1	2.32	0.62
1:D:213:ILE:HG12	1:D:216:PRO:HG3	1.82	0.62
1:A:329:THR:HB	1:A:349:VAL:HG13	1.81	0.62
1:D:206:ASP:HB2	1:D:207:PRO:CD	2.28	0.61
1:B:42:GLU:OE1	3:B:1666:HOH:O	2.16	0.61
1:B:283:HIS:CE1	1:C:253:LYS:HE2	2.35	0.61
1:A:274:ARG:NH1	1:A:278:ASP:OD2	2.33	0.61
1:D:8:LEU:HD13	1:D:366:ILE:HD11	1.82	0.61
1:C:205:LEU:C	1:C:207:PRO:HD2	2.21	0.61
1:D:139:MET:HG2	1:D:145:LEU:HB2	1.81	0.61
1:B:171:GLU:CD	1:B:174:ARG:HH21	2.02	0.61
1:A:29:ARG:CD	1:A:31:LEU:HD23	2.30	0.61
1:A:35:ARG:HG3	1:A:44:TRP:CZ2	2.36	0.61
1:D:68:ARG:HH11	1:D:68:ARG:CG	2.14	0.60
1:A:205:LEU:C	1:A:207:PRO:HD2	2.20	0.60
1:A:171:GLU:N	1:A:172:PRO:HD2	2.15	0.60
1:C:7:GLU:CD	1:C:35:ARG:HH12	2.04	0.60
1:A:65:HIS:HE1	3:B:1659:HOH:O	1.85	0.60
1:B:163:LYS:HE2	1:B:191:ASN:OD1	2.02	0.60
1:D:139:MET:HB2	1:D:168:TRP:HZ2	1.62	0.60
1:C:2:LYS:O	1:C:39:PRO:HD3	2.01	0.60
1:B:227:GLU:HA	1:B:230:ARG:NH1	2.17	0.60
1:A:38:THR:HB	1:A:39:PRO:CD	2.29	0.59
1:C:206:ASP:N	1:C:207:PRO:HD2	2.17	0.59
1:D:199:ALA:HB3	1:D:200:PRO:CD	2.29	0.59
1:C:142:ILE:N	1:C:143:PRO:HD2	2.18	0.59
1:D:194:TYR:CG	1:D:202:LEU:HD11	2.37	0.59
1:C:8:LEU:HD22	1:C:64:GLU:HG2	1.84	0.59
1:D:8:LEU:HD11	1:D:366:ILE:HD12	1.85	0.59
1:D:9:ARG:HG3	1:D:9:ARG:HH11	1.66	0.59
1:D:352:ILE:HB	1:D:355:LEU:CD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ARG:HA	1:D:208:PHE:CE2	2.38	0.59
1:A:32:LEU:O	1:A:33:LEU:HD23	2.03	0.59
3:A:1360:HOH:O	1:B:65:HIS:HE1	1.84	0.59
1:A:22:SER:HA	1:A:165:GLU:OE2	2.02	0.59
1:D:8:LEU:CD1	1:D:366:ILE:HD12	2.33	0.59
1:B:364:VAL:CG2	3:B:1615:HOH:O	2.50	0.59
1:C:87:THR:N	1:C:88:PRO:HD2	2.18	0.58
1:D:355:LEU:O	1:D:359:VAL:HG22	2.02	0.58
1:A:165:GLU:OE2	3:A:1352:HOH:O	2.17	0.58
1:A:169:ASP:O	1:A:172:PRO:HD2	2.02	0.58
1:C:87:THR:HB	1:C:88:PRO:CD	2.32	0.58
1:D:293:ILE:HG22	1:D:293:ILE:O	2.03	0.58
1:D:190:ALA:HB1	1:D:193:ALA:HB3	1.86	0.58
1:D:2:LYS:C	1:D:2:LYS:HD2	2.24	0.58
1:A:16:VAL:HB	1:A:323:PHE:O	2.04	0.58
1:D:7:GLU:HB2	1:D:365:TRP:HE3	1.68	0.58
1:D:160:ILE:O	1:D:186:LEU:HA	2.03	0.58
1:B:148:VAL:HA	3:B:1634:HOH:O	2.04	0.58
1:D:264:PRO:HG2	1:D:270:TYR:CE2	2.39	0.58
1:A:338:HIS:O	1:A:339:LEU:HD12	2.04	0.57
1:D:166:PRO:HD3	1:D:194:TYR:CZ	2.38	0.57
1:C:141:THR:CG2	1:C:144:GLN:H	2.13	0.57
1:B:140:ASP:HB2	1:B:144:GLN:OE1	2.04	0.57
1:C:8:LEU:HD22	1:C:64:GLU:CG	2.33	0.57
1:B:142:ILE:N	1:B:143:PRO:HD2	2.19	0.57
1:B:227:GLU:HA	1:B:230:ARG:HH11	1.70	0.57
1:C:217:LEU:HB2	1:C:225:HIS:CE1	2.39	0.57
1:C:220:GLU:CG	3:C:1656:HOH:O	2.43	0.57
1:C:171:GLU:N	1:C:172:PRO:HD2	2.20	0.57
1:B:171:GLU:HB2	1:B:172:PRO:HD3	1.87	0.57
1:D:363:LYS:NZ	1:D:363:LYS:HB3	2.19	0.57
1:A:12:GLN:NE2	1:A:28:VAL:HG11	2.20	0.56
1:D:8:LEU:CD1	1:D:366:ILE:CD1	2.83	0.56
1:C:9:ARG:NH2	1:C:360:THR:OG1	2.38	0.56
1:D:141:THR:HG22	1:D:144:GLN:CB	2.35	0.56
1:D:141:THR:CG2	1:D:144:GLN:HB2	2.34	0.56
1:B:141:THR:HB	1:B:143:PRO:HD2	1.85	0.56
1:D:249:ALA:O	1:D:253:LYS:HG3	2.05	0.56
1:D:7:GLU:CD	1:D:9:ARG:HH12	2.09	0.56
1:D:21:THR:HG21	1:D:23:PHE:CD1	2.39	0.56
2:C:1164:NPG:O62	3:C:1728:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:N	1:D:185:LEU:CD1	2.68	0.56
1:D:363:LYS:HZ3	1:D:363:LYS:CB	2.18	0.56
1:D:7:GLU:OE1	1:D:9:ARG:NH1	2.38	0.56
1:D:354:GLU:HG3	1:D:355:LEU:N	2.20	0.56
1:B:141:THR:OG1	1:B:144:GLN:HB3	2.05	0.56
1:B:199:ALA:HB3	1:B:200:PRO:CD	2.34	0.56
1:D:196:LEU:O	1:D:199:ALA:HB2	2.06	0.56
1:D:143:PRO:O	1:D:144:GLN:C	2.44	0.55
1:C:75:LEU:HD11	1:C:103:LEU:HD13	1.87	0.55
1:C:308:LEU:HB3	1:C:309:PRO:HD2	1.89	0.55
1:A:139:MET:HG3	1:A:145:LEU:HA	1.87	0.55
1:D:142:ILE:HB	1:D:143:PRO:HD3	1.87	0.55
1:D:171:GLU:HB2	1:D:172:PRO:HD3	1.89	0.55
1:D:194:TYR:N	1:D:194:TYR:HD1	2.05	0.55
1:B:321:ASP:HA	1:B:324:TYR:O	2.07	0.55
1:D:32:LEU:C	1:D:33:LEU:HD23	2.27	0.55
1:D:139:MET:HG3	1:D:145:LEU:CA	2.37	0.54
1:A:87:THR:HB	1:A:88:PRO:HD3	1.89	0.54
1:B:185:LEU:HD12	1:B:185:LEU:N	2.22	0.54
1:D:68:ARG:HH11	1:D:68:ARG:HG3	1.70	0.54
1:D:171:GLU:CB	1:D:172:PRO:CD	2.85	0.54
1:C:141:THR:CG2	1:C:143:PRO:CD	2.84	0.54
1:A:356:LEU:HD22	1:A:360:THR:OG1	2.08	0.54
1:B:163:LYS:HE3	1:B:189:ASP:OD2	2.08	0.54
1:C:96:HIS:O	1:C:100:LYS:HG3	2.07	0.54
1:C:249:ALA:O	1:C:253:LYS:HG3	2.07	0.54
1:C:190:ALA:HB3	1:C:216:PRO:HA	1.90	0.54
1:D:199:ALA:CB	1:D:200:PRO:HD3	2.36	0.54
1:C:112:LEU:HB3	1:C:117:ARG:O	2.08	0.54
1:A:331:PRO:HD3	3:A:1261:HOH:O	2.08	0.53
1:A:12:GLN:HE21	1:A:28:VAL:HG11	1.73	0.53
1:B:12:GLN:HE21	1:B:28:VAL:CG1	2.21	0.53
1:D:239:ASP:OD2	1:D:263:LYS:HE3	2.09	0.53
1:C:38:THR:CB	1:C:39:PRO:HD2	2.38	0.53
1:D:25:THR:HG22	1:D:26:GLN:N	2.24	0.53
1:C:293:ILE:HG13	2:C:1400:NPG:HD2	1.90	0.53
1:D:141:THR:HB	1:D:144:GLN:OE1	2.09	0.53
1:B:283:HIS:ND1	1:C:253:LYS:HE2	2.24	0.53
1:D:37:VAL:HG21	1:D:365:TRP:CH2	2.44	0.53
1:C:30:GLU:HB3	3:C:1704:HOH:O	2.08	0.53
1:A:169:ASP:O	1:A:173:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ILE:HB	1:D:168:TRP:O	2.08	0.52
1:A:33:LEU:CD2	1:A:46:GLU:HG3	2.39	0.52
1:C:204:ARG:NH1	1:C:204:ARG:HG2	2.16	0.52
1:D:333:VAL:HG12	1:D:334:LEU:O	2.08	0.52
1:D:205:LEU:C	1:D:207:PRO:CD	2.71	0.52
1:D:7:GLU:CD	1:D:9:ARG:NH1	2.63	0.52
1:C:75:LEU:CD1	1:C:103:LEU:HD13	2.39	0.52
1:B:109:ASP:O	1:B:113:ARG:HG3	2.09	0.52
1:D:214:GLU:C	1:D:216:PRO:HD3	2.30	0.52
1:D:293:ILE:CD1	2:D:1500:NPG:HE2	2.35	0.52
1:D:293:ILE:CD1	2:D:1500:NPG:CE2	2.87	0.52
1:C:9:ARG:NH2	1:C:356:LEU:HD13	2.24	0.52
2:A:1200:NPG:O12	2:A:1200:NPG:HD1	2.08	0.52
1:A:30:GLU:HG2	3:A:1300:HOH:O	2.10	0.52
1:A:349:VAL:CG1	1:A:350:ALA:N	2.72	0.52
1:A:334:LEU:HD12	1:A:339:LEU:CD1	2.40	0.52
1:D:334:LEU:CD1	1:D:339:LEU:HD13	2.40	0.52
1:A:159:ARG:C	1:A:159:ARG:HD2	2.30	0.52
1:A:206:ASP:OD1	3:A:1444:HOH:O	2.19	0.52
1:D:352:ILE:HD12	1:D:355:LEU:HD23	1.91	0.52
1:D:148:VAL:CG1	1:D:152:TYR:CE1	2.92	0.52
1:B:174:ARG:O	1:B:178:GLU:HB2	2.11	0.51
1:C:192:THR:HB	1:C:218:GLU:HA	1.92	0.51
1:D:127:ARG:NH2	1:D:308:LEU:O	2.44	0.51
1:D:195:THR:O	1:D:198:ASP:HB2	2.10	0.51
1:D:164:ILE:HG12	1:D:188:VAL:HB	1.92	0.51
1:A:8:LEU:HD23	1:A:32:LEU:HD22	1.92	0.51
1:D:216:PRO:HB2	1:D:217:LEU:HD23	1.91	0.51
1:A:192:THR:HB	1:A:218:GLU:HA	1.93	0.51
1:D:139:MET:HG3	1:D:145:LEU:N	2.25	0.51
1:D:171:GLU:CB	1:D:172:PRO:HD3	2.41	0.51
1:A:206:ASP:CB	1:A:207:PRO:HD3	2.41	0.51
1:A:85:LYS:C	1:A:88:PRO:HD2	2.31	0.51
1:C:65:HIS:HD2	2:C:1164:NPG:C2	2.23	0.51
1:C:59:TYR:OH	1:D:65:HIS:HD2	1.93	0.51
1:A:29:ARG:HD2	1:A:31:LEU:CD2	2.35	0.51
1:B:39:PRO:HG2	3:B:1409:HOH:O	2.11	0.51
1:A:169:ASP:C	1:A:172:PRO:HD2	2.32	0.50
1:D:135:SER:OG	1:D:161:LYS:HE2	2.12	0.50
1:A:199:ALA:N	1:A:200:PRO:CD	2.75	0.50
1:A:329:THR:HG21	1:A:349:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:O	1:A:293:ILE:HG22	2.12	0.50
1:D:328:ILE:O	1:D:351:PRO:CA	2.52	0.50
1:D:37:VAL:HB	1:D:365:TRP:HH2	1.75	0.50
1:D:185:LEU:N	1:D:185:LEU:HD13	2.25	0.50
1:D:142:ILE:HG22	1:D:146:LEU:HD12	1.94	0.50
1:D:293:ILE:CG1	2:D:1500:NPG:HD2	2.39	0.50
1:A:142:ILE:N	1:A:143:PRO:HD2	2.27	0.50
1:C:10:ARG:CD	1:C:32:LEU:HD11	2.36	0.50
1:B:199:ALA:N	1:B:200:PRO:HD2	2.26	0.50
1:D:195:THR:O	1:D:198:ASP:N	2.38	0.50
1:C:50:MET:CE	3:C:1475:HOH:O	2.56	0.50
1:D:363:LYS:NZ	1:D:363:LYS:HB2	2.26	0.49
1:C:87:THR:CB	1:C:88:PRO:CD	2.90	0.49
1:D:213:ILE:HG13	1:D:216:PRO:HG3	1.94	0.49
1:D:199:ALA:CB	1:D:200:PRO:CD	2.89	0.49
1:D:193:ALA:HB3	1:D:194:TYR:CE1	2.48	0.49
1:A:171:GLU:N	1:A:172:PRO:CD	2.75	0.49
1:A:9:ARG:CG	1:A:360:THR:HG23	2.42	0.49
1:D:308:LEU:CB	1:D:309:PRO:HD2	2.41	0.49
1:D:235:PRO:HB3	1:D:258:GLN:NE2	2.28	0.49
1:D:9:ARG:CG	1:D:9:ARG:HH11	2.26	0.49
1:A:161:LYS:HE3	1:A:189:ASP:HB2	1.93	0.49
1:A:11:VAL:HB	1:A:31:LEU:HD12	1.94	0.49
1:D:227:GLU:HA	1:D:230:ARG:NH1	2.27	0.49
1:B:137:GLY:HA2	1:B:163:LYS:HB2	1.93	0.49
1:A:352:ILE:O	1:A:355:LEU:N	2.45	0.49
1:D:263:LYS:NZ	2:D:1500:NPG:O11	2.44	0.49
1:A:139:MET:HG3	1:A:145:LEU:CA	2.43	0.49
1:B:146:LEU:O	1:B:180:PHE:HZ	1.96	0.49
1:D:141:THR:O	1:D:168:TRP:HH2	1.95	0.49
1:A:169:ASP:O	1:A:172:PRO:HG2	2.12	0.49
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.95	0.49
1:A:65:HIS:CE1	1:A:69:HIS:CD2	3.01	0.48
1:A:218:GLU:OE2	1:B:246:ARG:NE	2.46	0.48
1:D:277:HIS:CD2	1:D:310:ASN:HB3	2.48	0.48
1:B:5:GLY:HA3	1:B:365:TRP:CZ2	2.48	0.48
1:A:33:LEU:HD21	1:A:46:GLU:HG3	1.96	0.48
1:A:28:VAL:HG12	1:A:29:ARG:N	2.28	0.48
2:B:1163:NPG:H41	3:B:1403:HOH:O	2.14	0.48
1:B:261:ASN:C	1:B:261:ASN:OD1	2.51	0.48
1:D:293:ILE:HG13	2:D:1500:NPG:CD2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LEU:HG	1:D:337:GLY:HA2	1.95	0.48
1:D:19:PHE:HA	3:D:1603:HOH:O	2.13	0.48
1:D:288:TRP:HB3	1:D:313:LEU:HB2	1.95	0.48
1:D:10:ARG:NH2	1:D:61:ASP:OD1	2.43	0.48
1:B:204:ARG:O	1:B:207:PRO:HD2	2.14	0.48
1:C:141:THR:CG2	1:C:143:PRO:HD2	2.39	0.48
1:D:194:TYR:CB	1:D:202:LEU:HD11	2.43	0.48
1:D:194:TYR:CD2	1:D:202:LEU:HD21	2.49	0.48
1:D:321:ASP:HA	1:D:324:TYR:O	2.14	0.48
1:A:190:ALA:HB3	1:A:216:PRO:HA	1.95	0.48
1:D:46:GLU:OE2	1:D:294:GLU:HB3	2.14	0.48
1:C:95:GLY:O	1:C:100:LYS:HE3	2.14	0.48
1:D:293:ILE:N	2:D:1500:NPG:O62	2.40	0.47
1:A:141:THR:OG1	1:A:144:GLN:HB2	2.13	0.47
1:D:8:LEU:O	1:D:363:LYS:HA	2.14	0.47
1:D:37:VAL:HG21	1:D:365:TRP:CZ3	2.49	0.47
1:D:228:LEU:CD1	1:D:228:LEU:C	2.81	0.47
1:C:293:ILE:HG13	2:C:1400:NPG:CD2	2.44	0.47
1:D:87:THR:N	1:D:88:PRO:HD2	2.30	0.47
1:B:264:PRO:HG3	1:B:305:LEU:HD22	1.95	0.47
1:D:148:VAL:O	1:D:149:VAL:C	2.52	0.47
1:A:206:ASP:CB	1:A:207:PRO:CD	2.92	0.47
1:A:87:THR:N	1:A:88:PRO:HD2	2.30	0.47
1:A:97:ARG:O	1:A:268:GLY:HA2	2.15	0.47
1:D:190:ALA:O	1:D:193:ALA:HB2	2.14	0.47
1:B:171:GLU:N	1:B:172:PRO:HD2	2.30	0.47
1:D:141:THR:CG2	1:D:144:GLN:H	2.27	0.47
1:B:142:ILE:HB	1:B:143:PRO:HD3	1.97	0.47
1:D:33:LEU:HD13	1:D:297:LEU:HD12	1.96	0.47
1:B:78:ALA:HB3	1:B:81:ILE:CD1	2.41	0.47
1:D:68:ARG:NH1	1:D:68:ARG:CG	2.76	0.47
1:C:35:ARG:HD2	1:C:42:GLU:OE1	2.14	0.47
1:D:87:THR:HB	1:D:88:PRO:HD3	1.97	0.47
1:A:127:ARG:NH2	1:A:308:LEU:O	2.48	0.47
1:C:87:THR:CB	1:C:88:PRO:HD3	2.43	0.47
1:A:142:ILE:O	1:A:143:PRO:C	2.51	0.47
1:D:353:PRO:O	1:D:354:GLU:C	2.51	0.47
1:D:112:LEU:HB3	1:D:117:ARG:O	2.15	0.47
1:C:142:ILE:N	1:C:143:PRO:CD	2.78	0.46
1:D:199:ALA:N	1:D:200:PRO:HD2	2.30	0.46
1:D:171:GLU:HB2	1:D:172:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:CYS:SG	1:B:317:THR:O	2.74	0.46
1:D:235:PRO:C	1:D:236:ILE:HD13	2.35	0.46
1:D:33:LEU:C	1:D:34:LEU:HD23	2.35	0.46
1:C:21:THR:HG22	1:C:163:LYS:HE2	1.96	0.46
1:D:159:ARG:HD2	1:D:159:ARG:C	2.35	0.46
1:D:141:THR:HG23	1:D:142:ILE:N	2.30	0.46
1:D:148:VAL:HG12	1:D:152:TYR:CD1	2.51	0.46
1:D:166:PRO:HD3	1:D:194:TYR:CE1	2.51	0.46
1:B:10:ARG:NH2	1:B:61:ASP:HA	2.30	0.46
1:A:179:ARG:NH2	3:A:1441:HOH:O	2.25	0.46
1:D:363:LYS:HZ2	1:D:363:LYS:HB2	1.80	0.46
1:D:211:LEU:O	1:D:212:LEU:HB3	2.15	0.46
1:D:177:ARG:HD2	1:D:182:ASP:HA	1.98	0.46
1:D:162:LEU:HD12	1:D:186:LEU:HD11	1.96	0.46
1:D:143:PRO:O	1:D:144:GLN:O	2.34	0.46
1:D:325:LYS:HB3	3:D:1601:HOH:O	2.15	0.46
3:A:1456:HOH:O	1:B:220:GLU:HG2	2.14	0.46
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.76	0.46
1:D:350:ALA:HB1	1:D:351:PRO:CD	2.44	0.46
1:A:75:LEU:HD12	1:A:103:LEU:HD21	1.98	0.46
2:D:1500:NPG:O12	2:D:1500:NPG:HD1	2.17	0.45
1:D:87:THR:HB	1:D:88:PRO:CD	2.46	0.45
1:C:141:THR:HG22	1:C:144:GLN:N	2.17	0.45
1:D:37:VAL:CG2	1:D:365:TRP:CH2	2.99	0.45
1:D:18:PRO:CA	1:D:26:GLN:O	2.57	0.45
1:B:237:CYS:HA	1:B:259:ILE:O	2.16	0.45
1:D:216:PRO:HB2	1:D:217:LEU:CD2	2.47	0.45
1:B:192:THR:HB	1:B:218:GLU:HA	1.99	0.45
1:A:174:ARG:HA	1:A:208:PHE:CE2	2.52	0.45
1:A:18:PRO:HA	1:A:26:GLN:O	2.16	0.45
1:A:38:THR:CB	1:A:39:PRO:CD	2.90	0.45
1:D:11:VAL:HG13	1:D:359:VAL:HB	1.99	0.45
1:B:185:LEU:N	1:B:185:LEU:HD13	2.32	0.45
1:C:137:GLY:HA2	1:C:163:LYS:HG2	1.99	0.45
1:C:308:LEU:CB	1:C:309:PRO:CD	2.95	0.45
1:A:150:GLY:O	1:A:153:LEU:HB2	2.17	0.45
1:C:321:ASP:HA	1:C:324:TYR:O	2.16	0.45
1:D:141:THR:CG2	1:D:142:ILE:N	2.79	0.45
1:D:169:ASP:O	1:D:172:PRO:HD2	2.16	0.45
1:D:7:GLU:HG3	1:D:363:LYS:HG3	1.98	0.45
1:D:352:ILE:CB	1:D:355:LEU:HD22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:N	1:A:88:PRO:CD	2.79	0.45
1:B:179:ARG:HG2	1:B:180:PHE:CE1	2.52	0.45
1:A:36:ALA:O	1:A:42:GLU:HA	2.17	0.45
1:C:13:MET:HA	1:C:14:PRO:HD3	1.84	0.45
1:C:328:ILE:O	1:C:351:PRO:HA	2.16	0.45
1:B:12:GLN:HE22	1:B:28:VAL:HG11	1.71	0.45
1:C:159:ARG:C	1:C:159:ARG:HD2	2.37	0.45
1:D:30:GLU:O	1:D:60:ASN:ND2	2.46	0.45
1:D:174:ARG:O	1:D:178:GLU:HB2	2.17	0.45
1:C:141:THR:HG23	1:C:143:PRO:CG	2.47	0.45
1:D:25:THR:CG2	1:D:26:GLN:N	2.80	0.45
1:A:72:ILE:N	1:A:73:PRO:CD	2.79	0.45
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.99	0.45
1:A:125:SER:HG	1:A:307:SER:CB	2.29	0.44
1:B:177:ARG:HD3	1:B:177:ARG:HA	1.79	0.44
1:B:35:ARG:HD2	1:B:42:GLU:OE2	2.17	0.44
1:C:67:LEU:HA	1:C:71:LEU:HB2	1.99	0.44
1:B:29:ARG:HD2	1:B:31:LEU:HD21	1.98	0.44
1:C:87:THR:N	1:C:88:PRO:CD	2.81	0.44
1:A:22:SER:CB	1:A:165:GLU:HG3	2.47	0.44
1:C:141:THR:HG22	1:C:143:PRO:N	2.32	0.44
1:D:21:THR:HG22	1:D:23:PHE:N	2.26	0.44
1:D:190:ALA:O	1:D:193:ALA:CB	2.66	0.44
1:A:329:THR:CG2	1:A:349:VAL:CG1	2.93	0.44
1:D:65:HIS:O	1:D:69:HIS:HD2	2.01	0.44
1:D:139:MET:HG2	1:D:145:LEU:HD12	1.98	0.44
1:D:139:MET:HG3	1:D:145:LEU:HB2	1.99	0.44
1:D:264:PRO:CG	1:D:270:TYR:CE2	2.99	0.44
1:B:179:ARG:HG3	1:B:179:ARG:O	2.09	0.44
1:D:146:LEU:HD22	1:D:179:ARG:CG	2.45	0.44
1:B:139:MET:HG3	1:B:145:LEU:HA	1.99	0.44
1:B:113:ARG:NH2	1:B:349:VAL:O	2.51	0.44
1:A:319:ALA:HB1	1:A:332:PHE:O	2.17	0.44
1:D:209:GLY:HA3	3:D:1612:HOH:O	2.16	0.44
1:D:144:GLN:O	1:D:148:VAL:HG23	2.18	0.44
1:A:50:MET:HE2	3:A:1259:HOH:O	2.17	0.44
1:A:199:ALA:N	1:A:200:PRO:HD2	2.33	0.44
1:D:237:CYS:HA	1:D:259:ILE:O	2.18	0.44
1:C:32:LEU:HA	1:C:32:LEU:HD12	1.84	0.44
1:D:134:VAL:HG11	1:D:152:TYR:HB3	2.00	0.44
1:A:2:LYS:O	1:A:39:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:HB	1:B:365:TRP:HH2	1.83	0.44
1:C:34:LEU:O	1:C:44:TRP:HA	2.18	0.44
1:B:339:LEU:HA	1:B:339:LEU:HD12	1.87	0.44
1:B:364:VAL:HG23	3:B:1615:HOH:O	2.16	0.43
1:D:169:ASP:HB2	1:D:170:VAL:H	1.43	0.43
1:A:72:ILE:N	1:A:73:PRO:HD2	2.33	0.43
1:C:163:LYS:HE3	1:C:191:ASN:OD1	2.18	0.43
1:A:328:ILE:O	1:A:351:PRO:HA	2.18	0.43
1:C:163:LYS:HD2	1:C:163:LYS:HA	1.70	0.43
1:D:361:THR:O	1:D:362:ALA:HB2	2.17	0.43
1:C:365:TRP:C	1:C:365:TRP:CD1	2.92	0.43
1:B:171:GLU:OE2	1:B:174:ARG:NH2	2.51	0.43
1:D:363:LYS:HG2	1:D:364:VAL:H	1.82	0.43
1:D:261:ASN:OD1	1:D:261:ASN:C	2.57	0.43
1:D:185:LEU:HA	1:D:185:LEU:HD12	1.75	0.43
1:B:82:THR:O	1:B:86:VAL:HG23	2.19	0.43
1:D:352:ILE:CD1	1:D:355:LEU:HD23	2.49	0.43
1:C:293:ILE:HG13	2:C:1400:NPG:HE2	2.00	0.43
1:D:142:ILE:N	1:D:143:PRO:HD2	2.34	0.42
1:C:171:GLU:N	1:C:172:PRO:CD	2.80	0.42
1:A:261:ASN:OD1	1:A:261:ASN:C	2.57	0.42
1:B:199:ALA:CB	1:B:200:PRO:CD	2.95	0.42
1:D:356:LEU:O	1:D:359:VAL:HG23	2.19	0.42
1:C:293:ILE:HG13	2:C:1400:NPG:CE2	2.49	0.42
1:D:315:GLY:C	1:D:317:THR:H	2.22	0.42
1:A:301:ALA:HB2	1:A:347:LEU:CD2	2.49	0.42
1:B:20:ARG:HG2	1:B:138:ILE:HB	2.02	0.42
1:A:2:LYS:HG3	1:A:2:LYS:O	2.19	0.42
1:D:139:MET:CG	1:D:145:LEU:CB	2.93	0.42
1:D:9:ARG:NH1	1:D:9:ARG:CG	2.82	0.42
1:A:355:LEU:O	1:A:358:GLU:HB2	2.20	0.42
1:D:258:GLN:O	1:D:286:PRO:HD2	2.20	0.42
1:D:263:LYS:HD3	1:D:292:MET:SD	2.60	0.42
1:A:32:LEU:C	1:A:33:LEU:HD23	2.40	0.42
1:D:194:TYR:HB3	1:D:198:ASP:HB2	2.02	0.42
1:B:206:ASP:N	1:B:207:PRO:CD	2.82	0.42
1:A:356:LEU:CD2	1:A:360:THR:OG1	2.67	0.42
1:D:141:THR:HG22	1:D:144:GLN:N	2.32	0.42
1:D:78:ALA:HB3	1:D:81:ILE:HD11	1.94	0.42
1:C:353:PRO:O	1:C:354:GLU:C	2.58	0.42
1:B:355:LEU:HA	1:B:355:LEU:HD12	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:VAL:O	1:C:90:LEU:HG	2.19	0.42
1:B:199:ALA:N	1:B:200:PRO:CD	2.82	0.42
1:D:21:THR:HG21	1:D:23:PHE:CZ	2.54	0.42
1:B:7:GLU:HB3	1:B:35:ARG:HB3	2.02	0.42
1:B:299:ARG:HD3	1:B:318:SER:O	2.20	0.42
1:C:139:MET:HB2	1:C:168:TRP:CH2	2.54	0.42
1:D:165:GLU:HG2	1:D:166:PRO:N	2.35	0.42
1:C:308:LEU:HB3	1:C:309:PRO:CD	2.50	0.42
1:D:125:SER:HB2	1:D:307:SER:OG	2.20	0.42
1:D:328:ILE:HG13	1:D:329:THR:HG23	2.02	0.42
1:B:65:HIS:O	1:B:69:HIS:HD2	2.03	0.42
1:A:142:ILE:HB	1:A:143:PRO:HD3	2.02	0.42
1:A:355:LEU:O	1:A:359:VAL:HG22	2.20	0.42
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.88	0.42
1:D:354:GLU:HG3	1:D:355:LEU:H	1.85	0.41
1:C:354:GLU:HB3	3:C:1435:HOH:O	2.20	0.41
1:D:139:MET:CB	1:D:145:LEU:HB2	2.50	0.41
1:D:363:LYS:O	1:D:364:VAL:HG22	2.20	0.41
1:D:190:ALA:HB1	1:D:194:TYR:CE1	2.55	0.41
1:D:170:VAL:HA	1:D:205:LEU:CD2	2.50	0.41
1:C:7:GLU:OE1	1:C:35:ARG:NH1	2.54	0.41
1:B:163:LYS:CE	1:B:191:ASN:OD1	2.68	0.41
1:A:308:LEU:CB	1:A:309:PRO:HD2	2.49	0.41
1:B:280:CYS:HB3	1:B:285:ILE:O	2.20	0.41
1:C:185:LEU:HD23	1:C:185:LEU:N	2.35	0.41
1:D:175:ALA:O	1:D:178:GLU:HB3	2.20	0.41
1:A:82:THR:CG2	1:A:84:ALA:H	2.26	0.41
1:A:163:LYS:HD2	1:A:163:LYS:HA	1.83	0.41
1:C:206:ASP:HB2	1:C:207:PRO:HD3	2.02	0.41
1:C:7:GLU:CD	1:C:35:ARG:NH1	2.71	0.41
1:A:142:ILE:N	1:A:143:PRO:CD	2.84	0.41
1:B:87:THR:HB	1:B:88:PRO:HD3	2.01	0.41
1:D:227:GLU:HA	1:D:230:ARG:HH11	1.85	0.41
1:A:113:ARG:HG3	1:A:346:GLY:HA3	2.01	0.41
1:D:334:LEU:HD12	1:D:334:LEU:HA	1.78	0.41
1:C:125:SER:HA	1:C:308:LEU:HD12	2.03	0.41
1:A:25:THR:HG22	1:A:26:GLN:N	2.36	0.41
1:B:299:ARG:O	1:B:303:VAL:HG23	2.20	0.41
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.72	0.41
1:D:171:GLU:O	1:D:172:PRO:C	2.58	0.41
1:C:141:THR:HG23	1:C:143:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LEU:CD1	1:D:339:LEU:CD1	2.94	0.41
2:C:1164:NPG:HE2	1:D:62:GLY:HA2	2.02	0.41
1:A:210:LEU:HG	1:A:210:LEU:H	1.67	0.41
1:D:271:LEU:HA	1:D:271:LEU:HD23	1.74	0.41
1:D:2:LYS:O	1:D:39:PRO:HD3	2.20	0.41
1:D:196:LEU:O	1:D:199:ALA:CB	2.68	0.41
1:A:356:LEU:CD2	1:A:356:LEU:C	2.89	0.41
1:A:5:GLY:HA3	1:A:365:TRP:CZ2	2.56	0.41
1:C:10:ARG:HD3	1:C:64:GLU:OE2	2.21	0.41
1:D:81:ILE:HG22	1:D:81:ILE:O	2.21	0.41
1:C:191:ASN:C	1:C:192:THR:HG23	2.41	0.41
1:C:352:ILE:O	1:C:355:LEU:N	2.54	0.41
1:C:139:MET:HB2	1:C:168:TRP:CZ2	2.56	0.41
1:A:277:HIS:CD2	1:A:311:PHE:CE1	3.08	0.41
1:D:220:GLU:HA	3:D:1589:HOH:O	2.20	0.41
1:B:32:LEU:HB3	1:B:47:CYS:HB3	2.03	0.41
1:C:38:THR:O	1:C:39:PRO:C	2.58	0.41
1:B:8:LEU:O	1:B:363:LYS:HA	2.21	0.41
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.61	0.41
1:A:321:ASP:HA	1:A:324:TYR:O	2.21	0.41
1:D:142:ILE:HA	1:D:142:ILE:HD13	1.82	0.40
1:D:15:LEU:HD23	1:D:324:TYR:CE2	2.51	0.40
1:D:264:PRO:HG3	1:D:305:LEU:HD22	2.03	0.40
1:A:189:ASP:HA	1:A:214:GLU:HB3	2.02	0.40
1:B:29:ARG:HD2	1:B:31:LEU:HG	2.03	0.40
1:D:139:MET:CB	1:D:168:TRP:CH2	2.95	0.40
1:A:29:ARG:HH22	1:A:50:MET:HA	1.85	0.40
1:D:293:ILE:CD1	2:D:1500:NPG:CD2	3.00	0.40
1:D:33:LEU:HD23	1:D:33:LEU:N	2.37	0.40
1:B:132:CYS:O	1:B:158:VAL:HG22	2.21	0.40
1:B:277:HIS:CD2	1:B:311:PHE:CE1	3.09	0.40
1:A:177:ARG:HA	1:A:177:ARG:HD3	1.85	0.40
1:C:258:GLN:HB3	1:C:258:GLN:HE21	1.68	0.40
1:C:288:TRP:HB3	1:C:313:LEU:HB2	2.03	0.40
1:C:142:ILE:O	1:C:145:LEU:HB3	2.22	0.40
1:A:87:THR:CB	1:A:88:PRO:HD3	2.51	0.40
1:C:3:LEU:H	1:C:81:ILE:HD13	1.86	0.40
1:D:12:GLN:HG2	1:D:28:VAL:CG1	2.52	0.40
1:C:29:ARG:HG2	1:C:324:TYR:OH	2.22	0.40
1:C:352:ILE:HA	1:C:353:PRO:HD3	1.59	0.40
1:C:165:GLU:O	1:C:166:PRO:C	2.58	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:111:GLU:OE2	1:D:117:ARG:NH2[17_555]	1.85	0.35
3:A:1310:HOH:O	3:D:1604:HOH:O[17_555]	1.97	0.23

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	365/368 (99%)	350 (96%)	15 (4%)	0	100	100
1	B	366/368 (100%)	358 (98%)	8 (2%)	0	100	100
1	C	365/368 (99%)	349 (96%)	15 (4%)	1 (0%)	46	33
1	D	365/368 (99%)	334 (92%)	29 (8%)	2 (0%)	34	20
All	All	1461/1472 (99%)	1391 (95%)	67 (5%)	3 (0%)	52	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	144	GLN
1	C	353	PRO
1	D	39	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	290/291 (100%)	260 (90%)	30 (10%)	9 2
1	B	291/291 (100%)	268 (92%)	23 (8%)	15 5
1	C	290/291 (100%)	269 (93%)	21 (7%)	18 7
1	D	290/291 (100%)	254 (88%)	36 (12%)	6 1
All	All	1161/1164 (100%)	1051 (90%)	110 (10%)	11 3

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	4	SER
1	A	8	LEU
1	A	15	LEU
1	A	27	SER
1	A	29	ARG
1	A	30	GLU
1	A	31	LEU
1	A	32	LEU
1	A	34	LEU
1	A	35	ARG
1	A	79	GLU
1	A	80	ASP
1	A	85	LYS
1	A	116	GLU
1	A	127	ARG
1	A	142	ILE
1	A	155	GLU
1	A	163	LYS
1	A	169	ASP
1	A	177	ARG
1	A	178	GLU
1	A	179	ARG
1	A	227	GLU
1	A	322	ARG
1	A	343	THR
1	A	354	GLU
1	A	356	LEU
1	A	363	LYS
1	B	3	LEU
1	B	12	GLN
1	B	27	SER

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Mol	Chain	Res	Type
1	B	29	ARG
1	B	32	LEU
1	B	79	GLU
1	B	80	ASP
1	B	88	PRO
1	B	92	LYS
1	B	144	GLN
1	B	159	ARG
1	B	163	LYS
1	B	169	ASP
1	B	177	ARG
1	B	178	GLU
1	B	179	ARG
1	B	227	GLU
1	B	274	ARG
1	B	322	ARG
1	B	339	LEU
1	B	355	LEU
1	B	358	GLU
1	B	363	LYS
1	C	1	MET
1	C	2	LYS
1	C	8	LEU
1	C	9	ARG
1	C	103	LEU
1	C	113	ARG
1	C	119	PHE
1	C	126	VAL
1	C	142	ILE
1	C	163	LYS
1	C	174	ARG
1	C	177	ARG
1	C	185	LEU
1	C	204	ARG
1	C	213	ILE
1	C	217	LEU
1	C	233	GLN
1	C	322	ARG
1	C	354	GLU
1	C	356	LEU
1	C	363	LYS
1	D	2	LYS

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Mol	Chain	Res	Type
1	D	7	GLU
1	D	22	SER
1	D	27	SER
1	D	29	ARG
1	D	32	LEU
1	D	42	GLU
1	D	54	LEU
1	D	68	ARG
1	D	79	GLU
1	D	81	ILE
1	D	92	LYS
1	D	116	GLU
1	D	119	PHE
1	D	139	MET
1	D	141	THR
1	D	145	LEU
1	D	155	GLU
1	D	165	GLU
1	D	169	ASP
1	D	171	GLU
1	D	177	ARG
1	D	185	LEU
1	D	194	TYR
1	D	205	LEU
1	D	213	ILE
1	D	217	LEU
1	D	220	GLU
1	D	227	GLU
1	D	228	LEU
1	D	236	ILE
1	D	322	ARG
1	D	325	LYS
1	D	355	LEU
1	D	363	LYS
1	D	364	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	65	HIS
1	A	69	HIS

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Mol	Chain	Res	Type
1	A	258	GLN
1	A	283	HIS
1	B	12	GLN
1	B	65	HIS
1	B	258	GLN
1	C	12	GLN
1	C	69	HIS
1	C	258	GLN
1	D	65	HIS
1	D	69	HIS
1	D	258	GLN

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

6 ligands are modelled in this entry.

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	NPG	A	1200	-	12,18,18	1.42	2 (16%)	15,23,23	1.45	3 (20%)
2	NPG	B	1163	-	12,18,18	1.48	2 (16%)	15,23,23	3.04	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NPG	B	1300	-	12,18,18	1.42	2 (16%)	15,23,23	2.28	3 (20%)
2	NPG	C	1164	-	12,18,18	1.45	2 (16%)	15,23,23	3.16	6 (40%)
2	NPG	C	1400	-	12,18,18	1.39	2 (16%)	15,23,23	0.66	0
2	NPG	D	1500	-	12,18,18	1.33	2 (16%)	15,23,23	1.26	2 (13%)

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	NPG	A	1200	-	-	0/11/17/17	0/1/1/1
2	NPG	B	1163	-	-	0/11/17/17	0/1/1/1
2	NPG	B	1300	-	-	0/11/17/17	0/1/1/1
2	NPG	C	1164	-	-	0/11/17/17	0/1/1/1
2	NPG	C	1400	-	-	0/11/17/17	0/1/1/1
2	NPG	D	1500	-	-	0/11/17/17	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1163	NPG	CG-C1	-3.74	1.47	1.52
2	C	1164	NPG	CG-C1	-3.58	1.47	1.52
2	A	1200	NPG	CG-C1	-2.97	1.48	1.52
2	B	1300	NPG	CG-C1	-2.82	1.48	1.52
2	C	1400	NPG	CG-C1	-2.69	1.48	1.52
2	D	1500	NPG	CG-C1	-2.68	1.48	1.52
2	B	1163	NPG	C3-N1	2.20	1.38	1.34
2	C	1164	NPG	C3-N1	2.61	1.39	1.34
2	B	1300	NPG	C3-N1	2.74	1.39	1.34
2	D	1500	NPG	C3-N1	3.03	1.40	1.34
2	C	1400	NPG	C3-N1	3.30	1.40	1.34
2	A	1200	NPG	C3-N1	3.36	1.40	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1300	NPG	C4-C3-N1	-5.89	106.24	115.83
2	B	1300	NPG	C4-C5-C6	-4.37	104.74	112.75
2	B	1163	NPG	CD1-CG-C1	-4.28	113.49	120.77
2	B	1163	NPG	C5-C4-C3	-4.01	103.18	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1163	NPG	CG-C1-N1	-3.15	105.30	111.18
2	D	1500	NPG	C4-C5-C6	-2.92	107.40	112.75
2	B	1163	NPG	C4-C5-C6	-2.60	107.99	112.75
2	C	1164	NPG	CD1-CG-C1	-2.53	116.46	120.77
2	A	1200	NPG	C4-C5-C6	-2.45	108.25	112.75
2	C	1164	NPG	C4-C3-N1	-2.33	112.04	115.83
2	A	1200	NPG	C5-C4-C3	-2.30	107.36	113.01
2	C	1164	NPG	CG-C1-N1	-2.18	107.12	111.18
2	D	1500	NPG	C4-C3-N1	2.03	119.14	115.83
2	C	1164	NPG	CD2-CG-CD1	2.17	121.07	118.31
2	B	1163	NPG	CD2-CG-C1	2.28	124.65	120.77
2	B	1163	NPG	CD2-CG-CD1	2.45	121.44	118.31
2	C	1164	NPG	O31-C3-C4	2.53	126.34	121.98
2	A	1200	NPG	C4-C3-N1	3.01	120.74	115.83
2	B	1300	NPG	O31-C3-C4	3.42	127.89	121.98
2	B	1163	NPG	C2-C1-CG	8.29	125.00	112.97
2	C	1164	NPG	C2-C1-CG	10.59	128.34	112.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1200	NPG	1	0
2	B	1163	NPG	1	0
2	C	1164	NPG	3	0
2	C	1400	NPG	4	0
2	D	1500	NPG	12	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	367/368 (99%)	-0.40	1 (0%)	94	94	17, 37, 69, 96	0
1	B	368/368 (100%)	-0.47	2 (0%)	91	92	17, 27, 55, 91	0
1	C	367/368 (99%)	-0.50	3 (0%)	87	88	19, 30, 61, 97	0
1	D	367/368 (99%)	0.06	24 (6%)	22	24	15, 46, 89, 100	0
All	All	1469/1472 (99%)	-0.33	30 (2%)	68	70	15, 33, 78, 100	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	LEU	6.2
1	D	184	VAL	5.9
1	D	208	PHE	4.2
1	D	168	TRP	4.2
1	D	149	VAL	4.2
1	D	175	ALA	4.0
1	D	367	GLY	3.9
1	D	205	LEU	3.9
1	D	138	ILE	3.9
1	D	180	PHE	3.8
1	D	186	LEU	3.5
1	D	179	ARG	3.3
1	D	142	ILE	3.0
1	D	193	ALA	3.0
1	D	177	ARG	3.0
1	D	173	VAL	2.8
1	C	146	LEU	2.7
1	B	1	MET	2.6
1	D	232	ILE	2.5
1	D	176	VAL	2.4
1	D	19	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	178	GLU	2.3
1	A	15	LEU	2.2
1	C	142	ILE	2.2
1	D	153	LEU	2.2
1	C	149	VAL	2.2
1	D	148	VAL	2.1
1	D	139	MET	2.1
1	B	142	ILE	2.1
1	D	22	SER	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	NPG	B	1163	18/18	0.90	0.12	8.78	24,54,100,100	0
2	NPG	D	1500	18/18	0.82	0.25	3.07	50,84,100,100	0
2	NPG	A	1200	18/18	0.94	0.12	1.65	30,53,98,100	0
2	NPG	B	1300	18/18	0.94	0.11	1.56	29,44,65,67	0
2	NPG	C	1164	18/18	0.87	0.14	1.52	29,79,100,100	0
2	NPG	C	1400	18/18	0.97	0.07	-0.10	23,33,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.