Full wwPDB X-ray Structure Validation Report (i)

Dec 21, 2016 – 11:08 AM EST

PDB ID	:	1UP4
Title	:	Structure of the 6-phospho-beta glucosidase from Thermotoga maritima at 2.85 Angstrom resolution in the monoclinic form
Authors	:	Varrot, A.; Yip, V.; Withers, S.G.; Davies, G.J.
Deposited on	:	2003-09-26
Resolution	:	2.85 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:

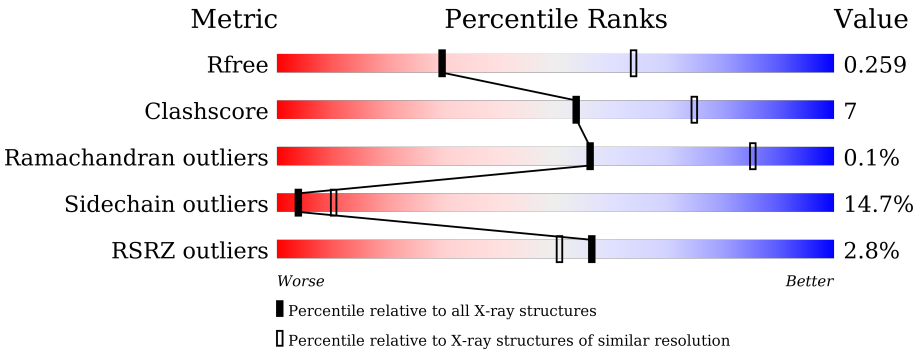
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	415	4% 69% 25% 5%
1	B	415	% 72% 22%
1	C	415	3% 72% 23%
1	D	415	3% 70% 22%
1	E	415	4% 73% 20% 5%
1	F	415	2% 71% 23%

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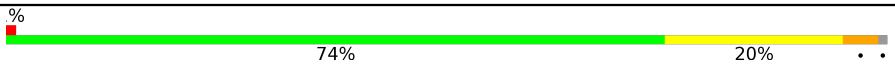
Mol	Chain	Length	Quality of chain
1	G	415	
1	H	415	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 26328 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 6-PHOSPHO-BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	Se	88	0	0
			3326	2143	554	620	2	7			
1	B	403	Total	C	N	O	S	Se	67	1	0
			3274	2112	544	609	2	7			
1	C	408	Total	C	N	O	S	Se	86	0	0
			3309	2133	551	616	2	7			
1	D	400	Total	C	N	O	S	Se	90	0	0
			3251	2099	539	604	2	7			
1	E	396	Total	C	N	O	S	Se	147	0	0
			3210	2073	533	595	2	7			
1	F	399	Total	C	N	O	S	Se	88	0	0
			3242	2092	538	603	2	7			
1	G	409	Total	C	N	O	S	Se	55	16	0
			3317	2137	552	619	2	7			
1	H	403	Total	C	N	O	S	Se	115	30	0
			3274	2111	542	612	2	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	16	Total	O	0	0
			16	16		
2	C	17	Total	O	0	0
			17	17		
2	D	14	Total	O	0	0
			14	14		
2	E	13	Total	O	0	0
			13	13		
2	F	13	Total	O	0	0
			13	13		

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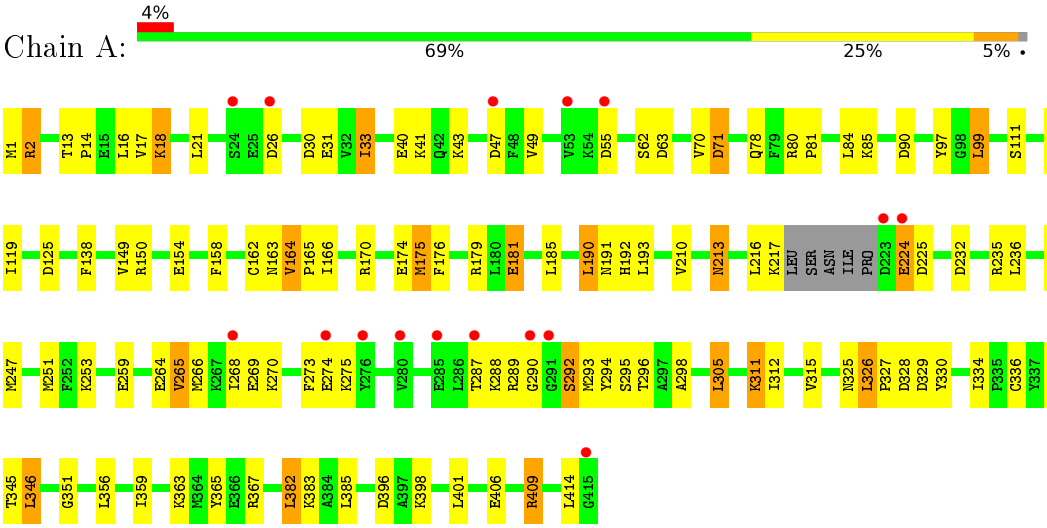
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	14	Total O 14 14	0	0
2	H	18	Total O 18 18	0	0

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.

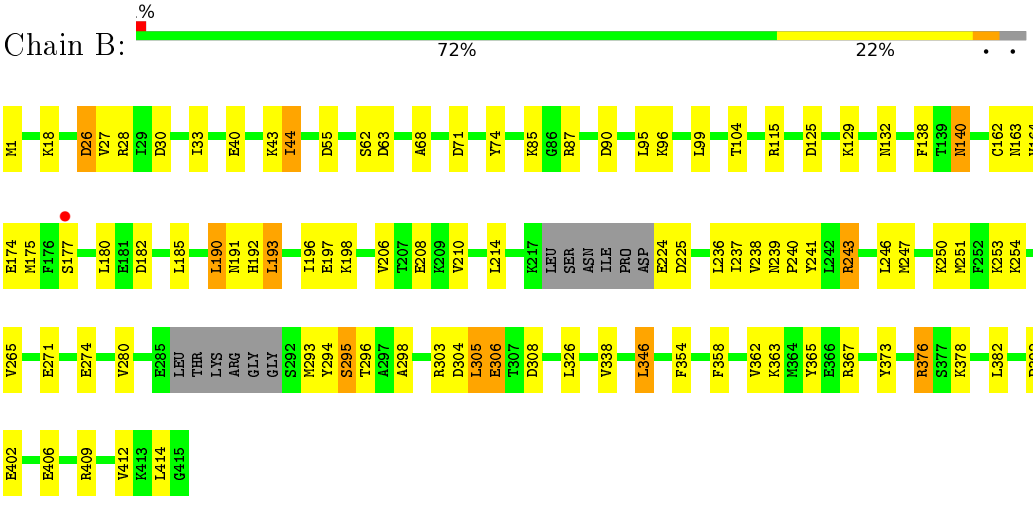
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain A:



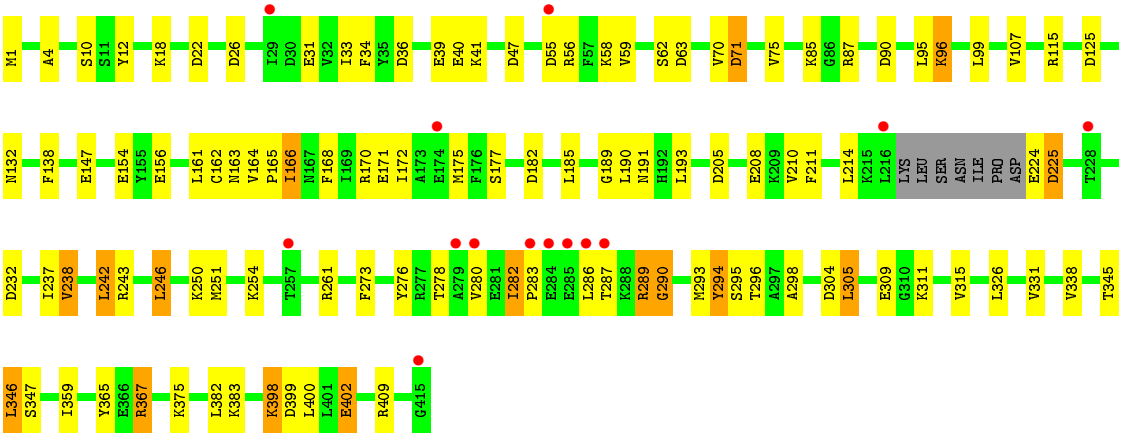
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain B:

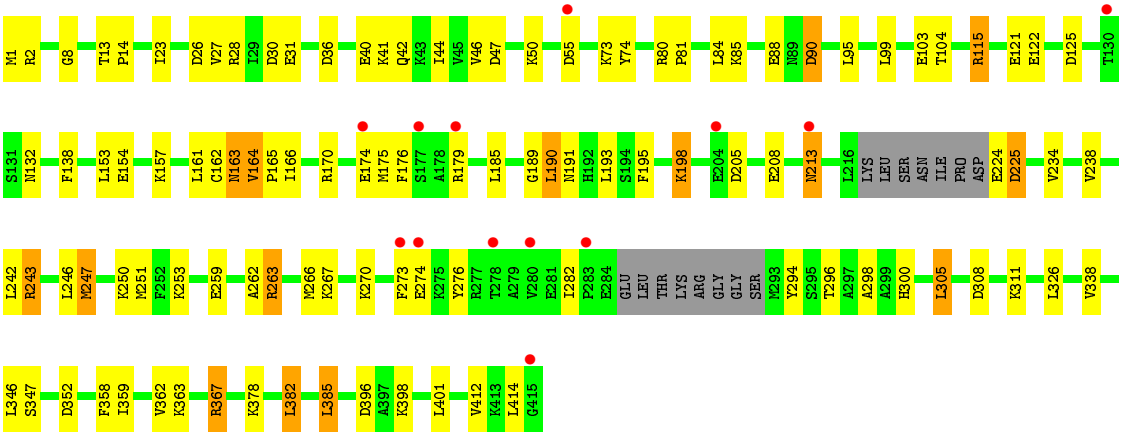


- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

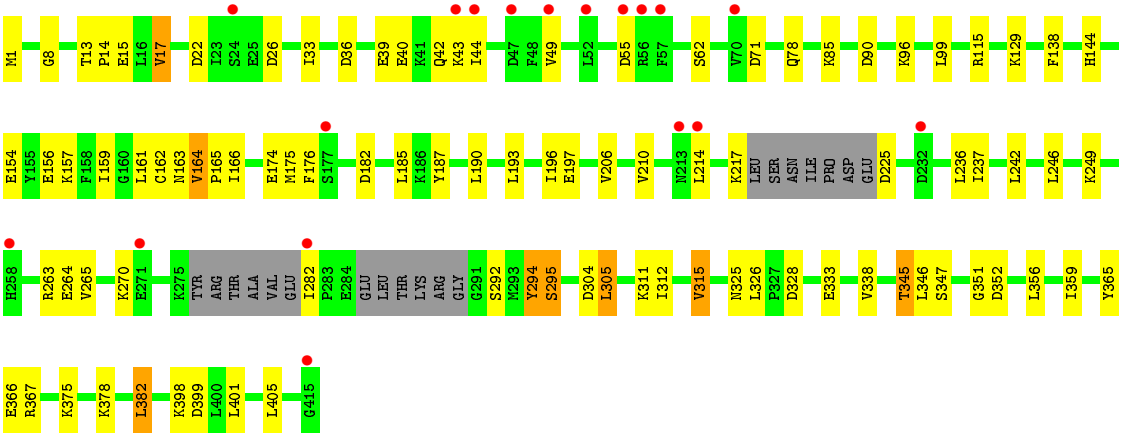
Chain C:



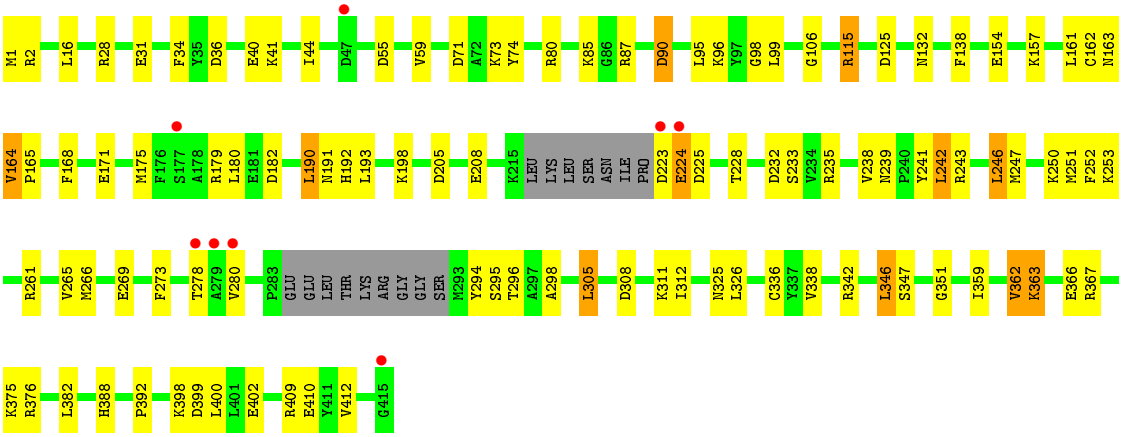
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

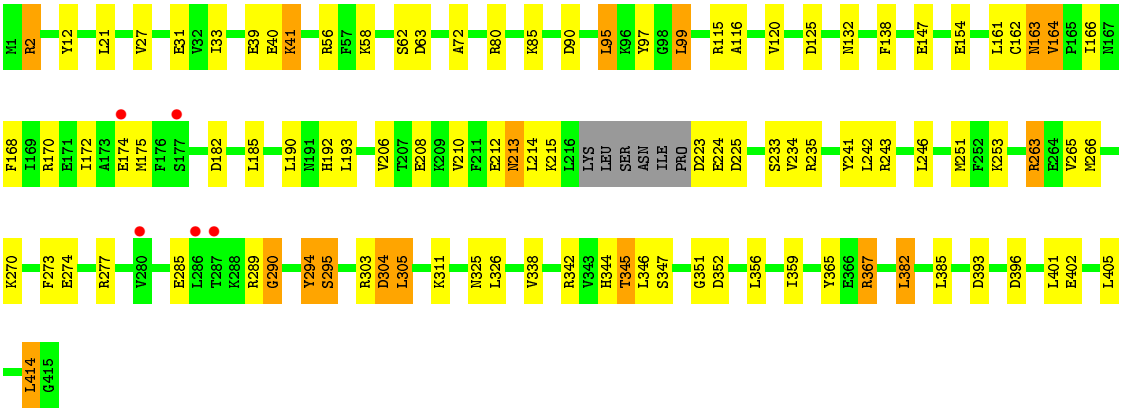


• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE



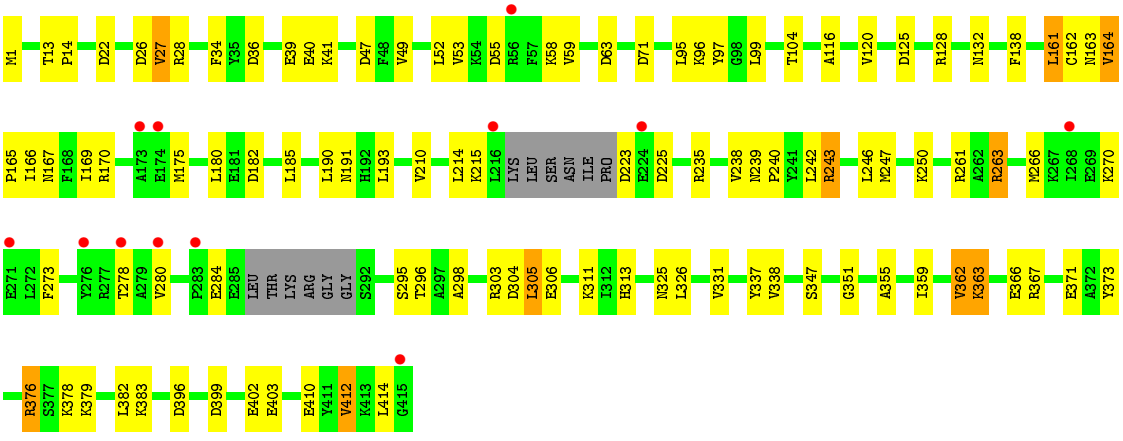
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain G:



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.05Å 188.31Å 125.63Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85 39.63 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.85) 97.8 (39.63-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.235 0.234 , 0.259	Depositor DCC
R_{free} test set	5150 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 29.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	26328	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.63	0/3385	0.83	9/4550 (0.2%)
1	B	0.67	0/3337	0.83	8/4487 (0.2%)
1	C	0.58	0/3368	0.80	13/4528 (0.3%)
1	D	0.58	0/3310	0.83	12/4452 (0.3%)
1	E	0.54	0/3266	0.78	8/4387 (0.2%)
1	F	0.61	0/3301	0.82	9/4440 (0.2%)
1	G	0.66	0/3376	0.85	8/4539 (0.2%)
1	H	0.60	0/3332	0.82	11/4480 (0.2%)
All	All	0.61	0/26675	0.82	78/35863 (0.2%)

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	63	ASP	CB-CG-OD2	8.05	125.55	118.30
1	H	125	ASP	CB-CG-OD2	7.50	125.05	118.30
1	E	182	ASP	CB-CG-OD2	6.74	124.36	118.30
1	C	232	ASP	CB-CG-OD2	6.55	124.20	118.30
1	H	399	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	63	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	396	ASP	CB-CG-OD2	6.44	124.10	118.30
1	F	90	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	71	ASP	CB-CG-OD2	6.35	124.01	118.30
1	H	396	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	125	ASP	CB-CG-OD2	6.27	123.94	118.30
1	F	125	ASP	CB-CG-OD2	6.25	123.93	118.30
1	C	63	ASP	CB-CG-OD2	6.18	123.87	118.30
1	F	36	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	182	ASP	CB-CG-OD2	6.14	123.83	118.30
1	E	304	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	55	ASP	CB-CG-OD2	6.06	123.76	118.30
1	G	225	ASP	CB-CG-OD2	6.04	123.73	118.30
1	C	304	ASP	CB-CG-OD2	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	328	ASP	CB-CG-OD2	5.92	123.63	118.30
1	H	22	ASP	CB-CG-OD2	5.84	123.56	118.30
1	C	225	ASP	CB-CG-OD2	5.84	123.55	118.30
1	F	182	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	90	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	396	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	232	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	182	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	399	ASP	CB-CG-OD2	5.71	123.44	118.30
1	H	182	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	125	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	352	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	30	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	308	ASP	CB-CG-OD2	5.67	123.41	118.30
1	G	393	ASP	CB-CG-OD2	5.64	123.37	118.30
1	C	47	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	352	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	36	ASP	CB-CG-OD2	5.50	123.25	118.30
1	G	125	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	22	ASP	CB-CG-OD2	5.48	123.24	118.30
1	D	36	ASP	CB-CG-OD2	5.47	123.22	118.30
1	H	36	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	63	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	328	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	47	ASP	CB-CG-OD2	5.42	123.17	118.30
1	C	22	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	115	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	H	71	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	125	ASP	CB-CG-OD2	5.39	123.15	118.30
1	F	308	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	26	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	71	ASP	CB-CG-OD2	5.37	123.13	118.30
1	G	352	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	367	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	H	223[H]	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	71	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	26	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	329	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	308	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	205	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	30	ASP	CB-CG-OD2	5.26	123.04	118.30
1	H	47	ASP	CB-CG-OD2	5.26	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	393	ASP	CB-CG-OD2	5.25	123.03	118.30
1	G	396	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	30	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	71	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	232	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	55	ASP	CB-CG-OD2	5.20	122.98	118.30
1	F	205	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	223	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	36	ASP	CB-CG-OD2	5.15	122.93	118.30
1	G	304	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	47	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	399	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	115	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	H	263	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	225	ASP	CB-CG-OD2	5.08	122.87	118.30
1	G	63	ASP	CB-CG-OD2	5.04	122.84	118.30
1	G	182	ASP	CB-CG-OD2	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	3326	0	3359	58	0
1	B	3274	0	3302	39	0
1	C	3309	0	3342	40	0
1	D	3251	0	3280	46	0
1	E	3210	0	3245	34	0
1	F	3242	0	3267	42	0
1	G	3317	0	3299	50	0
1	H	3274	0	3208	36	0
2	A	20	0	0	0	0
2	B	16	0	0	0	0
2	C	17	0	0	0	0
2	D	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	13	0	0	0	0
2	F	13	0	0	1	0
2	G	14	0	0	0	0
2	H	18	0	0	0	0
All	All	26328	0	26302	331	0

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 7.

All (331) 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:G:289:ARG:HG3	1:G:290:GLY:H	1.25	1.01
1:F:224:GLU:HG3	1:F:251:MSE:HE1	1.40	1.01
1:G:263:ARG:HH11	1:G:263:ARG:HG3	1.34	0.92
1:A:224:GLU:HG2	1:A:251:MSE:HE1	1.61	0.82
1:F:224:GLU:CG	1:F:251:MSE:HE1	2.11	0.80
1:G:263:ARG:HG3	1:G:263:ARG:NH1	1.92	0.80
1:B:138:PHE:HZ	1:B:298:ALA:HB2	1.47	0.80
1:C:398:LYS:O	1:C:402:GLU:HG2	1.83	0.79
1:G:263:ARG:CG	1:G:263:ARG:HH11	1.95	0.78
1:A:181:GLU:OE1	1:A:311:LYS:HE2	1.85	0.76
1:H:305:LEU:HD13	1:H:338:VAL:HG13	1.67	0.76
1:B:138:PHE:CZ	1:B:298:ALA:HB2	2.22	0.75
1:E:13:THR:O	1:E:17:VAL:HG23	1.85	0.75
1:A:409:ARG:HH11	1:A:409:ARG:HG3	1.51	0.74
1:D:138:PHE:HZ	1:D:298:ALA:HB2	1.53	0.73
1:E:8:GLY:HA3	1:E:42:GLN:HE21	1.53	0.73
1:D:243:ARG:HG2	1:D:247:MSE:HE2	1.68	0.72
1:H:162:CYS:HB2	1:H:191:ASN:HD21	1.54	0.71
1:D:162:CYS:HB2	1:D:191:ASN:HD21	1.56	0.69
1:A:2:ARG:HB2	1:A:31:GLU:HG2	1.75	0.68
1:G:224:GLU:HG3	1:G:251:MSE:HE1	1.75	0.68
1:G:289:ARG:HG3	1:G:290:GLY:N	2.06	0.67
1:A:383:LYS:HE2	1:B:354:PHE:HB2	1.77	0.66
1:C:107:VAL:HG11	1:C:400:LEU:HD21	1.77	0.66
1:G:382:LEU:HD13	1:G:401:LEU:HD22	1.76	0.66
1:A:162:CYS:HB2	1:A:191:ASN:HD21	1.60	0.66
1:G:41:LYS:HD3	1:G:273:PHE:CZ	2.31	0.65
1:F:305:LEU:HD13	1:F:338:VAL:HG13	1.78	0.65
1:D:84:LEU:HB2	1:D:266:MSE:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:PHE:CZ	1:D:298:ALA:HB2	2.31	0.64
1:C:164:VAL:HG22	1:C:165:PRO:HD3	1.78	0.64
1:B:162:CYS:SG	1:B:164:VAL:HG13	2.38	0.64
1:C:242:LEU:HD23	1:C:246:LEU:HD22	1.80	0.63
1:H:325:ASN:HD22	1:H:351:GLY:N	1.97	0.63
1:D:84:LEU:CB	1:D:266:MSE:HE3	2.28	0.63
1:D:382:LEU:HD13	1:D:401:LEU:HD22	1.80	0.63
1:G:90:ASP:OD1	1:G:115:ARG:NH2	2.32	0.63
1:E:312:ILE:HD11	1:H:337:TYR:CZ	2.33	0.62
1:G:382:LEU:HD13	1:G:401:LEU:CD2	2.29	0.62
1:A:409:ARG:HH11	1:A:409:ARG:CG	2.12	0.62
1:D:224:GLU:HG2	1:D:251:MSE:HE1	1.80	0.61
1:B:90:ASP:OD1	1:B:115:ARG:NH2	2.34	0.61
1:C:175:MSE:HE1	1:C:210:VAL:HA	1.82	0.61
1:G:305:LEU:HD13	1:G:338:VAL:CG1	2.30	0.61
1:D:162:CYS:SG	1:D:164:VAL:HG13	2.41	0.61
1:A:18:LYS:HA	1:A:21:LEU:HD12	1.82	0.61
1:A:406:GLU:O	1:A:409:ARG:HG2	2.01	0.61
1:G:90:ASP:CG	1:G:115:ARG:HH22	2.05	0.61
1:A:33:ILE:HD11	1:A:62:SER:HB2	1.81	0.60
1:F:224:GLU:HG3	1:F:251:MSE:CE	2.24	0.60
1:D:190:LEU:HD23	1:D:362:VAL:HG22	1.83	0.60
1:C:289:ARG:HG3	1:C:290:GLY:H	1.66	0.60
1:C:162:CYS:HB2	1:C:191:ASN:HD21	1.67	0.60
1:D:259:GLU:OE1	1:E:249:LYS:NZ	2.35	0.59
1:H:325:ASN:HD22	1:H:351:GLY:H	1.50	0.59
1:H:97:TYR:OH	1:H:403:GLU:OE1	2.21	0.59
1:B:190:LEU:CD2	1:B:362:VAL:HG22	2.33	0.59
1:B:247:MSE:HE2	1:B:251:MSE:HE3	1.84	0.58
1:A:162:CYS:HB2	1:A:191:ASN:ND2	2.18	0.58
1:C:238:VAL:HG22	1:C:242:LEU:HD13	1.85	0.58
1:D:162:CYS:HB2	1:D:191:ASN:ND2	2.16	0.58
1:D:81:PRO:O	1:D:115:ARG:HD2	2.03	0.58
1:H:190:LEU:HD13	1:H:359:ILE:HG23	1.86	0.57
1:E:13:THR:N	1:E:14:PRO:HD2	2.20	0.57
1:H:190:LEU:HD23	1:H:362:VAL:HG22	1.86	0.57
1:E:90:ASP:OD1	1:E:115:ARG:NH2	2.38	0.57
1:G:234:VAL:HA	1:H:383:LYS:HD2	1.87	0.57
1:H:190:LEU:CD2	1:H:362:VAL:HG22	2.35	0.57
1:A:325:ASN:ND2	1:A:351:GLY:O	2.38	0.56
1:G:190:LEU:HD13	1:G:359:ILE:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ILE:HD13	1:C:170:ARG:HH22	1.69	0.56
1:E:8:GLY:HA3	1:E:42:GLN:NE2	2.18	0.56
1:H:162:CYS:CB	1:H:191:ASN:HD21	2.18	0.56
1:A:179:ARG:NH1	1:A:181:GLU:OE2	2.39	0.56
1:G:168:PHE:CZ	1:G:172:ILE:HD11	2.40	0.56
1:D:213:ASN:N	1:D:213:ASN:HD22	2.04	0.56
1:B:33:ILE:HD11	1:B:62:SER:HB2	1.88	0.55
1:E:175:MSE:HE1	1:E:210:VAL:HA	1.88	0.55
1:F:162:CYS:HB2	1:F:191:ASN:HD21	1.70	0.55
1:G:21:LEU:HD22	1:G:56:ARG:CZ	2.37	0.55
1:G:138:PHE:CE1	1:G:294:TYR:HD2	2.25	0.55
1:G:325:ASN:HB3	1:G:356:LEU:HD21	1.88	0.55
1:A:305:LEU:HD13	1:A:338:VAL:HG13	1.89	0.55
1:D:358:PHE:O	1:D:362:VAL:HG13	2.07	0.55
1:G:138:PHE:CZ	1:G:161:LEU:HD23	2.41	0.55
1:H:164:VAL:HG13	1:H:165:PRO:HD3	1.88	0.55
1:B:190:LEU:HD23	1:B:362:VAL:HG22	1.89	0.55
1:G:175:MSE:HE1	1:G:210:VAL:HA	1.88	0.55
1:H:305:LEU:HD13	1:H:338:VAL:CG1	2.36	0.55
1:F:347:SER:OG	1:G:345:THR:HB	2.07	0.55
1:C:138:PHE:CZ	1:C:298:ALA:HB2	2.42	0.55
1:C:166:ILE:CD1	1:C:170:ARG:HH22	2.21	0.54
1:C:12:TYR:HB3	1:C:294:TYR:CE1	2.41	0.54
1:D:8:GLY:HA3	1:D:42:GLN:OE1	2.08	0.54
1:H:162:CYS:HB2	1:H:191:ASN:ND2	2.21	0.54
1:E:305:LEU:HD13	1:E:338:VAL:HG13	1.89	0.54
1:E:294:TYR:CD1	1:E:295:SER:N	2.76	0.54
1:F:138:PHE:CZ	1:F:298:ALA:HB2	2.43	0.54
1:A:78:GLN:O	1:A:78:GLN:HG2	2.09	0.53
1:F:269:GLU:O	1:F:273:PHE:HD1	1.91	0.53
1:H:175:MSE:HE1	1:H:210:VAL:HA	1.90	0.53
1:H:304:ASP:OD2	1:H:313:HIS:NE2	2.30	0.53
1:E:197:GLU:HG3	1:E:236:LEU:CD2	2.38	0.53
1:D:190:LEU:CD2	1:D:362:VAL:HG22	2.38	0.53
1:D:175:MSE:HE3	1:D:213:ASN:OD1	2.07	0.53
1:E:325:ASN:ND2	1:E:351:GLY:O	2.42	0.53
1:G:224:GLU:HG2	1:G:243:ARG:HH11	1.72	0.53
1:C:87:ARG:HH21	1:C:261:ARG:HG2	1.74	0.52
1:F:87:ARG:NH1	1:F:265:VAL:HG21	2.24	0.52
1:B:305:LEU:HD13	1:B:338:VAL:HG13	1.90	0.52
1:E:78:GLN:CG	1:E:78:GLN:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:LEU:HA	1:F:295:SER:HB2	1.91	0.52
1:A:138:PHE:CZ	1:A:298:ALA:HB2	2.45	0.52
1:E:325:ASN:HB3	1:E:356:LEU:HD21	1.92	0.52
1:F:242:LEU:HD12	1:F:246:LEU:HD22	1.92	0.52
1:B:162:CYS:SG	1:B:191:ASN:ND2	2.83	0.52
1:F:90:ASP:OD1	1:F:115:ARG:NH2	2.43	0.52
1:C:398:LYS:O	1:C:402:GLU:CG	2.56	0.52
1:H:355:ALA:O	1:H:359:ILE:HG13	2.10	0.52
1:A:382:LEU:HD13	1:A:401:LEU:CD2	2.39	0.51
1:B:104:THR:HG22	1:B:140[A]:ASN:OD1	2.10	0.51
1:G:224:GLU:HG2	1:G:243:ARG:NH1	2.24	0.51
1:C:162:CYS:HB2	1:C:191:ASN:ND2	2.24	0.51
1:D:305:LEU:HD13	1:D:338:VAL:HG13	1.92	0.51
1:G:303:ARG:NH1	1:G:304:ASP:OD1	2.41	0.51
1:B:224:GLU:OE1	1:B:254:LYS:HD2	2.11	0.51
1:C:90:ASP:OD2	1:C:115:ARG:NH2	2.43	0.51
1:C:162:CYS:CB	1:C:191:ASN:HD21	2.22	0.51
1:C:33:ILE:HD11	1:C:62:SER:HB2	1.92	0.51
1:F:34:PHE:HE2	1:F:59:VAL:HG13	1.75	0.51
1:A:90:ASP:CG	1:A:115:ARG:HH22	2.14	0.51
1:F:224:GLU:O	1:F:243:ARG:HD2	2.11	0.51
1:A:346:LEU:HD12	1:D:346:LEU:HD12	1.90	0.51
1:F:190:LEU:HD23	1:F:362:VAL:HG22	1.92	0.51
1:G:162:CYS:SG	1:G:163:ASN:N	2.83	0.51
1:B:392:PRO:HG3	1:B:400:LEU:HD23	1.92	0.51
1:C:138:PHE:HZ	1:C:298:ALA:HB2	1.76	0.51
1:D:46:VAL:O	1:D:50:LYS:HG3	2.11	0.51
1:C:170:ARG:NH2	1:C:293:MSE:SE	2.94	0.51
1:F:247:MSE:HE2	1:F:251:MSE:HE3	1.93	0.50
1:B:358:PHE:O	1:B:362:VAL:HG13	2.11	0.50
1:A:175:MSE:HE2	1:A:176:PHE:CE2	2.46	0.50
1:A:97:TYR:HB2	1:A:99:LEU:HD22	1.93	0.50
1:D:296:THR:HG23	1:D:300:HIS:CE1	2.47	0.50
1:G:175:MSE:HE3	1:G:213:ASN:OD1	2.12	0.50
1:A:13:THR:HB	1:A:14:PRO:HD3	1.94	0.50
1:B:295:SER:OG	1:B:296:THR:N	2.43	0.50
1:B:346:LEU:HD12	1:C:346:LEU:HD12	1.93	0.50
1:A:224:GLU:O	1:A:243:ARG:HD2	2.12	0.50
1:E:187:TYR:HE1	1:E:333:GLU:HG2	1.76	0.50
1:F:363:LYS:HE3	1:F:366:GLU:OE1	2.12	0.50
1:A:265:VAL:HA	1:A:268:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:LYS:HE2	1:E:405:LEU:HD13	1.94	0.50
1:D:90:ASP:OD1	1:D:115:ARG:NH2	2.41	0.49
1:F:162:CYS:HB2	1:F:191:ASN:ND2	2.26	0.49
1:G:274:GLU:OE2	1:G:277:ARG:NE	2.45	0.49
1:F:73:LYS:HG2	1:F:74:TYR:CE2	2.48	0.49
1:C:189:GLY:HA2	1:C:359:ILE:CD1	2.42	0.49
1:D:162:CYS:CB	1:D:191:ASN:HD21	2.23	0.49
1:G:294:TYR:CD1	1:G:295:SER:N	2.80	0.49
1:F:162:CYS:CB	1:F:191:ASN:HD21	2.26	0.49
1:G:138:PHE:CD1	1:G:294:TYR:HD2	2.30	0.49
1:F:138:PHE:HZ	1:F:298:ALA:HB2	1.77	0.49
1:F:168:PHE:O	1:F:171:GLU:HB2	2.13	0.49
1:H:138:PHE:CZ	1:H:298:ALA:HB2	2.47	0.49
1:E:345:THR:HB	1:H:347:SER:OG	2.13	0.49
1:A:162:CYS:CB	1:A:191:ASN:HD21	2.24	0.49
1:F:90:ASP:CG	1:F:115:ARG:HH22	2.16	0.48
1:B:175:MSE:HE1	1:B:210:VAL:HA	1.95	0.48
1:G:325:ASN:ND2	1:G:351:GLY:O	2.46	0.48
1:A:235:ARG:O	1:A:236:LEU:HD23	2.14	0.48
1:A:17:VAL:HG11	1:A:49:VAL:HG13	1.95	0.48
1:E:305:LEU:HD13	1:E:338:VAL:CG1	2.44	0.48
1:A:346:LEU:CD1	1:D:346:LEU:HD12	2.43	0.48
1:A:81:PRO:HB3	1:A:119:ILE:HD12	1.94	0.48
1:F:87:ARG:HH12	1:F:265:VAL:HG21	1.78	0.48
1:E:90:ASP:CG	1:E:115:ARG:HH22	2.17	0.48
1:C:295:SER:OG	1:C:296:THR:N	2.47	0.47
1:B:197:GLU:HG3	1:B:236:LEU:CD2	2.44	0.47
1:E:206:VAL:O	1:E:210:VAL:HG23	2.14	0.47
1:A:382:LEU:HD13	1:A:401:LEU:HD22	1.97	0.47
1:E:197:GLU:HG3	1:E:236:LEU:HD23	1.96	0.47
1:F:325:ASN:ND2	1:F:351:GLY:O	2.47	0.47
1:D:80:ARG:NH2	2:D:2003:HOH:O	2.48	0.47
1:A:191:ASN:O	1:A:192:HIS:HB2	2.15	0.47
1:A:175:MSE:HE2	1:A:176:PHE:CZ	2.49	0.47
1:A:138:PHE:HZ	1:A:298:ALA:HB2	1.78	0.47
1:F:392:PRO:HG3	1:F:400:LEU:HD23	1.95	0.47
1:G:147:GLU:OE2	1:G:367:ARG:NH1	2.40	0.47
1:A:16:LEU:HD22	1:A:78:GLN:OE1	2.15	0.47
1:B:303:ARG:HD2	1:B:304:ASP:OD1	2.14	0.47
1:B:193:LEU:HD11	1:B:358:PHE:HB3	1.95	0.47
1:B:162:CYS:HB2	1:B:191:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLY:HA2	1:C:359:ILE:HD11	1.97	0.47
1:F:239:ASN:O	1:F:242:LEU:HB2	2.15	0.47
1:A:90:ASP:OD1	1:A:115:ARG:NH2	2.48	0.46
1:H:239:ASN:OD1	1:H:240:PRO:HD2	2.15	0.46
1:D:14:PRO:HG2	1:D:276:TYR:CZ	2.50	0.46
1:D:73:LYS:HD3	1:D:74:TYR:CE2	2.50	0.46
1:E:33:ILE:HD11	1:E:62:SER:HB2	1.97	0.46
1:F:190:LEU:CD2	1:F:362:VAL:HG22	2.46	0.46
1:H:161:LEU:HA	1:H:161:LEU:HD12	1.57	0.46
1:B:306:GLU:HA	1:B:306:GLU:OE1	2.16	0.46
1:E:17:VAL:HG11	1:E:49:VAL:HG13	1.98	0.46
1:G:233:SER:HB3	1:H:379:LYS:O	2.15	0.46
1:A:326:LEU:HD11	1:A:356:LEU:HG	1.98	0.46
1:B:33:ILE:HD13	1:B:68:ALA:HA	1.96	0.46
1:F:80:ARG:HD3	2:F:2002:HOH:O	2.15	0.46
1:C:41:LYS:HD3	1:C:273:PHE:CZ	2.50	0.46
1:E:196:ILE:HB	1:E:237:ILE:HB	1.96	0.46
1:G:342:ARG:HD2	1:G:344:HIS:NE2	2.31	0.46
1:H:13:THR:HB	1:H:14:PRO:HD3	1.98	0.46
1:A:190:LEU:HD11	1:A:363:LYS:HE2	1.98	0.46
1:G:206:VAL:O	1:G:210:VAL:HG23	2.16	0.46
1:A:149:VAL:HG11	1:A:158:PHE:CD2	2.51	0.45
1:A:175:MSE:HE3	1:A:213:ASN:ND2	2.31	0.45
1:A:409:ARG:CG	1:A:409:ARG:NH1	2.74	0.45
1:C:96:LYS:HE2	1:C:96:LYS:HB3	1.66	0.45
1:B:87:ARG:NH1	1:B:265:VAL:HG21	2.31	0.45
1:H:49:VAL:O	1:H:53:VAL:HG23	2.17	0.45
1:D:247:MSE:HE3	1:D:251:MSE:HE3	1.98	0.45
1:E:138:PHE:CD1	1:E:294:TYR:HD2	2.35	0.45
1:H:412:VAL:HG23	1:H:414:LEU:HD13	1.99	0.45
1:B:125:ASP:OD2	1:B:129:LYS:NZ	2.49	0.45
1:G:168:PHE:CE2	1:G:172:ILE:HD11	2.52	0.45
1:A:269:GLU:O	1:A:273:PHE:HD2	1.98	0.45
1:E:382:LEU:HD13	1:E:401:LEU:HD22	1.99	0.45
1:H:163:ASN:O	1:H:167:ASN:ND2	2.50	0.45
1:A:259:GLU:OE2	1:A:264:GLU:HG2	2.16	0.45
1:A:78:GLN:O	1:A:78:GLN:CG	2.65	0.45
1:C:138:PHE:CZ	1:C:161:LEU:HD23	2.52	0.45
1:B:224:GLU:O	1:B:243:ARG:HD2	2.16	0.44
1:C:147:GLU:OE2	1:C:367:ARG:NH1	2.41	0.44
1:F:312:ILE:HD12	1:F:346:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD13	1:A:359:ILE:HG23	1.99	0.44
1:D:195:PHE:N	1:D:195:PHE:CD1	2.85	0.44
1:G:2:ARG:HB2	1:G:31:GLU:HG2	1.99	0.44
1:A:325:ASN:HB3	1:A:356:LEU:HD21	2.00	0.44
1:C:251:MSE:HE2	1:C:251:MSE:HA	1.99	0.44
1:D:121:GLU:HG3	1:D:153:LEU:HD21	1.99	0.44
1:E:175:MSE:HE2	1:E:176:PHE:CE2	2.52	0.44
1:F:190:LEU:HD13	1:F:359:ILE:HG23	1.99	0.44
1:G:12:TYR:HB3	1:G:294:TYR:CE1	2.52	0.44
1:E:17:VAL:HG21	1:E:49:VAL:HG22	1.99	0.44
1:F:164:VAL:N	1:F:165:PRO:CD	2.81	0.44
1:C:383:LYS:HD2	1:D:234:VAL:HA	1.98	0.44
1:D:253:LYS:HG3	1:F:253:LYS:NZ	2.33	0.44
1:E:159:ILE:HG23	1:E:315:VAL:HG13	1.99	0.44
1:E:190:LEU:HD13	1:E:359:ILE:HG23	1.99	0.44
1:A:175:MSE:HE1	1:A:210:VAL:HA	1.99	0.44
1:D:163:ASN:H	1:D:163:ASN:HD22	1.66	0.44
1:H:373:TYR:CZ	1:H:376:ARG:NH2	2.86	0.44
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.33	0.44
1:D:13:THR:HB	1:D:14:PRO:HD3	1.99	0.44
1:D:164:VAL:N	1:D:165:PRO:CD	2.81	0.44
1:G:116:ALA:O	1:G:120:VAL:HG13	2.17	0.44
1:E:164:VAL:HG22	1:E:165:PRO:HD3	1.99	0.43
1:G:405:LEU:HD21	1:G:414:LEU:HD22	2.00	0.43
1:B:90:ASP:CG	1:B:115:ARG:HH22	2.19	0.43
1:B:239:ASN:OD1	1:B:240:PRO:HD2	2.18	0.43
1:B:40:GLU:O	1:B:44:ILE:HD12	2.18	0.43
1:C:211:PHE:CE1	1:C:237:ILE:HG13	2.53	0.43
1:F:192:HIS:HD2	1:F:241:TYR:CE1	2.36	0.43
1:H:243:ARG:HG2	1:H:247:MSE:SE	2.68	0.43
1:C:305:LEU:HD13	1:C:338:VAL:HG13	2.01	0.43
1:E:144:HIS:CD2	1:E:366:GLU:HG2	2.54	0.43
1:B:192:HIS:HD2	1:B:241:TYR:CE1	2.37	0.43
1:D:175:MSE:HE2	1:D:176:PHE:CE2	2.52	0.43
1:F:2:ARG:HG3	1:F:31:GLU:HG3	2.01	0.43
1:D:385:LEU:HD22	1:D:401:LEU:HD13	2.01	0.43
1:F:41:LYS:HG2	1:F:273:PHE:CE2	2.54	0.43
1:H:116:ALA:O	1:H:120:VAL:HG13	2.18	0.43
1:D:103:GLU:HG2	1:D:104:THR:HG23	2.00	0.43
1:F:106:GLY:HA2	1:F:388:HIS:CE1	2.54	0.43
1:A:363:LYS:HA	1:A:363:LYS:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:LYS:NZ	1:D:205:ASP:OD2	2.51	0.43
1:H:34:PHE:HE2	1:H:59:VAL:HG13	1.83	0.43
1:A:84:LEU:HD13	1:A:266:MSE:HG3	2.00	0.43
1:G:33:ILE:HD11	1:G:62:SER:HB2	2.01	0.43
1:B:74:TYR:OH	1:B:306:GLU:OE1	2.30	0.42
1:H:138:PHE:CE1	1:H:161:LEU:HB3	2.54	0.42
1:H:27:VAL:HG21	1:H:306:GLU:CB	2.48	0.42
1:B:90:ASP:CG	1:B:115:ARG:NH2	2.73	0.42
1:C:147:GLU:HA	1:C:331:VAL:HG21	2.00	0.42
1:C:294:TYR:CD1	1:C:295:SER:N	2.86	0.42
1:D:189:GLY:HA2	1:D:359:ILE:HD11	2.00	0.42
1:E:162:CYS:SG	1:E:164:VAL:HG13	2.59	0.42
1:G:2:ARG:HG2	1:G:72:ALA:HA	2.01	0.42
1:H:96:LYS:HE3	1:H:403:GLU:OE2	2.20	0.42
1:C:4:ALA:HB3	1:C:75:VAL:HG22	2.00	0.42
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.85	0.42
1:G:208:GLU:O	1:G:212:GLU:HG2	2.20	0.42
1:A:325:ASN:HD22	1:A:351:GLY:N	2.18	0.42
1:B:373:TYR:CZ	1:B:376:ARG:NH2	2.88	0.42
1:F:346:LEU:CD1	1:G:346:LEU:HD12	2.49	0.42
1:B:190:LEU:HD23	1:B:362:VAL:CG2	2.49	0.42
1:G:95:LEU:HD12	1:G:95:LEU:HA	1.81	0.42
1:G:97:TYR:HB2	1:G:99:LEU:HD22	2.01	0.42
1:A:117:PHE:HB2	1:A:118:PRO:HD3	2.02	0.42
1:C:34:PHE:HE1	1:C:59:VAL:HG13	1.85	0.42
1:D:88:GLU:HG3	1:D:262:ALA:HB3	2.02	0.41
1:H:363:LYS:HE3	1:H:366:GLU:OE1	2.20	0.41
1:B:90:ASP:OD2	1:B:115:ARG:NH2	2.43	0.41
1:A:170:ARG:NH2	1:A:293:MSE:HG3	2.36	0.41
1:G:162:CYS:SG	1:G:164:VAL:HG13	2.60	0.41
1:A:243:ARG:HG2	1:A:247:MSE:SE	2.70	0.41
1:C:276:TYR:OH	1:C:286:LEU:HD22	2.20	0.41
1:D:190:LEU:HD23	1:D:362:VAL:CG2	2.49	0.41
1:E:161:LEU:HA	1:E:161:LEU:HD12	1.79	0.41
1:G:192:HIS:CD2	1:G:241:TYR:CE2	3.08	0.41
1:B:170:ARG:O	1:B:174:GLU:HG2	2.19	0.41
1:B:206:VAL:O	1:B:210:VAL:HG23	2.20	0.41
1:D:2:ARG:NE	1:D:31:GLU:OE2	2.42	0.41
1:C:70:VAL:HG13	1:C:71:ASP:N	2.36	0.41
1:D:162:CYS:SG	1:D:163:ASN:N	2.94	0.41
1:F:312:ILE:HA	1:F:336:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ARG:HH11	1:G:115:ARG:HD2	1.74	0.41
1:B:196:ILE:HB	1:B:237:ILE:HB	2.01	0.41
1:G:161:LEU:HA	1:G:161:LEU:HD12	1.93	0.41
1:H:331:VAL:O	1:H:363:LYS:NZ	2.53	0.41
1:A:164:VAL:N	1:A:165:PRO:CD	2.84	0.41
1:C:282:ILE:HA	1:C:283:PRO:HD3	1.87	0.41
1:A:312:ILE:HA	1:A:336:CYS:O	2.20	0.41
1:F:98:GLY:HA2	1:F:252:PHE:CZ	2.56	0.41
1:H:49:VAL:HA	1:H:52:LEU:HD12	2.02	0.41
1:A:70:VAL:HG13	1:A:71:ASP:N	2.36	0.40
1:D:263:ARG:HH22	1:F:399:ASP:CG	2.24	0.40
1:A:327:PRO:HG2	1:A:330:TYR:CE1	2.55	0.40
1:F:164:VAL:N	1:F:165:PRO:HD2	2.36	0.40
1:C:168:PHE:CZ	1:C:172:ILE:HD11	2.56	0.40
1:G:138:PHE:CZ	1:G:294:TYR:CD2	3.10	0.40

There are no symmetry-related clashes.

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	406/415 (98%)	390 (96%)	14 (3%)	2 (0%)	34 67
1	B	398/415 (96%)	390 (98%)	8 (2%)	0	100 100
1	C	404/415 (97%)	392 (97%)	11 (3%)	1 (0%)	52 82
1	D	394/415 (95%)	386 (98%)	8 (2%)	0	100 100
1	E	388/415 (94%)	380 (98%)	8 (2%)	0	100 100
1	F	393/415 (95%)	386 (98%)	7 (2%)	0	100 100
1	G	405/415 (98%)	392 (97%)	12 (3%)	1 (0%)	52 82
1	H	397/415 (96%)	389 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3185/3320 (96%)	3105 (98%)	76 (2%)	4 (0%)	56 85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	GLY
1	G	290	GLY
1	A	292	SER
1	C	290	GLY

5.3.2 Protein sidechains

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	362/360 (101%)	305 (84%)	57 (16%)	3 8
1	B	357/360 (99%)	304 (85%)	53 (15%)	4 10
1	C	360/360 (100%)	306 (85%)	54 (15%)	3 9
1	D	354/360 (98%)	300 (85%)	54 (15%)	3 9
1	E	350/360 (97%)	303 (87%)	47 (13%)	5 12
1	F	353/360 (98%)	299 (85%)	54 (15%)	3 9
1	G	361/360 (100%)	316 (88%)	45 (12%)	6 15
1	H	357/360 (99%)	302 (85%)	55 (15%)	3 9
All	All	2854/2880 (99%)	2435 (85%)	419 (15%)	4 10

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	ARG
1	A	18	LYS
1	A	26	ASP
1	A	33	ILE
1	A	40	GLU

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Mol	Chain	Res	Type
1	A	41	LYS
1	A	43	LYS
1	A	55	ASP
1	A	80	ARG
1	A	85	LYS
1	A	99	LEU
1	A	111	SER
1	A	154	GLU
1	A	163	ASN
1	A	164	VAL
1	A	166	ILE
1	A	174	GLU
1	A	175	MSE
1	A	181	GLU
1	A	185	LEU
1	A	190	LEU
1	A	193	LEU
1	A	213	ASN
1	A	216	LEU
1	A	217	LYS
1	A	224	GLU
1	A	225	ASP
1	A	242	LEU
1	A	246	LEU
1	A	253	LYS
1	A	265	VAL
1	A	270	LYS
1	A	274	GLU
1	A	275	LYS
1	A	287	THR
1	A	288	LYS
1	A	289	ARG
1	A	292	SER
1	A	294	TYR
1	A	295	SER
1	A	296	THR
1	A	305	LEU
1	A	311	LYS
1	A	315	VAL
1	A	326	LEU
1	A	334	ILE
1	A	342	ARG

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Mol	Chain	Res	Type
1	A	345	THR
1	A	346	LEU
1	A	365	TYR
1	A	367	ARG
1	A	382	LEU
1	A	385	LEU
1	A	398	LYS
1	A	409	ARG
1	A	414	LEU
1	B	1	MSE
1	B	18	LYS
1	B	26	ASP
1	B	27	VAL
1	B	28	ARG
1	B	43	LYS
1	B	44	ILE
1	B	85	LYS
1	B	95	LEU
1	B	96	LYS
1	B	99	LEU
1	B	132	ASN
1	B	140[A]	ASN
1	B	140[B]	ASN
1	B	163	ASN
1	B	177	SER
1	B	180	LEU
1	B	185	LEU
1	B	190	LEU
1	B	193	LEU
1	B	198	LYS
1	B	208	GLU
1	B	214	LEU
1	B	225	ASP
1	B	238	VAL
1	B	243	ARG
1	B	246	LEU
1	B	250	LYS
1	B	253	LYS
1	B	261	ARG
1	B	263	ARG
1	B	264	GLU
1	B	271	GLU

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Mol	Chain	Res	Type
1	B	274	GLU
1	B	280	VAL
1	B	293	MSE
1	B	294	TYR
1	B	295	SER
1	B	305	LEU
1	B	306	GLU
1	B	326	LEU
1	B	346	LEU
1	B	363	LYS
1	B	365	TYR
1	B	367	ARG
1	B	376	ARG
1	B	378	LYS
1	B	382	LEU
1	B	402	GLU
1	B	406	GLU
1	B	409	ARG
1	B	412	VAL
1	B	414	LEU
1	C	1	MSE
1	C	10	SER
1	C	18	LYS
1	C	31	GLU
1	C	39	GLU
1	C	40	GLU
1	C	55	ASP
1	C	56	ARG
1	C	58	LYS
1	C	85	LYS
1	C	95	LEU
1	C	96	LYS
1	C	99	LEU
1	C	132	ASN
1	C	154	GLU
1	C	156	GLU
1	C	163	ASN
1	C	166	ILE
1	C	171	GLU
1	C	177	SER
1	C	185	LEU
1	C	190	LEU

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Mol	Chain	Res	Type
1	C	193	LEU
1	C	208	GLU
1	C	214	LEU
1	C	224	GLU
1	C	225	ASP
1	C	238	VAL
1	C	242	LEU
1	C	243	ARG
1	C	246	LEU
1	C	250	LYS
1	C	254	LYS
1	C	278	THR
1	C	280	VAL
1	C	282	ILE
1	C	287	THR
1	C	289	ARG
1	C	294	TYR
1	C	305	LEU
1	C	309	GLU
1	C	311	LYS
1	C	315	VAL
1	C	326	LEU
1	C	345	THR
1	C	346	LEU
1	C	347	SER
1	C	365	TYR
1	C	367	ARG
1	C	375	LYS
1	C	382	LEU
1	C	398	LYS
1	C	402	GLU
1	C	409	ARG
1	D	1	MSE
1	D	23	ILE
1	D	26	ASP
1	D	27	VAL
1	D	28	ARG
1	D	40	GLU
1	D	41	LYS
1	D	44	ILE
1	D	85	LYS
1	D	95	LEU

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Mol	Chain	Res	Type
1	D	99	LEU
1	D	122	GLU
1	D	132	ASN
1	D	154	GLU
1	D	157	LYS
1	D	161	LEU
1	D	163	ASN
1	D	164	VAL
1	D	166	ILE
1	D	170	ARG
1	D	174	GLU
1	D	179	ARG
1	D	185	LEU
1	D	190	LEU
1	D	193	LEU
1	D	198	LYS
1	D	208	GLU
1	D	213	ASN
1	D	225	ASP
1	D	238	VAL
1	D	242	LEU
1	D	243	ARG
1	D	246	LEU
1	D	247	MSE
1	D	250	LYS
1	D	263	ARG
1	D	267	LYS
1	D	270	LYS
1	D	273	PHE
1	D	274	GLU
1	D	282	ILE
1	D	294	TYR
1	D	305	LEU
1	D	311	LYS
1	D	326	LEU
1	D	347	SER
1	D	363	LYS
1	D	367	ARG
1	D	378	LYS
1	D	382	LEU
1	D	385	LEU
1	D	398	LYS

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Mol	Chain	Res	Type
1	D	412	VAL
1	D	414	LEU
1	E	1	MSE
1	E	15	GLU
1	E	17	VAL
1	E	26	ASP
1	E	39	GLU
1	E	40	GLU
1	E	43	LYS
1	E	44	ILE
1	E	55	ASP
1	E	85	LYS
1	E	96	LYS
1	E	99	LEU
1	E	129	LYS
1	E	154	GLU
1	E	156	GLU
1	E	157	LYS
1	E	163	ASN
1	E	164	VAL
1	E	166	ILE
1	E	174	GLU
1	E	185	LEU
1	E	193	LEU
1	E	214	LEU
1	E	217	LYS
1	E	225	ASP
1	E	242	LEU
1	E	246	LEU
1	E	263	ARG
1	E	264	GLU
1	E	265	VAL
1	E	270	LYS
1	E	282	ILE
1	E	292	SER
1	E	294	TYR
1	E	295	SER
1	E	305	LEU
1	E	311	LYS
1	E	315	VAL
1	E	326	LEU
1	E	345	THR

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Mol	Chain	Res	Type
1	E	346	LEU
1	E	347	SER
1	E	365	TYR
1	E	367	ARG
1	E	375	LYS
1	E	382	LEU
1	E	398	LYS
1	F	1	MSE
1	F	28	ARG
1	F	40	GLU
1	F	44	ILE
1	F	55	ASP
1	F	71	ASP
1	F	85	LYS
1	F	95	LEU
1	F	96	LYS
1	F	99	LEU
1	F	132	ASN
1	F	154	GLU
1	F	157	LYS
1	F	161	LEU
1	F	163	ASN
1	F	164	VAL
1	F	175	MSE
1	F	179	ARG
1	F	180	LEU
1	F	190	LEU
1	F	193	LEU
1	F	198	LYS
1	F	208	GLU
1	F	224	GLU
1	F	225	ASP
1	F	228	THR
1	F	233	SER
1	F	235	ARG
1	F	238	VAL
1	F	242	LEU
1	F	246	LEU
1	F	250	LYS
1	F	261	ARG
1	F	266	MSE
1	F	278	THR

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Mol	Chain	Res	Type
1	F	280	VAL
1	F	294	TYR
1	F	296	THR
1	F	305	LEU
1	F	311	LYS
1	F	326	LEU
1	F	342	ARG
1	F	346	LEU
1	F	362	VAL
1	F	363	LYS
1	F	367	ARG
1	F	375	LYS
1	F	376	ARG
1	F	382	LEU
1	F	398	LYS
1	F	402	GLU
1	F	409	ARG
1	F	410	GLU
1	F	412	VAL
1	G	2	ARG
1	G	27	VAL
1	G	39	GLU
1	G	40[G]	GLU
1	G	41	LYS
1	G	58[G]	LYS
1	G	80	ARG
1	G	85	LYS
1	G	95	LEU
1	G	99	LEU
1	G	132	ASN
1	G	154	GLU
1	G	163	ASN
1	G	164	VAL
1	G	166	ILE
1	G	170[G]	ARG
1	G	174	GLU
1	G	185	LEU
1	G	193	LEU
1	G	213	ASN
1	G	214	LEU
1	G	215	LYS
1	G	223[G]	ASP

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Mol	Chain	Res	Type
1	G	235	ARG
1	G	242	LEU
1	G	246	LEU
1	G	253[G]	LYS
1	G	263	ARG
1	G	265	VAL
1	G	266	MSE
1	G	270	LYS
1	G	285	GLU
1	G	294	TYR
1	G	295	SER
1	G	305	LEU
1	G	311	LYS
1	G	326	LEU
1	G	345	THR
1	G	347	SER
1	G	365	TYR
1	G	367	ARG
1	G	382	LEU
1	G	385	LEU
1	G	402	GLU
1	G	414	LEU
1	H	1	MSE
1	H	26	ASP
1	H	27	VAL
1	H	28	ARG
1	H	39	GLU
1	H	40[H]	GLU
1	H	41[H]	LYS
1	H	55[H]	ASP
1	H	58[H]	LYS
1	H	95	LEU
1	H	99	LEU
1	H	104	THR
1	H	128	ARG
1	H	132	ASN
1	H	161	LEU
1	H	164	VAL
1	H	166	ILE
1	H	169	ILE
1	H	170[H]	ARG
1	H	180	LEU

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Mol	Chain	Res	Type
1	H	185	LEU
1	H	193	LEU
1	H	214	LEU
1	H	215[H]	LYS
1	H	225	ASP
1	H	235	ARG
1	H	238	VAL
1	H	242	LEU
1	H	243	ARG
1	H	246	LEU
1	H	250[H]	LYS
1	H	261	ARG
1	H	263	ARG
1	H	266	MSE
1	H	270	LYS
1	H	273	PHE
1	H	278	THR
1	H	280	VAL
1	H	284[H]	GLU
1	H	295	SER
1	H	296	THR
1	H	303	ARG
1	H	305	LEU
1	H	311	LYS
1	H	326	LEU
1	H	362	VAL
1	H	363	LYS
1	H	367	ARG
1	H	371	GLU
1	H	376	ARG
1	H	378	LYS
1	H	382	LEU
1	H	402[H]	GLU
1	H	410	GLU
1	H	412	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	192	HIS
1	A	213	ASN

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Mol	Chain	Res	Type
1	A	320	ASN
1	B	163	ASN
1	B	167	ASN
1	B	191	ASN
1	B	192	HIS
1	B	320	ASN
1	C	320	ASN
1	D	163	ASN
1	D	191	ASN
1	D	213	ASN
1	D	320	ASN
1	D	353	HIS
1	E	42	GLN
1	E	167	ASN
1	E	191	ASN
1	E	320	ASN
1	F	192	HIS
1	F	320	ASN
1	G	192	HIS
1	G	320	ASN
1	H	213	ASN
1	H	320	ASN
1	H	325	ASN

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

There are no ligands in this entry.

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	403/415 (97%)	0.16	16 (3%)	42	34	14, 20, 35, 43	22 (5%)
1	B	396/415 (95%)	0.05	3 (0%)	87	86	13, 20, 32, 43	19 (4%)
1	C	401/415 (96%)	0.18	14 (3%)	48	40	14, 20, 34, 43	24 (5%)
1	D	393/415 (94%)	0.13	13 (3%)	50	43	14, 19, 32, 43	25 (6%)
1	E	389/415 (93%)	0.26	18 (4%)	36	30	14, 19, 33, 43	35 (8%)
1	F	392/415 (94%)	0.02	8 (2%)	68	64	13, 20, 32, 44	23 (5%)
1	G	402/415 (96%)	0.12	5 (1%)	81	78	13, 20, 34, 46	16 (3%)
1	H	396/415 (95%)	0.19	12 (3%)	54	47	14, 19, 32, 43	29 (7%)
All	All	3172/3320 (95%)	0.14	89 (2%)	56	51	13, 20, 34, 46	193 (6%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	GLY	5.7
1	F	177	SER	4.3
1	E	55	ASP	4.3
1	E	47	ASP	4.0
1	F	280	VAL	3.9
1	C	286	LEU	3.9
1	A	287	THR	3.8
1	G	287	THR	3.8
1	E	44	ILE	3.8
1	D	174	GLU	3.7
1	E	282	ILE	3.7
1	C	284	GLU	3.6
1	A	415	GLY	3.5
1	H	280	VAL	3.4
1	A	47	ASP	3.3
1	A	285	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	287	THR	3.2
1	A	276	TYR	3.1
1	C	415	GLY	3.1
1	B	177	SER	3.0
1	F	278	THR	2.9
1	A	274	GLU	2.8
1	G	177	SER	2.8
1	G	174	GLU	2.8
1	A	55	ASP	2.7
1	E	56	ARG	2.7
1	B	173	ALA	2.6
1	F	47	ASP	2.6
1	F	415	GLY	2.6
1	G	286	LEU	2.6
1	C	55	ASP	2.6
1	H	216	LEU	2.6
1	E	49	VAL	2.6
1	C	280	VAL	2.6
1	A	223	ASP	2.5
1	A	268	ILE	2.5
1	A	290	GLY	2.5
1	D	273	PHE	2.5
1	C	216	LEU	2.5
1	C	257	THR	2.5
1	A	224	GLU	2.5
1	H	415	GLY	2.5
1	D	177	SER	2.5
1	C	285	GLU	2.4
1	E	52	LEU	2.4
1	H	283	PRO	2.4
1	A	53	VAL	2.4
1	D	213	ASN	2.4
1	E	57	PHE	2.4
1	E	177	SER	2.4
1	H	173	ALA	2.3
1	A	24	SER	2.3
1	C	29	ILE	2.3
1	E	213	ASN	2.3
1	D	283	PRO	2.3
1	E	70	VAL	2.3
1	E	415	GLY	2.3
1	H	174	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	278	THR	2.2
1	D	179	ARG	2.2
1	E	258	HIS	2.2
1	F	279	ALA	2.2
1	G	280	VAL	2.2
1	D	204	GLU	2.2
1	E	43	LYS	2.2
1	D	278	THR	2.2
1	F	224	GLU	2.2
1	E	24	SER	2.2
1	C	174	GLU	2.1
1	E	214	LEU	2.1
1	E	271	GLU	2.1
1	H	271	GLU	2.1
1	C	279	ALA	2.1
1	C	228	THR	2.1
1	A	280	VAL	2.1
1	F	223	ASP	2.1
1	A	291	GLY	2.1
1	H	224	GLU	2.1
1	D	274	GLU	2.0
1	D	55	ASP	2.0
1	H	268	ILE	2.0
1	H	276	TYR	2.0
1	D	280	VAL	2.0
1	H	56	ARG	2.0
1	E	232	ASP	2.0
1	B	262	ALA	2.0
1	D	130	THR	2.0
1	C	283	PRO	2.0
1	A	26	ASP	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.