Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:24 PM GMT

PDB ID	:	3X0X
Title	:	Crystal structure of apo-DszC from Rhodococcus erythropolis D-1
Authors	:	Guan, L.J.; Lee, W.C.; Wang, S.P.; Ohtsuka, J.; Tanokura, M.
Deposited on	:	2014-10-23
Resolution	:	2.11 Å(reported)

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

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

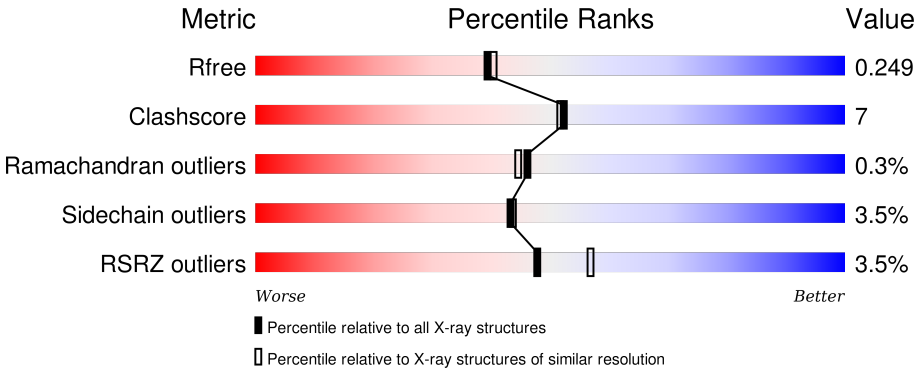
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.11 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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	417	84% 12%
1	B	417	82% 13%
1	C	417	81% 13%
1	D	417	82% 13%
1	E	417	80% 15%

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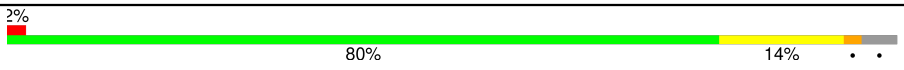
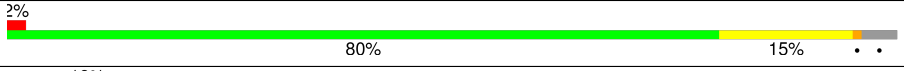
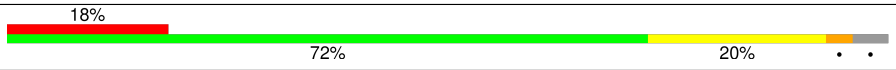
Mol	Chain	Length	Quality of chain
1	F	417	
1	G	417	
1	H	417	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25802 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 DszC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	B	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	D	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	C	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	E	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	F	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	G	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			
1	H	400	Total	C	N	O	S	0	0	0
			3054	1918	545	587	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	189	Total	O	0	0
			189	189		
2	B	223	Total	O	0	0
			223	223		
2	D	196	Total	O	0	0
			196	196		
2	C	196	Total	O	0	0
			196	196		
2	E	191	Total	O	0	0
			191	191		
2	F	153	Total	O	0	0
			153	153		

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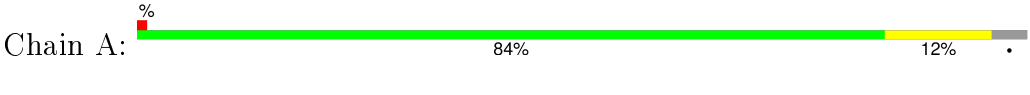
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	146	Total O 146 146	0	0
2	H	76	Total O 76 76	0	0

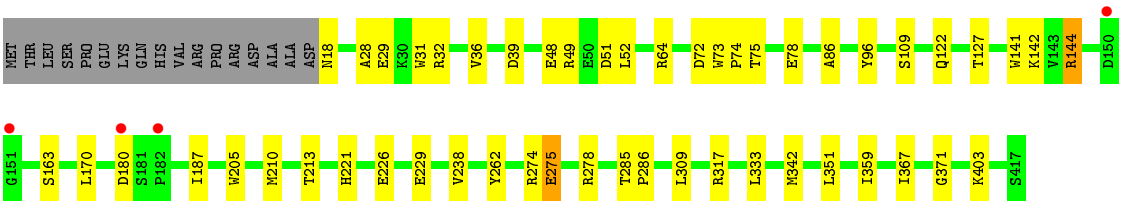
3 Residue-property plots (i)

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: DszC

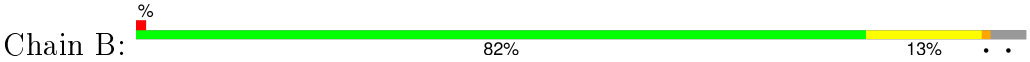
Chain A:





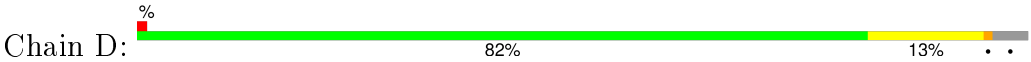
- Molecule 1: DszC

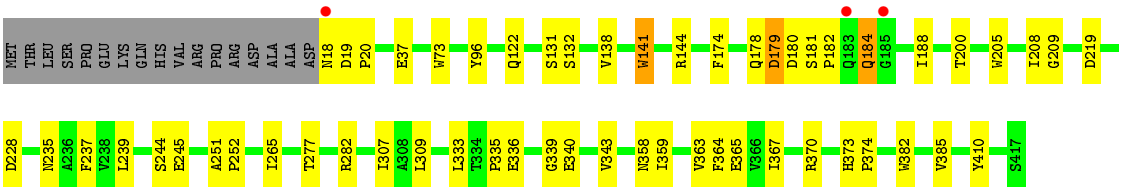
Chain B:



- Molecule 1: DszC

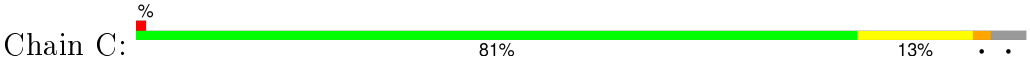
Chain D:

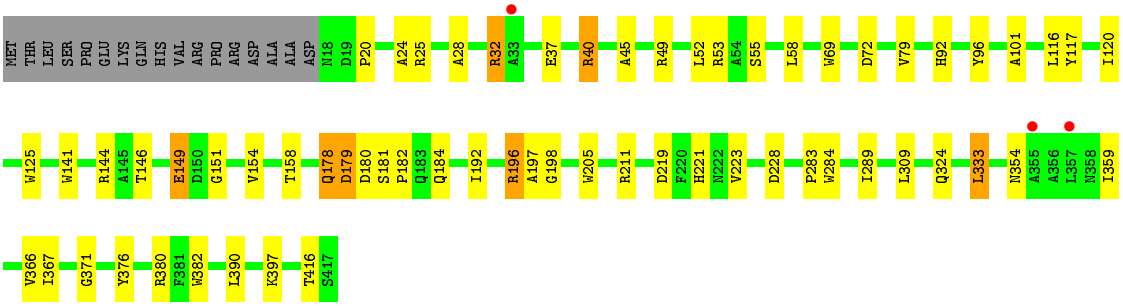




- Molecule 1: DszC

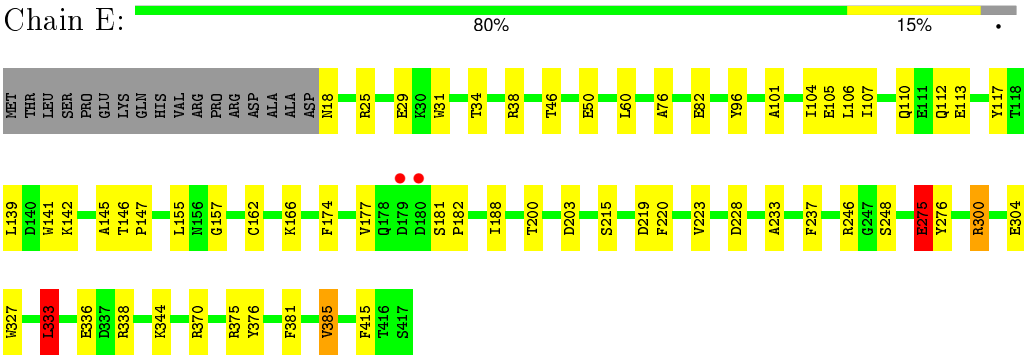
Chain C:





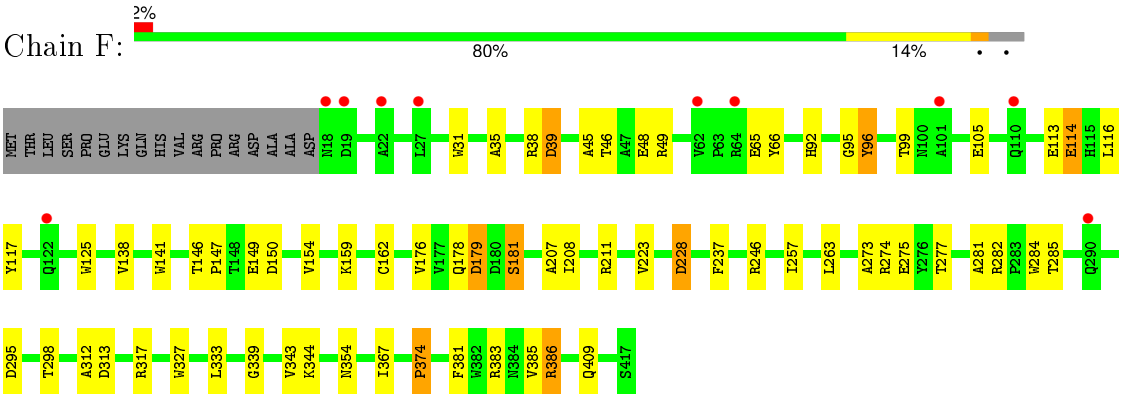
• Molecule 1: DszC

Chain E:



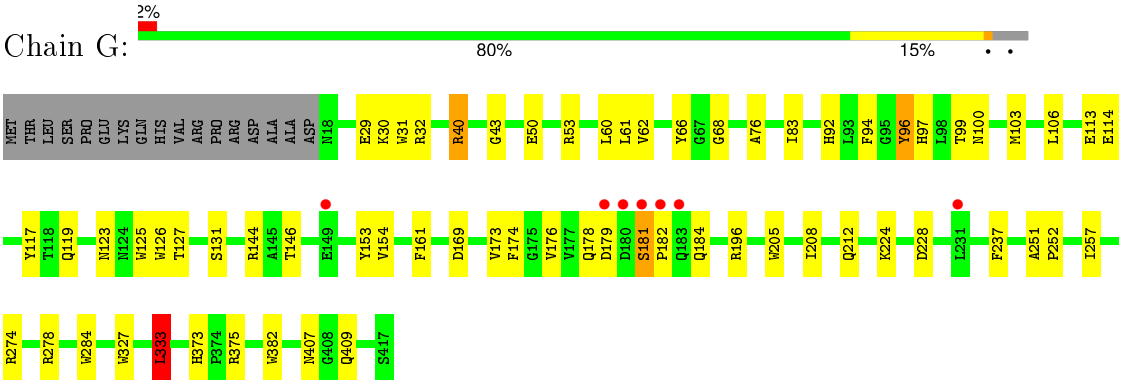
• Molecule 1: DszC

Chain F:



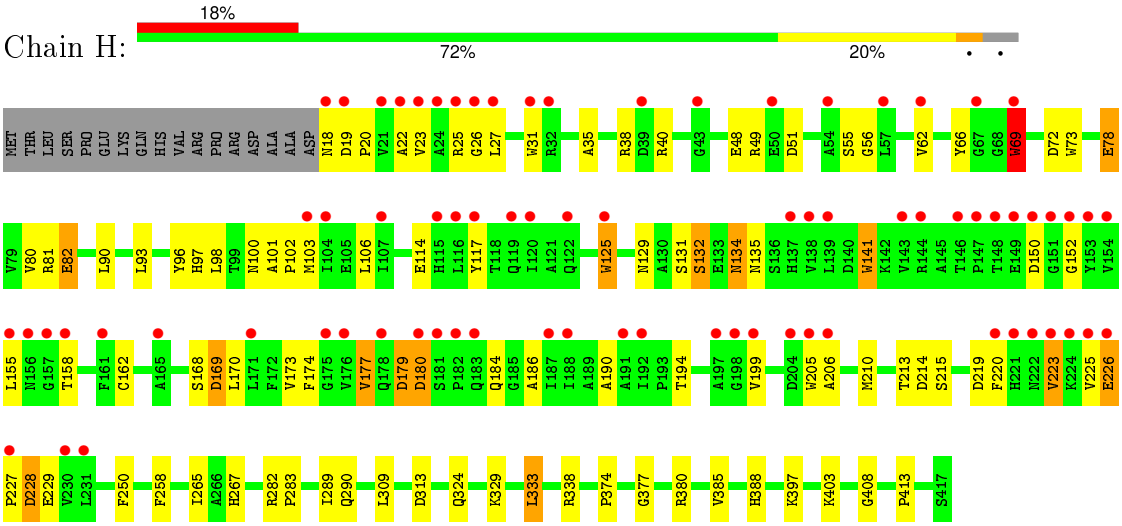
• Molecule 1: DszC

Chain G:



• Molecule 1: DszC

Chain H:


18%
72%
20%
MET THR LEU SER PRO GLU LYS GLN HIS VAL ARG PRO ARG ASP ALA ALA ASP N18 D19 P20 V21 A22 V23 A24 R25 G26 L27 W31 R32 A35 R38 D39 R40 G43 E48 R49 E50 D51 A54 S55 G56 L57 V62 Y66 G67 G68 M69 D72 W73 E78
V79 V80 R81 E82 L90 L93 Y96 H97 L98 T99 N100 A101 P102 M103 I104 E105 L106 I107 E114 H115 L116 Y117 T118 Q119 I120 A121 Q122 W125 N129 A130 S131 S132 E133 N134 N135 S136 H137 V138 L139 D140 W141 K142 V143 R144 A145 T146 P147 T148 E149 D150 G151 G152 Y153 V154
L155 N156 G157 T158 F161 C162 A165 S168 D169 L170 L171 F172 V173 F174 G175 V176 V177 Q178 D179 D180 S181 P182 Q183 Q184 G185 A186 I187 I188 A189 A190 A191 I192 P193 T194 A197 G198 V199 D204 W205 A206 M210 T213 D214 S215 D219 F220 H221 N222 V223 K224 V225 E226
P227 D228 E229 V230 L231 F250 F258 I265 A266 H267 R282 P283 I289 Q290 I309 D313 Q324 K329 I333 R338 P374 G377 R380 V385 H388 K397 K403 G408 P413 S417

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.13Å 123.25Å 184.27Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	43.91 – 2.11 43.91 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.91-2.11) 98.2 (43.91-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.253 0.184 , 0.249	Depositor DCC
R_{free} test set	8996 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 179460 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25802	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 2.99% 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

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	0.89	4/3129 (0.1%)	0.86	3/4265 (0.1%)
1	B	0.94	4/3129 (0.1%)	0.90	5/4265 (0.1%)
1	C	0.96	5/3129 (0.2%)	0.90	4/4265 (0.1%)
1	D	0.92	5/3129 (0.2%)	0.87	0/4265
1	E	0.91	4/3129 (0.1%)	0.88	3/4265 (0.1%)
1	F	0.87	4/3129 (0.1%)	0.85	1/4265 (0.0%)
1	G	0.85	6/3129 (0.2%)	0.84	1/4265 (0.0%)
1	H	0.78	4/3129 (0.1%)	0.77	2/4265 (0.0%)
All	All	0.89	36/25032 (0.1%)	0.86	19/34120 (0.1%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	275	GLU	CD-OE2	7.89	1.34	1.25
1	F	141	TRP	CD2-CE2	6.69	1.49	1.41
1	B	125	TRP	CD2-CE2	6.33	1.49	1.41
1	C	382	TRP	CD2-CE2	6.17	1.48	1.41
1	B	205	TRP	CD2-CE2	6.14	1.48	1.41
1	A	205	TRP	CD2-CE2	6.09	1.48	1.41
1	G	205	TRP	CD2-CE2	6.01	1.48	1.41
1	E	327	TRP	CD2-CE2	5.97	1.48	1.41
1	C	205	TRP	CD2-CE2	5.97	1.48	1.41
1	B	73	TRP	CD2-CE2	5.82	1.48	1.41
1	E	141	TRP	CD2-CE2	5.80	1.48	1.41
1	A	262	TYR	CB-CG	-5.73	1.43	1.51
1	H	125	TRP	CD2-CE2	5.71	1.48	1.41
1	D	205	TRP	CD2-CE2	5.68	1.48	1.41
1	H	69	TRP	CD2-CE2	5.64	1.48	1.41
1	A	73	TRP	CD2-CE2	5.63	1.48	1.41
1	D	73	TRP	CD2-CE2	5.60	1.48	1.41
1	D	365	GLU	CG-CD	5.54	1.60	1.51
1	F	125	TRP	CD2-CE2	5.48	1.48	1.41
1	G	382	TRP	CD2-CE2	5.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	141	TRP	CD2-CE2	5.39	1.47	1.41
1	D	382	TRP	CD2-CE2	5.28	1.47	1.41
1	H	205	TRP	CD2-CE2	5.27	1.47	1.41
1	C	141	TRP	CD2-CE2	5.22	1.47	1.41
1	D	141	TRP	CD2-CE2	5.22	1.47	1.41
1	A	141	TRP	CD2-CE2	5.21	1.47	1.41
1	F	327	TRP	CD2-CE2	5.21	1.47	1.41
1	F	284	TRP	CD2-CE2	5.21	1.47	1.41
1	B	382	TRP	CD2-CE2	5.19	1.47	1.41
1	G	125	TRP	CD2-CE2	5.18	1.47	1.41
1	G	126	TRP	CD2-CE2	5.17	1.47	1.41
1	E	31	TRP	CD2-CE2	5.10	1.47	1.41
1	C	284	TRP	CD2-CE2	5.08	1.47	1.41
1	C	125	TRP	CD2-CE2	5.05	1.47	1.41
1	G	31	TRP	CD2-CE2	5.04	1.47	1.41
1	G	284	TRP	CD2-CE2	5.01	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	F	386	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	H	333	LEU	CA-CB-CG	6.42	130.05	115.30
1	E	300	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	385	VAL	CB-CA-C	-6.20	99.63	111.40
1	B	49	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	342	MET	CG-SD-CE	5.66	109.25	100.20
1	C	333	LEU	CA-CB-CG	5.62	128.24	115.30
1	B	333	LEU	CA-CB-CG	5.58	128.13	115.30
1	G	333	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	38	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	E	333	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	211	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	39	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	317	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	366	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	C	380	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	H	90	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	51	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	3054	0	2932	26	0
1	B	3054	0	2932	36	0
1	C	3054	0	2932	31	0
1	D	3054	0	2932	36	0
1	E	3054	0	2932	40	0
1	F	3054	0	2932	48	0
1	G	3054	0	2932	36	0
1	H	3054	0	2932	76	0
2	A	189	0	0	10	0
2	B	223	0	0	8	0
2	C	196	0	0	3	0
2	D	196	0	0	7	0
2	E	191	0	0	7	0
2	F	153	0	0	3	0
2	G	146	0	0	1	0
2	H	76	0	0	9	0
All	All	25802	0	23456	319	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 (319) 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:H:31:TRP:O	1:H:38:ARG:NH2	1.87	1.08
1:D:282:ARG:HD2	1:D:370:ARG:NH1	1.73	1.02
1:G:97:HIS:ND1	1:G:127:THR:HG22	1.75	1.01
1:E:370:ARG:HD3	1:G:161:PHE:CZ	2.06	0.91
1:B:181:SER:HB2	1:B:182:PRO:HD2	1.52	0.89
1:H:101:ALA:HB3	1:H:102:PRO:HD3	1.55	0.89
1:D:282:ARG:CD	1:D:370:ARG:NH1	2.43	0.81
1:D:282:ARG:HD2	1:D:370:ARG:HH12	1.47	0.80
1:H:377:GLY:O	1:H:380:ARG:NH1	2.14	0.80
1:D:282:ARG:CD	1:D:370:ARG:HH12	1.96	0.79
1:F:31:TRP:HB3	1:F:38:ARG:HH22	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:VAL:HG23	1:H:223:VAL:HG11	1.67	0.77
1:E:155:LEU:HB2	1:E:223:VAL:HB	1.66	0.76
1:H:62:VAL:HG13	1:H:117:TYR:HD2	1.51	0.75
1:F:31:TRP:HB3	1:F:38:ARG:NH2	2.01	0.74
1:E:370:ARG:HD3	1:G:161:PHE:HZ	1.55	0.72
1:D:282:ARG:HD2	1:D:370:ARG:HH11	1.54	0.71
1:G:181:SER:HB2	1:G:182:PRO:CD	2.21	0.70
1:H:56:GLY:O	1:H:69:TRP:NE1	2.22	0.69
1:D:181:SER:HB2	1:D:182:PRO:HD2	1.73	0.69
1:B:180:ASP:N	1:B:180:ASP:OD1	2.26	0.68
1:B:354:ASN:ND2	2:B:642:HOH:O	2.19	0.68
1:H:132:SER:OG	1:H:134:ASN:OD1	2.09	0.67
1:F:45:ALA:O	1:F:49:ARG:HG3	1.95	0.66
1:E:106:LEU:HD22	1:E:246:ARG:O	1.95	0.66
1:B:280:GLN:OE1	1:F:409:GLN:HG3	1.96	0.66
1:F:99:THR:HG22	1:F:257:ILE:HD13	1.78	0.65
1:A:221:HIS:ND1	2:A:566:HOH:O	2.29	0.65
1:G:181:SER:HB2	1:G:182:PRO:HD2	1.77	0.65
1:H:173:VAL:O	1:H:174:PHE:HD1	1.79	0.65
1:D:277:THR:HG23	2:D:580:HOH:O	1.96	0.65
1:H:177:VAL:CG1	1:H:186:ALA:HB3	2.27	0.65
1:H:66:TYR:CE1	1:H:114:GLU:HA	2.32	0.64
1:C:376:TYR:OH	2:C:563:HOH:O	2.15	0.64
1:H:380:ARG:NH2	2:H:553:HOH:O	2.27	0.64
1:H:155:LEU:HB2	1:H:223:VAL:HG23	1.79	0.64
1:F:113:GLU:O	1:F:117:TYR:HB2	1.98	0.64
1:H:82:GLU:OE2	1:H:82:GLU:HA	1.96	0.63
1:G:61:LEU:HD21	1:G:76:ALA:HB2	1.81	0.63
1:F:381:PHE:O	1:F:385:VAL:HG23	1.99	0.62
1:H:152:GLY:HA3	1:H:225:VAL:O	1.99	0.62
1:E:300:ARG:O	1:E:304:GLU:HG3	2.00	0.62
1:G:99:THR:HG22	1:G:257:ILE:HD12	1.82	0.62
1:H:132:SER:HB2	1:H:141:TRP:CH2	2.35	0.61
1:H:329:LYS:NZ	2:H:523:HOH:O	2.25	0.61
1:H:81:ARG:HH22	1:H:313:ASP:CG	2.03	0.60
1:H:413:PRO:O	2:H:566:HOH:O	2.17	0.60
1:H:31:TRP:HZ2	1:H:51:ASP:HB2	1.66	0.59
1:A:142:LYS:NZ	2:A:583:HOH:O	2.35	0.59
1:A:48:GLU:OE2	2:A:649:HOH:O	2.15	0.59
1:F:207:ALA:HA	1:H:374:PRO:HD3	1.84	0.59
1:H:380:ARG:NH1	2:H:553:HOH:O	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:226:GLU:HB3	1:H:228:ASP:OD1	2.03	0.58
1:G:106:LEU:HD21	1:G:327:TRP:HZ3	1.69	0.58
1:F:105:GLU:HG2	1:F:246:ARG:HH12	1.68	0.58
1:B:92:HIS:HE1	2:B:651:HOH:O	1.85	0.58
1:B:226:GLU:HG2	1:B:229:GLU:OE1	2.04	0.58
1:C:158:THR:OG1	1:C:219:ASP:OD1	2.13	0.57
1:C:144:ARG:HD2	1:C:178:GLN:HG2	1.86	0.57
1:D:200:THR:HB	1:D:219:ASP:HB2	1.85	0.57
1:F:317:ARG:NH2	2:F:558:HOH:O	2.37	0.57
1:H:177:VAL:HG13	1:H:186:ALA:HB3	1.87	0.57
1:A:49:ARG:NH2	2:A:542:HOH:O	2.05	0.57
1:H:132:SER:HB2	1:H:141:TRP:HH2	1.69	0.57
1:E:34:THR:HG21	2:E:669:HOH:O	2.04	0.57
1:H:180:ASP:HA	1:H:184:GLN:NE2	2.19	0.57
1:E:375:ARG:NH1	2:E:579:HOH:O	2.36	0.57
1:A:317:ARG:HD3	2:A:646:HOH:O	2.06	0.56
1:B:148:THR:HG22	1:B:152:GLY:N	2.20	0.56
1:E:18:ASN:N	2:E:525:HOH:O	2.38	0.56
1:H:220:PHE:HD1	1:H:223:VAL:HG21	1.70	0.55
1:C:149:GLU:C	1:C:151:GLY:H	2.08	0.55
1:C:28:ALA:O	1:C:32:ARG:HD3	2.07	0.55
1:E:174:PHE:HE2	1:E:415:PHE:CE1	2.25	0.55
1:C:181:SER:HB2	1:C:182:PRO:HD2	1.88	0.55
1:H:100:ASN:OD1	1:H:129:ASN:HB3	2.07	0.55
1:D:37:GLU:HB2	2:D:599:HOH:O	2.05	0.55
1:H:35:ALA:HB1	2:H:555:HOH:O	2.06	0.55
1:F:105:GLU:CG	1:F:246:ARG:HH12	2.20	0.55
1:B:115:HIS:ND1	2:B:631:HOH:O	2.33	0.55
1:E:34:THR:HG23	1:E:38:ARG:HE	1.71	0.54
1:F:31:TRP:HB3	1:F:38:ARG:NH1	2.22	0.54
1:B:344:LYS:HD3	2:B:697:HOH:O	2.05	0.54
1:G:100:ASN:HB2	1:G:127:THR:HG21	1.89	0.54
1:C:37:GLU:OE2	1:C:40:ARG:NH1	2.40	0.54
1:F:39:ASP:O	1:F:211:ARG:NH1	2.40	0.54
1:H:103:MET:HA	1:H:106:LEU:HD12	1.87	0.54
1:H:38:ARG:HD3	1:H:48:GLU:HG2	1.90	0.54
1:D:235:ASN:O	1:D:239:LEU:HG	2.07	0.54
1:E:375:ARG:NH2	1:E:376:TYR:OH	2.40	0.54
1:G:106:LEU:HD21	1:G:327:TRP:CZ3	2.43	0.53
1:C:146:THR:OG1	1:C:154:VAL:CG1	2.57	0.53
1:F:31:TRP:HB3	1:F:38:ARG:CZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:O	1:C:55:SER:OG	2.24	0.53
1:D:181:SER:HB2	1:D:182:PRO:CD	2.39	0.53
1:C:116:LEU:O	1:C:120:ILE:HG13	2.08	0.53
1:A:274:ARG:NH1	1:A:278:ARG:NH1	2.56	0.53
1:F:374:PRO:HG2	1:H:206:ALA:HB1	1.90	0.53
1:G:53:ARG:NH2	1:G:169:ASP:OD2	2.41	0.53
1:F:263:LEU:HD21	1:F:312:ALA:HB1	1.91	0.53
1:H:23:VAL:HG11	1:H:55:SER:HB2	1.89	0.53
1:B:116:LEU:O	1:B:120:ILE:HG13	2.09	0.52
1:G:119:GLN:O	1:G:123:ASN:HB2	2.09	0.52
1:G:100:ASN:OD1	1:G:127:THR:HG23	2.10	0.52
1:H:31:TRP:CZ2	1:H:51:ASP:HB2	2.45	0.52
1:B:181:SER:CB	1:B:182:PRO:HD2	2.34	0.52
1:H:226:GLU:HB2	1:H:229:GLU:HG3	1.92	0.52
1:D:174:PHE:HA	1:D:188:ILE:O	2.08	0.52
1:F:66:TYR:CE1	1:F:114:GLU:HG3	2.45	0.52
1:G:113:GLU:O	1:G:117:TYR:HB2	2.10	0.52
1:A:31:TRP:HH2	1:A:52:LEU:HG	1.76	0.51
1:B:72:ASP:HB2	1:B:324:GLN:OE1	2.09	0.51
1:G:99:THR:HG22	1:G:257:ILE:CD1	2.41	0.51
1:D:358:ASN:HB2	2:D:642:HOH:O	2.10	0.51
1:F:38:ARG:HD3	1:F:48:GLU:CD	2.30	0.51
1:H:19:ASP:HB2	1:H:20:PRO:HD2	1.93	0.51
1:H:49:ARG:NH1	1:H:93:LEU:HD11	2.26	0.51
1:C:196:ARG:HG3	1:C:197:ALA:N	2.24	0.51
1:E:317:ARG:HD3	2:E:582:HOH:O	2.11	0.50
1:B:18:ASN:N	1:E:18:ASN:HD21	2.10	0.50
1:H:210:MET:CE	1:H:388:HIS:HB2	2.42	0.50
1:H:173:VAL:HG13	1:H:190:ALA:HB3	1.93	0.50
1:H:283:PRO:HG3	1:H:290:GLN:O	2.11	0.50
1:E:101:ALA:O	1:E:104:ILE:HD12	2.12	0.50
1:C:354:ASN:ND2	2:C:584:HOH:O	2.45	0.50
1:C:146:THR:OG1	1:C:154:VAL:HG12	2.11	0.50
1:A:285:THR:N	1:A:286:PRO:CD	2.75	0.50
1:G:333:LEU:HD13	1:G:333:LEU:O	2.11	0.50
1:F:92:HIS:NE2	1:F:96:TYR:HD2	2.09	0.50
1:E:381:PHE:O	1:E:385:VAL:HG23	2.11	0.50
1:F:31:TRP:HB3	1:F:38:ARG:HH12	1.76	0.50
1:H:265:ILE:HG21	1:H:385:VAL:HG23	1.94	0.50
1:G:146:THR:O	1:G:153:TYR:HA	2.11	0.50
1:G:61:LEU:HD21	1:G:76:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLY:O	1:F:99:THR:HG23	2.12	0.49
1:F:149:GLU:CD	1:F:149:GLU:H	2.15	0.49
1:B:122:GLN:HG2	2:B:717:HOH:O	2.11	0.49
1:G:251:ALA:HB3	1:G:252:PRO:HD3	1.95	0.49
1:G:60:LEU:HD21	1:G:76:ALA:HA	1.94	0.49
1:A:403:LYS:NZ	2:A:679:HOH:O	2.21	0.49
1:E:333:LEU:HD13	1:E:333:LEU:O	2.13	0.49
1:H:23:VAL:CG1	1:H:55:SER:HB2	2.43	0.49
1:A:74:PRO:O	1:A:78:GLU:HG2	2.12	0.49
1:B:176:VAL:HG12	1:B:178:GLN:HG3	1.95	0.48
1:G:43:GLY:O	1:G:212:GLN:HG2	2.13	0.48
1:H:25:ARG:HG2	1:H:25:ARG:O	2.12	0.48
1:E:313:ASP:OD2	2:E:585:HOH:O	2.20	0.48
1:C:92:HIS:HE1	2:C:615:HOH:O	1.95	0.48
1:A:226:GLU:HG2	1:A:229:GLU:OE1	2.13	0.48
1:E:174:PHE:CE2	1:E:415:PHE:CE1	3.01	0.48
1:C:179:ASP:OD1	1:C:180:ASP:N	2.47	0.48
1:H:27:LEU:O	1:H:31:TRP:HB2	2.13	0.48
1:H:173:VAL:C	1:H:174:PHE:HD1	2.15	0.48
1:D:339:GLY:O	1:D:343:VAL:HG23	2.14	0.48
1:D:340:GLU:OE2	1:D:410:TYR:OH	2.25	0.48
1:F:274:ARG:NH2	1:F:275:GLU:OE1	2.47	0.48
1:B:45:ALA:O	1:B:49:ARG:HG3	2.14	0.47
1:H:162:CYS:O	1:H:215:SER:HA	2.15	0.47
1:A:144:ARG:NE	2:A:652:HOH:O	2.46	0.47
1:B:226:GLU:HG3	2:B:632:HOH:O	2.15	0.47
1:E:139:LEU:HD13	2:E:684:HOH:O	2.14	0.47
1:A:210:MET:HB3	1:A:213:THR:CG2	2.45	0.47
1:G:373:HIS:ND1	1:G:375:ARG:HG2	2.30	0.47
1:D:144:ARG:NH2	2:D:671:HOH:O	2.47	0.47
1:A:309:LEU:HG	1:A:359:ILE:CD1	2.46	0.46
1:F:38:ARG:HD3	1:F:48:GLU:OE2	2.15	0.46
1:A:210:MET:HB3	1:A:213:THR:HG21	1.97	0.46
1:A:275:GLU:HG2	2:A:553:HOH:O	2.15	0.46
1:H:179:ASP:O	1:H:184:GLN:NE2	2.48	0.46
1:G:40:ARG:NH1	2:G:595:HOH:O	2.48	0.46
1:H:40:ARG:NH1	2:H:512:HOH:O	2.48	0.46
1:D:244:SER:HB3	1:D:335:PRO:HA	1.97	0.46
1:B:99:THR:HG22	1:B:257:ILE:CD1	2.46	0.46
1:E:200:THR:OG1	1:E:219:ASP:HB2	2.16	0.46
1:H:101:ALA:HB3	1:H:102:PRO:CD	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:ARG:HB2	1:G:32:ARG:HH11	1.81	0.46
1:F:317:ARG:NH1	2:F:629:HOH:O	2.15	0.46
1:D:122:GLN:NE2	2:D:627:HOH:O	2.48	0.46
1:C:45:ALA:O	1:C:49:ARG:HG3	2.16	0.46
1:D:138:VAL:HA	1:D:141:TRP:CD1	2.51	0.45
1:G:100:ASN:O	1:G:103:MET:HB3	2.16	0.45
1:H:180:ASP:HA	1:H:184:GLN:HE21	1.81	0.45
1:C:149:GLU:C	1:C:151:GLY:N	2.69	0.45
1:G:407:ASN:HB2	1:G:409:GLN:HG3	1.96	0.45
1:F:179:ASP:HB3	1:F:181:SER:H	1.80	0.45
1:H:282:ARG:NE	2:H:570:HOH:O	2.49	0.45
1:B:181:SER:HB2	1:B:182:PRO:CD	2.35	0.45
1:E:142:LYS:O	1:E:157:GLY:HA3	2.16	0.45
1:H:73:TRP:HD1	1:H:324:GLN:OE1	1.99	0.45
1:H:199:VAL:HG22	1:H:220:PHE:CE1	2.52	0.45
1:F:146:THR:HA	1:F:147:PRO:HD3	1.86	0.45
1:H:403:LYS:HD2	2:H:564:HOH:O	2.17	0.45
1:F:66:TYR:HE1	1:F:114:GLU:HG3	1.81	0.45
1:H:210:MET:HE3	1:H:388:HIS:HB2	1.97	0.45
1:F:49:ARG:HE	1:F:49:ARG:HB3	1.48	0.45
1:F:149:GLU:OE1	1:F:149:GLU:N	2.37	0.45
1:A:109:SER:OG	2:A:636:HOH:O	2.18	0.45
1:F:386:ARG:HA	1:F:386:ARG:NE	2.32	0.45
1:B:187:ILE:HD12	1:B:238:VAL:CG2	2.47	0.45
1:B:138:VAL:CG1	1:B:187:ILE:HD11	2.47	0.45
1:F:154:VAL:HA	1:F:223:VAL:O	2.17	0.45
1:D:363:VAL:O	1:D:367:ILE:HG13	2.16	0.44
1:A:36:VAL:HB	2:A:658:HOH:O	2.18	0.44
1:C:397:LYS:NZ	1:C:416:THR:O	2.35	0.44
1:H:78:GLU:HA	1:H:78:GLU:OE1	2.18	0.44
1:G:196:ARG:NH1	1:G:224:LYS:O	2.49	0.44
1:E:60:LEU:HD21	1:E:76:ALA:HA	1.98	0.44
1:H:22:ALA:O	1:H:26:GLY:N	2.48	0.44
1:B:367:ILE:CG2	1:B:371:GLY:HA3	2.47	0.44
1:G:83:ILE:HD12	1:G:94:PHE:CD2	2.53	0.44
1:B:31:TRP:HZ3	1:B:83:ILE:HG23	1.83	0.44
1:B:138:VAL:HG11	1:B:187:ILE:HD11	2.00	0.44
1:E:220:PHE:HD2	1:E:223:VAL:HG21	1.82	0.44
1:A:351:LEU:HG	1:D:307:ILE:CG2	2.48	0.44
1:B:81:ARG:HH22	1:B:313:ASP:CG	2.22	0.43
1:B:24:ALA:HB2	1:B:79:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ALA:HB2	1:C:79:VAL:HG13	1.99	0.43
1:H:173:VAL:HG22	1:H:174:PHE:N	2.32	0.43
1:D:358:ASN:ND2	2:D:642:HOH:O	2.33	0.43
1:F:149:GLU:N	1:F:149:GLU:CD	2.72	0.43
1:E:107:ILE:HD13	1:E:237:PHE:CE2	2.53	0.43
1:H:168:SER:O	1:H:194:THR:HB	2.18	0.43
1:H:101:ALA:CB	1:H:102:PRO:HD3	2.37	0.43
1:B:188:ILE:N	1:B:188:ILE:HD13	2.32	0.43
1:E:145:ALA:O	1:E:177:VAL:HA	2.17	0.43
1:H:380:ARG:CZ	2:H:553:HOH:O	2.55	0.43
1:H:62:VAL:HG13	1:H:117:TYR:CD2	2.42	0.43
1:H:125:TRP:HA	1:H:169:ASP:OD2	2.18	0.43
1:E:131:SER:OG	1:E:132:SER:N	2.48	0.43
1:C:53:ARG:HA	1:C:58:LEU:HD12	2.00	0.43
1:D:131:SER:OG	1:D:132:SER:N	2.52	0.43
1:F:273:ALA:HA	1:F:367:ILE:HD11	2.01	0.43
1:H:97:HIS:CD2	1:H:98:LEU:HD23	2.54	0.43
1:D:144:ARG:HG3	1:D:178:GLN:HB2	2.00	0.43
1:E:146:THR:HA	1:E:147:PRO:HD3	1.91	0.43
1:B:18:ASN:N	1:E:18:ASN:ND2	2.67	0.42
1:G:274:ARG:NH1	1:G:278:ARG:NH1	2.66	0.42
1:D:336:GLU:O	1:D:340:GLU:HG2	2.19	0.42
1:C:72:ASP:HB2	1:C:324:GLN:OE1	2.18	0.42
1:F:159:LYS:HG2	1:F:162:CYS:SG	2.59	0.42
1:E:25:ARG:NH1	1:E:82:GLU:OE2	2.52	0.42
1:E:275:GLU:HG2	1:E:276:TYR:N	2.32	0.42
1:F:263:LEU:HD13	1:F:313:ASP:OD1	2.20	0.42
1:G:32:ARG:HH11	1:G:32:ARG:CB	2.32	0.42
1:D:184:GLN:C	1:D:184:GLN:HE21	2.23	0.42
1:G:131:SER:HB2	1:G:174:PHE:CE2	2.55	0.42
1:C:20:PRO:HG3	1:C:69:TRP:CE3	2.54	0.42
1:F:176:VAL:HB	1:F:178:GLN:NE2	2.34	0.42
1:D:179:ASP:O	1:D:184:GLN:HG3	2.20	0.42
1:D:364:PHE:HB3	1:C:390:LEU:HD11	2.00	0.42
1:H:97:HIS:O	1:H:100:ASN:HB2	2.19	0.42
1:H:150:ASP:OD2	1:H:227:PRO:HD3	2.20	0.42
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.80	0.42
1:D:309:LEU:HG	1:D:359:ILE:CD1	2.50	0.42
1:C:40:ARG:HB3	1:C:40:ARG:CZ	2.47	0.42
1:E:177:VAL:HG23	1:E:188:ILE:HG12	2.01	0.42
1:C:283:PRO:HB2	1:C:289:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ILE:CG2	1:C:371:GLY:HA3	2.50	0.42
1:H:213:THR:O	1:H:214:ASP:C	2.59	0.42
1:E:181:SER:HB2	1:E:182:PRO:HD2	2.02	0.42
1:D:208:ILE:HG13	1:D:209:GLY:N	2.34	0.42
1:F:295:ASP:HB3	1:F:298:THR:HB	2.02	0.41
1:F:99:THR:CG2	1:F:257:ILE:HD13	2.48	0.41
1:H:258:PHE:CG	1:H:388:HIS:HE1	2.37	0.41
1:E:112:GLN:O	1:E:113:GLU:C	2.57	0.41
1:A:187:ILE:HD12	1:A:238:VAL:HG23	2.02	0.41
1:H:283:PRO:HB2	1:H:289:ILE:O	2.21	0.41
1:E:166:LYS:HE3	1:E:203:ASP:HB2	2.02	0.41
1:F:138:VAL:HG12	1:F:176:VAL:HG11	2.03	0.41
1:B:246:ARG:NE	1:B:330:GLY:HA2	2.35	0.41
1:G:176:VAL:HG12	1:G:178:GLN:HG3	2.02	0.41
1:B:273:ALA:CB	1:B:363:VAL:HB	2.51	0.41
1:H:170:LEU:HD12	1:H:170:LEU:HA	1.94	0.41
1:A:72:ASP:OD1	1:A:75:THR:CB	2.68	0.41
1:A:187:ILE:HD12	1:A:238:VAL:CG2	2.50	0.41
1:D:251:ALA:O	1:D:252:PRO:C	2.58	0.41
1:D:373:HIS:CG	1:D:374:PRO:HD2	2.55	0.41
1:D:265:ILE:HG21	1:D:385:VAL:HG23	2.01	0.41
1:B:18:ASN:HA	2:B:661:HOH:O	2.19	0.41
1:A:29:GLU:HG2	1:A:32:ARG:HH22	1.85	0.41
1:C:198:GLY:O	1:C:221:HIS:N	2.38	0.41
1:G:66:TYR:HE1	1:G:114:GLU:HG2	1.86	0.41
1:F:31:TRP:CB	1:F:38:ARG:HH22	2.26	0.41
1:H:22:ALA:O	1:H:25:ARG:N	2.54	0.41
1:E:119:GLN:NE2	2:E:590:HOH:O	2.54	0.41
1:C:192:ILE:HG21	1:C:192:ILE:HD13	1.79	0.41
1:E:336:GLU:CD	1:E:336:GLU:N	2.74	0.41
1:G:92:HIS:O	1:G:96:TYR:HB2	2.21	0.41
1:C:154:VAL:HA	1:C:223:VAL:O	2.20	0.41
1:B:131:SER:O	1:B:159:LYS:HE2	2.21	0.41
1:H:338:ARG:O	1:H:338:ARG:HD3	2.21	0.41
1:F:228:ASP:OD1	1:F:228:ASP:N	2.51	0.41
1:F:354:ASN:HB2	2:F:600:HOH:O	2.21	0.41
1:C:309:LEU:HG	1:C:359:ILE:CD1	2.51	0.41
1:H:27:LEU:HD22	1:H:31:TRP:CH2	2.56	0.41
1:E:101:ALA:HB1	1:E:117:TYR:HE1	1.86	0.41
1:F:277:THR:HA	1:F:281:ALA:HB2	2.02	0.41
1:F:282:ARG:NH2	1:H:135:ASN:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ASN:HB3	2:D:622:HOH:O	2.20	0.41
1:A:367:ILE:CG2	1:A:371:GLY:HA3	2.51	0.41
1:F:208:ILE:O	1:F:383:ARG:HD2	2.20	0.41
1:D:19:ASP:HA	1:D:20:PRO:HD2	1.92	0.40
1:H:267:HIS:CD2	1:H:309:LEU:HD13	2.56	0.40
1:G:62:VAL:HB	1:G:68:GLY:HA3	2.03	0.40
1:A:28:ALA:HB1	1:A:86:ALA:HB2	2.02	0.40
1:C:101:ALA:HB1	1:C:117:TYR:CE1	2.57	0.40
1:B:273:ALA:HB2	1:B:363:VAL:HB	2.04	0.40
1:H:80:VAL:HG12	1:H:80:VAL:O	2.21	0.40
1:E:139:LEU:HD23	1:E:139:LEU:HA	1.94	0.40
1:B:32:ARG:NE	2:B:633:HOH:O	2.48	0.40
1:E:162:CYS:O	1:E:215:SER:HA	2.21	0.40
1:H:73:TRP:CD1	1:H:324:GLN:OE1	2.73	0.40
1:B:27:LEU:HD22	1:B:51:ASP:HB3	2.02	0.40
1:G:181:SER:CB	1:G:182:PRO:CD	2.96	0.40
1:D:18:ASN:O	1:D:20:PRO:HD3	2.22	0.40
1:A:127:THR:HA	1:A:170:LEU:O	2.21	0.40
1:E:248:SER:OG	1:E:338:ARG:HG3	2.22	0.40
1:F:116:LEU:HD23	1:F:116:LEU:HA	1.88	0.40
1:F:339:GLY:O	1:F:343:VAL:HG23	2.22	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	398/417 (95%)	381 (96%)	17 (4%)	0	100	100
1	B	398/417 (95%)	388 (98%)	10 (2%)	0	100	100
1	C	398/417 (95%)	384 (96%)	13 (3%)	1 (0%)	46	44
1	D	398/417 (95%)	388 (98%)	9 (2%)	1 (0%)	46	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	398/417 (95%)	385 (97%)	12 (3%)	1 (0%)	46 44
1	F	398/417 (95%)	383 (96%)	12 (3%)	3 (1%)	24 17
1	G	398/417 (95%)	381 (96%)	16 (4%)	1 (0%)	46 44
1	H	398/417 (95%)	365 (92%)	29 (7%)	4 (1%)	19 12
All	All	3184/3336 (95%)	3055 (96%)	118 (4%)	11 (0%)	46 44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	179	ASP
1	G	181	SER
1	H	131	SER
1	D	179	ASP
1	H	179	ASP
1	H	134	ASN
1	H	408	GLY
1	F	35	ALA
1	F	179	ASP
1	F	374	PRO
1	E	233	ALA

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	308/323 (95%)	299 (97%)	9 (3%)	50 52
1	B	308/323 (95%)	301 (98%)	7 (2%)	58 62
1	C	308/323 (95%)	298 (97%)	10 (3%)	46 48
1	D	308/323 (95%)	301 (98%)	7 (2%)	58 62
1	E	308/323 (95%)	298 (97%)	10 (3%)	46 48
1	F	308/323 (95%)	296 (96%)	12 (4%)	39 38
1	G	308/323 (95%)	294 (96%)	14 (4%)	34 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	308/323 (95%)	290 (94%)	18 (6%)	25 21
All	All	2464/2584 (95%)	2377 (96%)	87 (4%)	43 44

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	64	ARG
1	A	96	TYR
1	A	122	GLN
1	A	144	ARG
1	A	163	SER
1	A	180	ASP
1	A	275	GLU
1	A	333	LEU
1	B	96	TYR
1	B	148	THR
1	B	180	ASP
1	B	219	ASP
1	B	228	ASP
1	B	237	PHE
1	B	333	LEU
1	D	96	TYR
1	D	180	ASP
1	D	184	GLN
1	D	228	ASP
1	D	237	PHE
1	D	245	GLU
1	D	333	LEU
1	C	25	ARG
1	C	32	ARG
1	C	40	ARG
1	C	96	TYR
1	C	149	GLU
1	C	178	GLN
1	C	184	GLN
1	C	196	ARG
1	C	228	ASP
1	C	333	LEU
1	E	29	GLU
1	E	46	THR
1	E	50	GLU

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Mol	Chain	Res	Type
1	E	96	TYR
1	E	105	GLU
1	E	110	GLN
1	E	228	ASP
1	E	275	GLU
1	E	333	LEU
1	E	344	LYS
1	F	39	ASP
1	F	46	THR
1	F	65	GLU
1	F	96	TYR
1	F	114	GLU
1	F	150	ASP
1	F	181	SER
1	F	228	ASP
1	F	237	PHE
1	F	285	THR
1	F	333	LEU
1	F	344	LYS
1	G	29	GLU
1	G	30	LYS
1	G	40	ARG
1	G	50	GLU
1	G	96	TYR
1	G	144	ARG
1	G	154	VAL
1	G	173	VAL
1	G	179	ASP
1	G	184	GLN
1	G	208	ILE
1	G	228	ASP
1	G	237	PHE
1	G	333	LEU
1	H	18	ASN
1	H	69	TRP
1	H	72	ASP
1	H	78	GLU
1	H	82	GLU
1	H	96	TYR
1	H	132	SER
1	H	158	THR
1	H	169	ASP

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Mol	Chain	Res	Type
1	H	177	VAL
1	H	180	ASP
1	H	219	ASP
1	H	223	VAL
1	H	226	GLU
1	H	228	ASP
1	H	250	PHE
1	H	333	LEU
1	H	397	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	321	HIS
1	D	184	GLN
1	D	409	GLN
1	C	178	GLN
1	E	280	GLN
1	G	137	HIS
1	H	18	ASN
1	H	184	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	400/417 (95%)	-0.15	4 (1%) 84 87	17, 35, 56, 84	0
1	B	400/417 (95%)	-0.15	5 (1%) 79 84	16, 30, 54, 108	0
1	C	400/417 (95%)	0.05	3 (0%) 87 90	17, 34, 57, 104	0
1	D	400/417 (95%)	-0.05	3 (0%) 87 90	16, 33, 56, 95	0
1	E	400/417 (95%)	-0.00	2 (0%) 91 93	17, 34, 60, 105	0
1	F	400/417 (95%)	0.13	10 (2%) 61 67	19, 39, 67, 109	0
1	G	400/417 (95%)	0.01	7 (1%) 71 76	20, 40, 63, 101	0
1	H	400/417 (95%)	0.82	77 (19%) 2 2	20, 57, 94, 125	0
All	All	3200/3336 (95%)	0.08	111 (3%) 48 57	16, 36, 72, 125	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	151	GLY	6.5
1	H	147	PRO	5.9
1	H	148	THR	5.5
1	G	182	PRO	5.4
1	H	150	ASP	5.3
1	H	175	GLY	5.2
1	H	18	ASN	5.1
1	H	197	ALA	4.9
1	H	180	ASP	4.9
1	B	180	ASP	4.9
1	H	156	ASN	4.7
1	H	146	THR	4.2
1	H	154	VAL	4.2
1	H	139	LEU	4.2
1	H	120	ILE	4.1
1	H	149	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	224	LYS	4.0
1	B	179	ASP	4.0
1	H	155	LEU	4.0
1	H	54	ALA	3.9
1	H	144	ARG	3.9
1	B	181	SER	3.9
1	H	221	HIS	3.6
1	D	183	GLN	3.6
1	H	157	GLY	3.5
1	H	220	PHE	3.5
1	F	27	LEU	3.5
1	H	227	PRO	3.5
1	H	117	TYR	3.4
1	G	180	ASP	3.4
1	H	182	PRO	3.3
1	H	223	VAL	3.3
1	H	125	TRP	3.3
1	H	225	VAL	3.3
1	F	18	ASN	3.3
1	G	149	GLU	3.3
1	B	183	GLN	3.3
1	H	188	ILE	3.2
1	H	67	GLY	3.2
1	H	62	VAL	3.2
1	H	31	TRP	3.2
1	H	178	GLN	3.1
1	H	24	ALA	3.0
1	F	101	ALA	3.0
1	E	179	ASP	3.0
1	H	26	GLY	3.0
1	H	152	GLY	3.0
1	H	231	LEU	3.0
1	B	182	PRO	3.0
1	H	183	GLN	2.9
1	H	22	ALA	2.9
1	H	23	VAL	2.9
1	H	32	ARG	2.8
1	H	205	TRP	2.8
1	H	176	VAL	2.7
1	H	25	ARG	2.7
1	F	290	GLN	2.7
1	G	231	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	104	ILE	2.7
1	H	50	GLU	2.7
1	F	110	GLN	2.6
1	H	119	GLN	2.6
1	A	150	ASP	2.6
1	H	143	VAL	2.6
1	H	158	THR	2.6
1	G	179	ASP	2.6
1	A	151	GLY	2.5
1	C	355	ALA	2.5
1	H	161	PHE	2.5
1	H	181	SER	2.5
1	H	153	TYR	2.5
1	H	191	ALA	2.5
1	C	357	LEU	2.5
1	H	206	ALA	2.4
1	F	62	VAL	2.4
1	H	192	ILE	2.4
1	E	180	ASP	2.4
1	H	137	HIS	2.4
1	D	18	ASN	2.4
1	F	19	ASP	2.4
1	H	21	VAL	2.3
1	D	185	GLY	2.3
1	F	122	GLN	2.3
1	H	165	ALA	2.3
1	H	204	ASP	2.3
1	H	222	ASN	2.3
1	G	181	SER	2.2
1	H	187	ILE	2.2
1	A	180	ASP	2.2
1	H	138	VAL	2.2
1	F	22	ALA	2.2
1	H	57	LEU	2.2
1	H	116	LEU	2.2
1	H	171	LEU	2.2
1	H	230	VAL	2.2
1	H	19	ASP	2.2
1	H	198	GLY	2.2
1	H	43	GLY	2.1
1	H	27	LEU	2.1
1	F	64	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	39	ASP	2.1
1	A	182	PRO	2.1
1	H	199	VAL	2.1
1	H	107	ILE	2.1
1	H	122	GLN	2.1
1	G	183	GLN	2.0
1	H	115	HIS	2.0
1	H	69	TRP	2.0
1	C	33	ALA	2.0
1	H	226	GLU	2.0
1	H	103	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.