Full wwPDB X-ray Structure Validation Report

Sep 10, 2023 – 03:06 PM EDT

PDB ID	:	4JHM
Title	:	Crystal structure of a putative mandelate racemase/muconate lactonizing enzyme from Pseudovibrio sp.
Authors	:	Hegde, R.P.; Toro, R.; Burley, S.K.; Almo, S.C.; Ramagopal, U.A.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2013-03-05
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

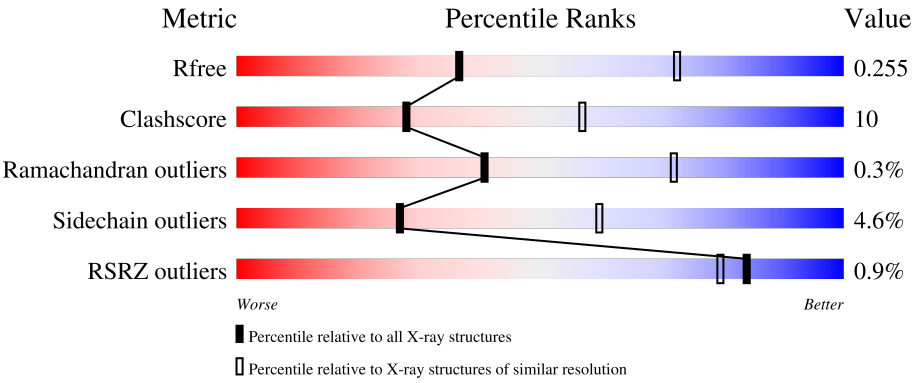
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	384	76% 20%
1	B	384	81% 15%
1	C	384	75% 20%
1	D	384	74% 21%
1	E	384	73% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	384	73% 22%
1	G	384	% 72% 23%
1	H	384	3% 76% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23568 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 Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	Se	0	0	0
			2946	1876	482	566	10	12			
1	B	375	Total	C	N	O	S	Se	0	1	0
			2960	1886	484	568	10	12			
1	C	374	Total	C	N	O	S	Se	0	0	0
			2940	1874	479	565	10	12			
1	D	375	Total	C	N	O	S	Se	0	0	0
			2942	1873	481	566	10	12			
1	E	374	Total	C	N	O	S	Se	0	2	0
			2951	1880	480	569	10	12			
1	F	375	Total	C	N	O	S	Se	0	1	0
			2945	1875	479	569	10	12			
1	G	375	Total	C	N	O	S	Se	0	0	0
			2944	1876	480	566	10	12			
1	H	374	Total	C	N	O	S	Se	0	0	0
			2932	1868	477	565	10	12			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP B6R2Z8
A	0	SER	-	expression tag	UNP B6R2Z8
A	1	LEU	-	expression tag	UNP B6R2Z8
A	375	GLU	-	expression tag	UNP B6R2Z8
A	376	GLY	-	expression tag	UNP B6R2Z8
A	377	HIS	-	expression tag	UNP B6R2Z8
A	378	HIS	-	expression tag	UNP B6R2Z8
A	379	HIS	-	expression tag	UNP B6R2Z8
A	380	HIS	-	expression tag	UNP B6R2Z8
A	381	HIS	-	expression tag	UNP B6R2Z8
A	382	HIS	-	expression tag	UNP B6R2Z8
B	-1	MSE	-	expression tag	UNP B6R2Z8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP B6R2Z8
B	1	LEU	-	expression tag	UNP B6R2Z8
B	375	GLU	-	expression tag	UNP B6R2Z8
B	376	GLY	-	expression tag	UNP B6R2Z8
B	377	HIS	-	expression tag	UNP B6R2Z8
B	378	HIS	-	expression tag	UNP B6R2Z8
B	379	HIS	-	expression tag	UNP B6R2Z8
B	380	HIS	-	expression tag	UNP B6R2Z8
B	381	HIS	-	expression tag	UNP B6R2Z8
B	382	HIS	-	expression tag	UNP B6R2Z8
C	-1	MSE	-	expression tag	UNP B6R2Z8
C	0	SER	-	expression tag	UNP B6R2Z8
C	1	LEU	-	expression tag	UNP B6R2Z8
C	375	GLU	-	expression tag	UNP B6R2Z8
C	376	GLY	-	expression tag	UNP B6R2Z8
C	377	HIS	-	expression tag	UNP B6R2Z8
C	378	HIS	-	expression tag	UNP B6R2Z8
C	379	HIS	-	expression tag	UNP B6R2Z8
C	380	HIS	-	expression tag	UNP B6R2Z8
C	381	HIS	-	expression tag	UNP B6R2Z8
C	382	HIS	-	expression tag	UNP B6R2Z8
D	-1	MSE	-	expression tag	UNP B6R2Z8
D	0	SER	-	expression tag	UNP B6R2Z8
D	1	LEU	-	expression tag	UNP B6R2Z8
D	375	GLU	-	expression tag	UNP B6R2Z8
D	376	GLY	-	expression tag	UNP B6R2Z8
D	377	HIS	-	expression tag	UNP B6R2Z8
D	378	HIS	-	expression tag	UNP B6R2Z8
D	379	HIS	-	expression tag	UNP B6R2Z8
D	380	HIS	-	expression tag	UNP B6R2Z8
D	381	HIS	-	expression tag	UNP B6R2Z8
D	382	HIS	-	expression tag	UNP B6R2Z8
E	-1	MSE	-	expression tag	UNP B6R2Z8
E	0	SER	-	expression tag	UNP B6R2Z8
E	1	LEU	-	expression tag	UNP B6R2Z8
E	375	GLU	-	expression tag	UNP B6R2Z8
E	376	GLY	-	expression tag	UNP B6R2Z8
E	377	HIS	-	expression tag	UNP B6R2Z8
E	378	HIS	-	expression tag	UNP B6R2Z8
E	379	HIS	-	expression tag	UNP B6R2Z8
E	380	HIS	-	expression tag	UNP B6R2Z8
E	381	HIS	-	expression tag	UNP B6R2Z8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	382	HIS	-	expression tag	UNP B6R2Z8
F	-1	MSE	-	expression tag	UNP B6R2Z8
F	0	SER	-	expression tag	UNP B6R2Z8
F	1	LEU	-	expression tag	UNP B6R2Z8
F	375	GLU	-	expression tag	UNP B6R2Z8
F	376	GLY	-	expression tag	UNP B6R2Z8
F	377	HIS	-	expression tag	UNP B6R2Z8
F	378	HIS	-	expression tag	UNP B6R2Z8
F	379	HIS	-	expression tag	UNP B6R2Z8
F	380	HIS	-	expression tag	UNP B6R2Z8
F	381	HIS	-	expression tag	UNP B6R2Z8
F	382	HIS	-	expression tag	UNP B6R2Z8
G	-1	MSE	-	expression tag	UNP B6R2Z8
G	0	SER	-	expression tag	UNP B6R2Z8
G	1	LEU	-	expression tag	UNP B6R2Z8
G	375	GLU	-	expression tag	UNP B6R2Z8
G	376	GLY	-	expression tag	UNP B6R2Z8
G	377	HIS	-	expression tag	UNP B6R2Z8
G	378	HIS	-	expression tag	UNP B6R2Z8
G	379	HIS	-	expression tag	UNP B6R2Z8
G	380	HIS	-	expression tag	UNP B6R2Z8
G	381	HIS	-	expression tag	UNP B6R2Z8
G	382	HIS	-	expression tag	UNP B6R2Z8
H	-1	MSE	-	expression tag	UNP B6R2Z8
H	0	SER	-	expression tag	UNP B6R2Z8
H	1	LEU	-	expression tag	UNP B6R2Z8
H	375	GLU	-	expression tag	UNP B6R2Z8
H	376	GLY	-	expression tag	UNP B6R2Z8
H	377	HIS	-	expression tag	UNP B6R2Z8
H	378	HIS	-	expression tag	UNP B6R2Z8
H	379	HIS	-	expression tag	UNP B6R2Z8
H	380	HIS	-	expression tag	UNP B6R2Z8
H	381	HIS	-	expression tag	UNP B6R2Z8
H	382	HIS	-	expression tag	UNP B6R2Z8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 1 1	0	0
2	C	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

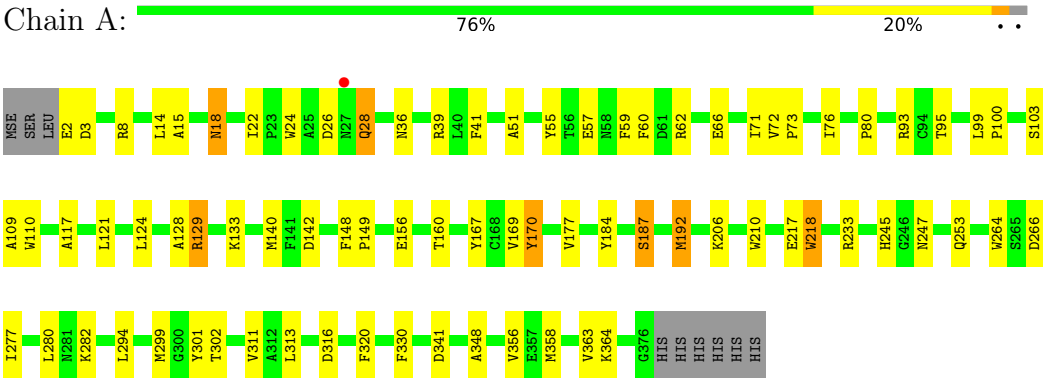
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O 1 1	0	0
2	E	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0
2	G	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

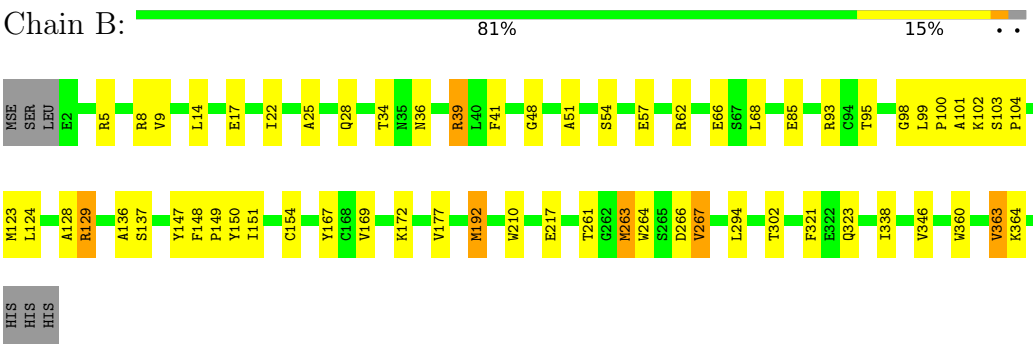
• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain A:



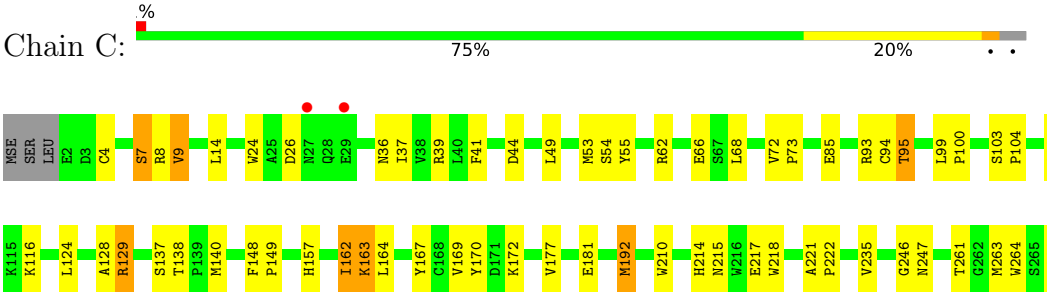
• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

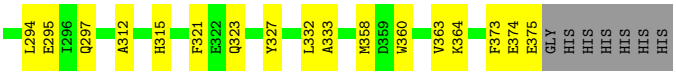
Chain B:



• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

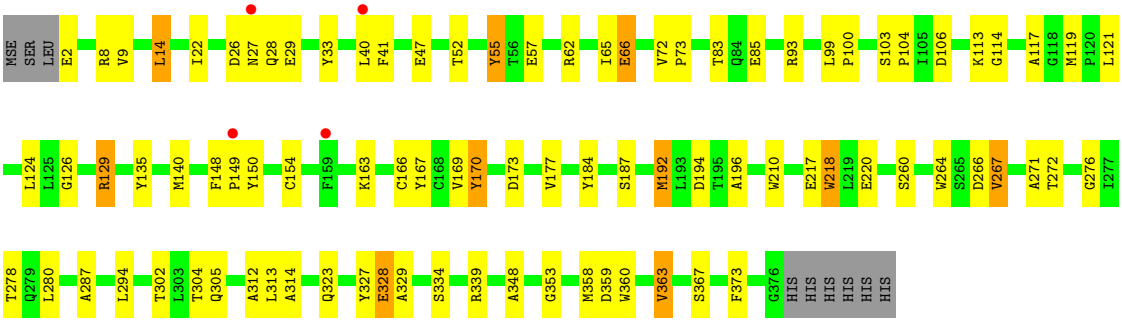
Chain C:





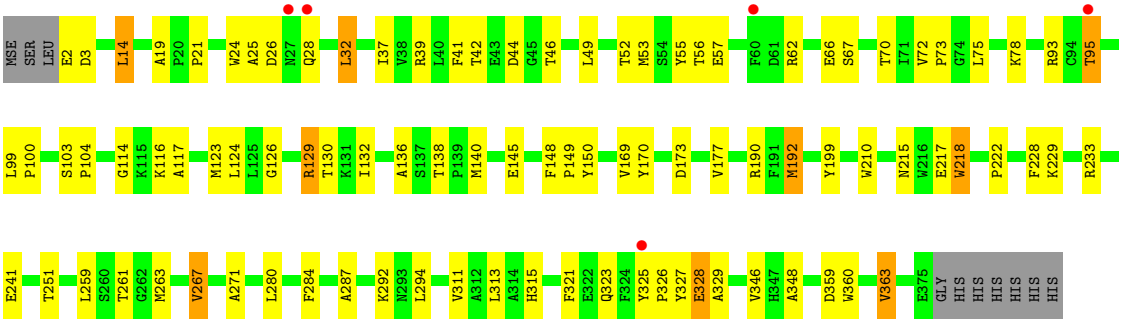
• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain D:



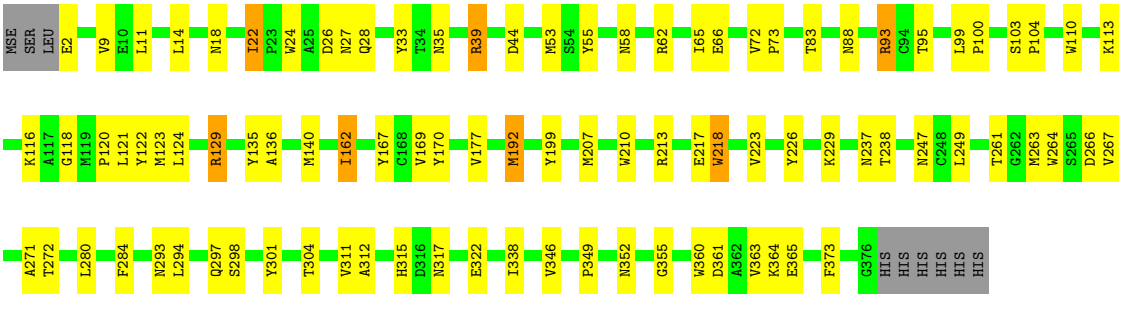
• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain E:



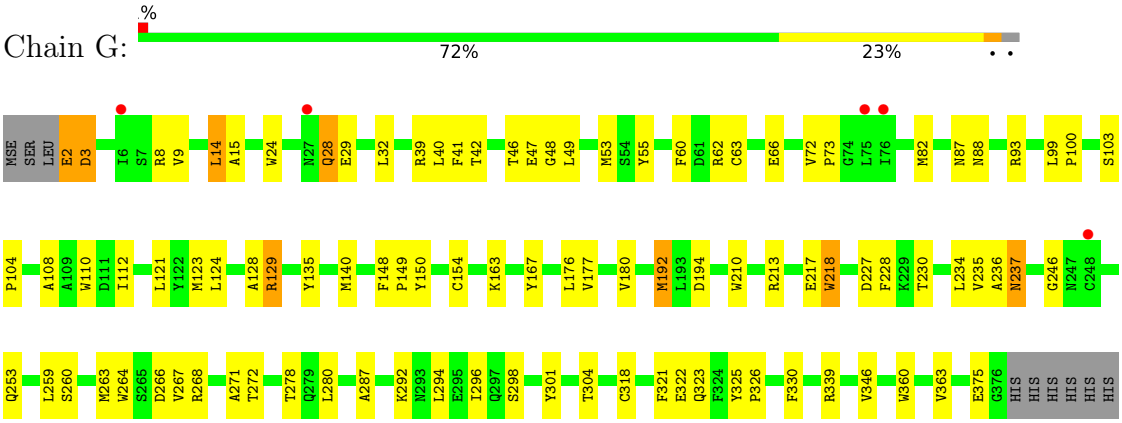
• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain F:



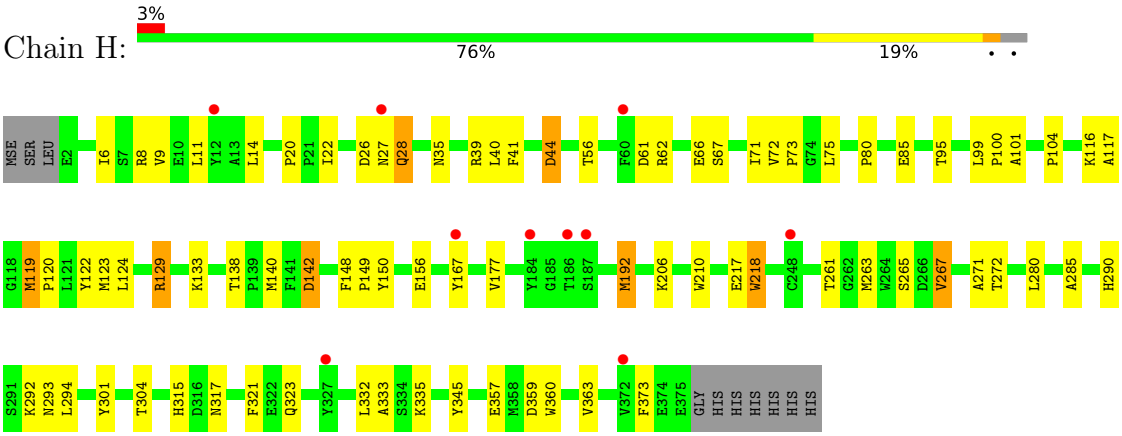
• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain G:



• Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	201.79Å 117.31Å 143.13Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	39.41 – 2.80 39.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.41-2.80) 98.6 (39.41-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.253 0.195 , 0.255	Depositor DCC
R_{free} test set	3989 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23568	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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	0.27	0/3009	0.46	0/4072
1	B	0.28	0/3026	0.49	0/4092
1	C	0.28	0/3003	0.46	0/4064
1	D	0.26	0/3005	0.44	0/4068
1	E	0.26	0/3017	0.44	0/4084
1	F	0.26	0/3008	0.45	0/4073
1	G	0.27	0/3007	0.45	0/4069
1	H	0.26	0/2995	0.44	0/4056
All	All	0.27	0/24070	0.46	0/32578

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2946	0	2808	57	0
1	B	2960	0	2835	48	0
1	C	2940	0	2805	60	0
1	D	2942	0	2797	63	0
1	E	2951	0	2806	70	0
1	F	2945	0	2790	63	0
1	G	2944	0	2808	67	0
1	H	2932	0	2783	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
All	All	23568	0	22432	457	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 10.

All (457) 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:B:25:ALA:HB3	1:B:28:GLN:HG2	1.58	0.85
1:C:177:VAL:HG12	1:C:210:TRP:CH2	2.12	0.84
1:E:321:PHE:HE2	1:E:323:GLN:HG2	1.46	0.81
1:E:66:GLU:HG2	1:F:62:ARG:HB2	1.61	0.81
1:D:272:THR:HG21	1:D:304:THR:HG23	1.63	0.81
1:C:177:VAL:CG1	1:C:210:TRP:CZ3	2.67	0.78
1:G:321:PHE:CE2	1:G:323:GLN:HG2	2.20	0.77
1:F:136:ALA:HB3	1:F:162:ILE:HG22	1.68	0.76
1:C:374:GLU:O	1:C:375:GLU:HB2	1.84	0.76
1:B:261:THR:OG1	1:B:263:MSE:HE3	1.85	0.76
1:A:62:ARG:HB2	1:B:66:GLU:CG	2.19	0.73
1:G:66:GLU:HG2	1:H:62:ARG:HB2	1.70	0.72
1:B:177:VAL:HG12	1:B:210:TRP:CH2	2.25	0.72
1:B:177:VAL:CG1	1:B:210:TRP:CZ3	2.73	0.71
1:D:334:SER:CB	1:D:358:MSE:HE2	2.19	0.71
1:D:334:SER:HB2	1:D:358:MSE:HE2	1.71	0.71
1:E:321:PHE:CE2	1:E:323:GLN:HG2	2.26	0.70
1:B:360:TRP:HA	1:B:363:VAL:HG13	1.74	0.70
1:A:26:ASP:HA	1:A:140:MSE:HE1	1.73	0.70
1:F:123:MSE:HE2	1:G:82:MSE:HE3	1.75	0.69
1:F:177:VAL:CG1	1:F:210:TRP:CZ3	2.76	0.68
1:A:192:MSE:HG3	1:A:217:GLU:HB3	1.74	0.68
1:G:177:VAL:CG1	1:G:210:TRP:CZ3	2.76	0.68
1:A:267:VAL:HG22	1:A:294:LEU:HG	1.76	0.68
1:A:71:ILE:HD11	1:A:95:THR:HG21	1.77	0.67
1:H:20:PRO:O	1:H:22:ILE:HD12	1.94	0.67
1:B:123:MSE:O	1:C:113:LYS:HE2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:ASP:N	1:H:44:ASP:OD1	2.27	0.67
1:E:66:GLU:CG	1:F:62:ARG:HB2	2.24	0.67
1:C:128:ALA:C	1:C:129:ARG:HG3	2.15	0.66
1:E:173:ASP:OD2	1:E:199:TYR:OH	2.13	0.66
1:G:3:ASP:OD1	1:G:3:ASP:N	2.29	0.65
1:G:192:MSE:HG3	1:G:217:GLU:HB3	1.78	0.64
1:G:39:ARG:NH1	1:G:47:GLU:OE1	2.29	0.64
1:A:62:ARG:HB2	1:B:66:GLU:HG2	1.79	0.64
1:A:18:ASN:N	1:A:18:ASN:HD22	1.96	0.64
1:A:28:GLN:N	1:A:28:GLN:HE21	1.95	0.64
1:B:25:ALA:CB	1:B:28:GLN:HG2	2.28	0.64
1:G:237:ASN:N	1:G:237:ASN:HD22	1.95	0.63
1:D:126:GLY:O	1:D:314:ALA:O	2.16	0.63
1:G:298:SER:OG	1:G:322:GLU:O	2.17	0.62
1:F:272:THR:HG21	1:F:304:THR:HG23	1.82	0.62
1:H:360:TRP:HA	1:H:363:VAL:CG1	2.29	0.62
1:F:129:ARG:NH1	1:F:315:HIS:O	2.32	0.62
1:C:177:VAL:CG1	1:C:210:TRP:CH2	2.82	0.62
1:D:360:TRP:HA	1:D:363:VAL:CG1	2.29	0.62
1:F:2[A]:GLU:HG3	1:G:123:MSE:HE1	1.82	0.62
1:F:199:TYR:O	1:F:223:VAL:HG12	1.99	0.62
1:C:44:ASP:OD2	1:C:116:LYS:NZ	2.22	0.61
1:E:25:ALA:HB3	1:E:28[A]:GLN:CD	2.21	0.61
1:E:26:ASP:O	1:E:28[B]:GLN:NE2	2.33	0.61
1:E:177:VAL:CG1	1:E:210:TRP:CZ3	2.83	0.61
1:G:148:PHE:HB2	1:G:149:PRO:HD3	1.83	0.61
1:H:133:LYS:HE3	1:H:345:TYR:CE1	2.35	0.61
1:E:233:ARG:NH1	1:G:235:VAL:O	2.32	0.61
1:C:192:MSE:HG3	1:C:217:GLU:HB3	1.81	0.61
1:D:114:GLY:HA2	1:D:124:LEU:HD11	1.82	0.60
1:E:261:THR:OG1	1:E:263:MSE:HE3	2.02	0.60
1:E:360:TRP:HA	1:E:363:VAL:CG1	2.30	0.60
1:F:11:LEU:HB3	1:F:65:ILE:HD11	1.83	0.60
1:F:271:ALA:HB2	1:F:280:LEU:HD22	1.84	0.60
1:H:148:PHE:HB2	1:H:149:PRO:HD3	1.84	0.60
1:A:233:ARG:NH1	1:C:235:VAL:O	2.35	0.59
1:B:68:LEU:HD21	1:B:101:ALA:O	2.02	0.59
1:C:8:ARG:HD3	1:C:41:PHE:CD1	2.36	0.59
1:F:140:MSE:HE3	1:F:167:TYR:HA	1.84	0.59
1:H:9:VAL:HG22	1:H:373:PHE:HB2	1.84	0.59
1:F:26:ASP:O	1:F:28:GLN:OE1	2.20	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ARG:HB2	1:D:66:GLU:HG2	1.83	0.59
1:B:192:MSE:HG3	1:B:217:GLU:HB3	1.85	0.59
1:A:128:ALA:C	1:A:129:ARG:HG3	2.23	0.59
1:D:177:VAL:CG1	1:D:210:TRP:CZ3	2.86	0.58
1:F:177:VAL:HG12	1:F:210:TRP:CH2	2.38	0.58
1:C:9:VAL:HG13	1:C:373:PHE:HB2	1.85	0.58
1:H:26:ASP:HA	1:H:140:MSE:HE1	1.85	0.58
1:A:140:MSE:HE3	1:A:167:TYR:HA	1.85	0.58
1:D:271:ALA:HB2	1:D:280:LEU:HD22	1.84	0.58
1:H:138:THR:HG22	1:H:150:TYR:HE1	1.68	0.58
1:F:361:ASP:O	1:F:365:GLU:HB2	2.04	0.58
1:F:22:ILE:HG23	1:F:33:TYR:CE1	2.38	0.58
1:G:321:PHE:HE2	1:G:323:GLN:HG2	1.69	0.58
1:B:169:VAL:HG13	1:B:169:VAL:O	2.03	0.58
1:E:129:ARG:NH2	1:E:132:ILE:HD12	2.19	0.57
1:H:335:LYS:HB2	1:H:357:GLU:HB3	1.86	0.57
1:A:110:TRP:HB3	1:A:121:LEU:HD11	1.86	0.57
1:D:26:ASP:HA	1:D:140:MSE:HE1	1.87	0.57
1:D:113:LYS:NZ	1:E:123:MSE:O	2.31	0.57
1:H:26:ASP:C	1:H:27:ASN:HD22	2.07	0.57
1:E:44:ASP:OD2	1:E:116:LYS:HE2	2.04	0.57
1:H:290:HIS:O	1:H:292:LYS:HG2	2.05	0.57
1:H:271:ALA:HB2	1:H:280:LEU:HD22	1.87	0.56
1:D:114:GLY:HA3	1:D:353:GLY:HA2	1.87	0.56
1:H:177:VAL:CG1	1:H:210:TRP:CZ3	2.88	0.56
1:A:62:ARG:HB2	1:B:66:GLU:HG3	1.87	0.56
1:E:136:ALA:HA	1:E:323:GLN:O	2.06	0.56
1:E:177:VAL:CG1	1:E:210:TRP:CH2	2.88	0.56
1:H:9:VAL:HG12	1:H:40:LEU:CD2	2.36	0.56
1:G:129:ARG:NH2	1:G:318:CYS:O	2.36	0.56
1:G:177:VAL:HG12	1:G:210:TRP:CH2	2.41	0.56
1:E:192:MSE:HG3	1:E:217:GLU:HB3	1.87	0.55
1:F:177:VAL:CG1	1:F:210:TRP:CH2	2.88	0.55
1:F:284:PHE:CD1	1:F:294:LEU:HD13	2.41	0.55
1:B:62:ARG:O	1:B:66:GLU:HB2	2.06	0.55
1:B:128:ALA:C	1:B:129:ARG:HG3	2.26	0.55
1:G:236:ALA:C	1:G:237:ASN:HD22	2.10	0.55
1:E:129:ARG:NH1	1:E:315:HIS:O	2.38	0.55
1:G:39:ARG:HD2	1:G:41:PHE:CE2	2.41	0.55
1:E:39:ARG:HD2	1:E:41:PHE:CE1	2.42	0.55
1:G:271:ALA:HB2	1:G:280:LEU:HD22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LEU:HD22	1:E:292:LYS:HD2	1.89	0.55
1:F:280:LEU:HD23	1:F:311:VAL:HG21	1.89	0.55
1:D:8:ARG:HB3	1:D:41:PHE:HB2	1.89	0.55
1:D:106:ASP:OD1	1:D:278:THR:OG1	2.21	0.55
1:F:44:ASP:OD2	1:F:116:LYS:NZ	2.35	0.55
1:H:99:LEU:N	1:H:100:PRO:CD	2.70	0.55
1:F:110:TRP:HB3	1:F:121:LEU:HD11	1.89	0.54
1:H:138:THR:HG22	1:H:150:TYR:CE1	2.42	0.54
1:A:177:VAL:CG1	1:A:210:TRP:CH2	2.90	0.54
1:F:266:ASP:C	1:F:266:ASP:OD1	2.46	0.54
1:D:99:LEU:N	1:D:100:PRO:CD	2.71	0.54
1:E:114:GLY:HA2	1:E:124:LEU:HD11	1.89	0.54
1:H:9:VAL:HG12	1:H:40:LEU:HD23	1.90	0.54
1:G:321:PHE:CD2	1:G:346:VAL:HG11	2.42	0.54
1:H:44:ASP:OD2	1:H:116:LYS:NZ	2.31	0.54
1:H:101:ALA:O	1:H:104:PRO:HD2	2.08	0.54
1:C:162:ILE:HD11	1:C:164:LEU:HD23	1.90	0.54
1:D:148:PHE:HB2	1:D:149:PRO:HD3	1.90	0.54
1:H:9:VAL:CG2	1:H:373:PHE:HB2	2.38	0.54
1:A:177:VAL:CG1	1:A:210:TRP:CZ3	2.91	0.53
1:C:363:VAL:HG23	1:C:364:LYS:N	2.21	0.53
1:A:99:LEU:N	1:A:100:PRO:CD	2.71	0.53
1:G:163:LYS:HE3	1:G:194:ASP:HB2	1.89	0.53
1:D:135:TYR:CE1	1:D:163:LYS:HD3	2.43	0.53
1:E:99:LEU:N	1:E:100:PRO:CD	2.72	0.53
1:G:110:TRP:HB3	1:G:121:LEU:HD11	1.89	0.53
1:D:72:VAL:N	1:D:73:PRO:CD	2.72	0.53
1:D:121:LEU:HD12	1:D:124:LEU:HD12	1.91	0.53
1:B:150:TYR:CE1	1:B:154:CYS:SG	3.02	0.53
1:D:2:GLU:O	1:D:2:GLU:HG3	2.09	0.53
1:A:177:VAL:HG13	1:A:210:TRP:CH2	2.44	0.53
1:E:67:SER:OG	1:E:95:THR:HG21	2.09	0.53
1:F:22:ILE:HG13	1:F:22:ILE:O	2.07	0.53
1:A:66:GLU:CG	1:B:62:ARG:HB2	2.39	0.53
1:G:49:LEU:O	1:G:108:ALA:HA	2.09	0.53
1:D:359:ASP:O	1:D:363:VAL:HG12	2.08	0.52
1:B:266:ASP:OD1	1:B:266:ASP:C	2.47	0.52
1:C:66:GLU:HG3	1:D:62:ARG:HB3	1.89	0.52
1:C:66:GLU:CG	1:D:62:ARG:HB3	2.40	0.52
1:C:129:ARG:NH1	1:C:315:HIS:O	2.43	0.52
1:G:62:ARG:O	1:G:66:GLU:HB2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:THR:OG1	1:C:263:MSE:HE3	2.09	0.52
1:D:192:MSE:HG3	1:D:217:GLU:HB3	1.90	0.52
1:D:323:GLN:HE22	1:D:339:ARG:HA	1.74	0.52
1:G:230:THR:O	1:G:234:LEU:HG	2.10	0.52
1:G:99:LEU:N	1:G:100:PRO:CD	2.73	0.52
1:A:313:LEU:HD23	1:A:348:ALA:HB2	1.92	0.52
1:H:9:VAL:HG21	1:H:72:VAL:HB	1.92	0.52
1:A:264:TRP:HB3	1:A:266:ASP:O	2.10	0.52
1:D:302:THR:HA	1:D:305:GLN:HG3	1.93	0.52
1:G:14:LEU:HD22	1:G:363:VAL:HG23	1.92	0.52
1:B:22:ILE:HD12	1:B:22:ILE:O	2.10	0.51
1:H:9:VAL:HG11	1:H:75:LEU:HD12	1.91	0.51
1:A:133:LYS:O	1:A:320:PHE:HA	2.10	0.51
1:G:360:TRP:HA	1:G:363:VAL:HG12	1.92	0.51
1:H:71:ILE:C	1:H:73:PRO:HD2	2.31	0.51
1:C:99:LEU:N	1:C:100:PRO:CD	2.73	0.51
1:A:8:ARG:HD3	1:A:41:PHE:CD2	2.45	0.51
1:C:49:LEU:O	1:C:108:ALA:HA	2.10	0.51
1:D:271:ALA:O	1:D:276:GLY:HA2	2.11	0.51
1:H:267:VAL:HG22	1:H:294:LEU:HG	1.93	0.51
1:E:177:VAL:HG12	1:E:210:TRP:CH2	2.46	0.51
1:A:177:VAL:HG13	1:A:210:TRP:CZ3	2.46	0.51
1:F:26:ASP:O	1:F:27:ASN:HB2	2.11	0.51
1:B:39:ARG:HG3	1:B:360:TRP:CH2	2.46	0.50
1:B:321:PHE:CE2	1:B:323:GLN:HG2	2.45	0.50
1:C:37:ILE:HD11	1:C:358:MSE:HE2	1.92	0.50
1:H:72:VAL:N	1:H:73:PRO:CD	2.74	0.50
1:A:15:ALA:HB1	1:A:60:PHE:CE1	2.47	0.50
1:A:110:TRP:CD1	1:A:277:ILE:HB	2.46	0.50
1:C:363:VAL:CG2	1:C:364:LYS:N	2.73	0.50
1:G:2:GLU:HA	1:G:2:GLU:OE2	2.11	0.50
1:G:218:TRP:C	1:G:218:TRP:CD1	2.84	0.50
1:B:177:VAL:CG1	1:B:210:TRP:CH2	2.92	0.50
1:E:145:GLU:HA	1:E:148:PHE:CE2	2.46	0.50
1:C:157:HIS:HE2	1:C:327:TYR:HH	1.57	0.50
1:G:301:TYR:HA	1:G:330:PHE:HB3	1.93	0.50
1:H:335:LYS:HD2	1:H:357:GLU:HG2	1.93	0.50
1:D:267:VAL:HG13	1:D:294:LEU:HA	1.93	0.50
1:C:114:GLY:HA2	1:C:124:LEU:HD11	1.92	0.50
1:A:124:LEU:HD22	1:H:124:LEU:CD2	2.42	0.50
1:B:36:ASN:O	1:B:51:ALA:HA	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:VAL:N	1:F:73:PRO:CD	2.75	0.49
1:D:150:TYR:CE1	1:D:154:CYS:SG	3.05	0.49
1:E:313:LEU:CD2	1:E:348:ALA:HB2	2.42	0.49
1:A:72:VAL:N	1:A:73:PRO:CD	2.75	0.49
1:B:321:PHE:HE2	1:B:323:GLN:HG2	1.77	0.49
1:D:9:VAL:HG22	1:D:373:PHE:HB2	1.94	0.49
1:E:138:THR:HG22	1:E:150:TYR:CE1	2.48	0.49
1:H:192:MSE:HE3	1:H:217:GLU:HG2	1.95	0.49
1:A:148:PHE:HB2	1:A:149:PRO:HD3	1.95	0.49
1:H:192:MSE:HG3	1:H:217:GLU:HB3	1.95	0.48
1:C:62:ARG:HB2	1:D:66:GLU:CG	2.43	0.48
1:D:129:ARG:NH1	1:D:312:ALA:O	2.45	0.48
1:E:57:GLU:OE1	1:F:93:ARG:NH1	2.46	0.48
1:H:177:VAL:CG1	1:H:210:TRP:CH2	2.96	0.48
1:H:272:THR:HG21	1:H:304:THR:OG1	2.13	0.48
1:A:57:GLU:O	1:A:59:PHE:N	2.45	0.48
1:C:266:ASP:C	1:C:266:ASP:OD1	2.52	0.48
1:G:267:VAL:HG13	1:G:294:LEU:HA	1.95	0.48
1:E:32:LEU:N	1:E:56:THR:O	2.38	0.48
1:G:72:VAL:N	1:G:73:PRO:CD	2.76	0.48
1:G:296:ILE:HD11	1:G:321:PHE:HA	1.96	0.48
1:H:8:ARG:HB3	1:H:41:PHE:HB2	1.96	0.48
1:C:177:VAL:HG11	1:C:210:TRP:CZ3	2.46	0.48
1:D:163:LYS:HE3	1:D:194:ASP:HB2	1.95	0.48
1:E:199:TYR:HB2	1:E:222:PRO:O	2.13	0.48
1:E:284:PHE:CE1	1:E:311:VAL:HG12	2.49	0.48
1:F:11:LEU:HB3	1:F:65:ILE:CD1	2.43	0.48
1:E:360:TRP:HA	1:E:363:VAL:HG12	1.94	0.48
1:E:190:ARG:NH2	1:E:215:ASN:O	2.45	0.48
1:G:177:VAL:HG11	1:G:210:TRP:CZ3	2.48	0.48
1:H:62:ARG:O	1:H:66:GLU:HB2	2.13	0.48
1:B:148:PHE:HB2	1:B:149:PRO:HD3	1.95	0.48
1:D:302:THR:HA	1:D:305:GLN:CG	2.44	0.48
1:F:129:ARG:NH1	1:F:312:ALA:O	2.46	0.48
1:A:80:PRO:O	1:A:109:ALA:HB1	2.13	0.48
1:B:267:VAL:HG22	1:B:294:LEU:HG	1.96	0.48
1:F:298:SER:OG	1:F:322:GLU:O	2.32	0.48
1:F:272:THR:CG2	1:F:304:THR:HG23	2.43	0.47
1:E:325:TYR:CD1	1:E:326:PRO:HA	2.49	0.47
1:C:140:MSE:HE3	1:C:167:TYR:CE2	2.49	0.47
1:E:321:PHE:CD2	1:E:346:VAL:HG11	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:ASN:N	1:F:18:ASN:HD22	2.12	0.47
1:G:246:GLY:HA3	1:G:268:ARG:HG2	1.95	0.47
1:A:26:ASP:CA	1:A:140:MSE:HE1	2.42	0.47
1:H:129:ARG:NH1	1:H:315:HIS:O	2.47	0.47
1:D:264:TRP:HB3	1:D:266:ASP:O	2.14	0.47
1:F:62:ARG:O	1:F:65:ILE:HG22	2.15	0.47
1:A:313:LEU:CD2	1:A:348:ALA:HB2	2.44	0.47
1:E:75:LEU:O	1:E:78:LYS:HB2	2.14	0.47
1:E:271:ALA:HB2	1:E:280:LEU:HD22	1.96	0.47
1:G:272:THR:HG21	1:G:304:THR:HG23	1.96	0.47
1:H:20:PRO:O	1:H:22:ILE:CD1	2.63	0.47
1:A:133:LYS:HE2	1:A:160:THR:HG21	1.96	0.47
1:B:99:LEU:N	1:B:100:PRO:CD	2.78	0.47
1:F:35:ASN:HB2	1:F:301:TYR:CE2	2.50	0.47
1:D:327:TYR:O	1:D:329:ALA:N	2.48	0.47
1:F:267:VAL:HG13	1:F:294:LEU:HG	1.96	0.47
1:C:169:VAL:O	1:C:170:TYR:C	2.53	0.47
1:D:14:LEU:HD22	1:D:363:VAL:HG23	1.97	0.47
1:D:267:VAL:HG11	1:D:287:ALA:HB2	1.97	0.47
1:H:359:ASP:O	1:H:363:VAL:HG12	2.15	0.47
1:C:68:LEU:O	1:C:72:VAL:HG13	2.15	0.46
1:F:99:LEU:N	1:F:100:PRO:CD	2.78	0.46
1:F:103:SER:N	1:F:104:PRO:CD	2.78	0.46
1:G:323:GLN:HE22	1:G:339:ARG:HA	1.80	0.46
1:D:26:ASP:HB2	1:D:167:TYR:HB3	1.97	0.46
1:D:103:SER:HB2	1:D:104:PRO:HD3	1.97	0.46
1:E:267:VAL:HG11	1:E:287:ALA:HB2	1.97	0.46
1:F:9:VAL:HG22	1:F:373:PHE:HB2	1.98	0.46
1:G:128:ALA:C	1:G:129:ARG:HG3	2.35	0.46
1:A:363:VAL:HG23	1:A:364:LYS:N	2.30	0.46
1:D:177:VAL:CG1	1:D:210:TRP:CH2	2.98	0.46
1:E:72:VAL:N	1:E:73:PRO:CD	2.78	0.46
1:G:177:VAL:CG1	1:G:210:TRP:CH2	2.98	0.46
1:C:36:ASN:ND2	1:C:54:SER:OG	2.48	0.46
1:C:103:SER:N	1:C:104:PRO:CD	2.78	0.46
1:F:83:THR:HG23	1:F:113:LYS:HD2	1.96	0.46
1:G:9:VAL:HG12	1:G:40:LEU:CD2	2.46	0.46
1:G:259:LEU:HD22	1:G:292:LYS:HG3	1.97	0.46
1:B:103:SER:N	1:B:104:PRO:CD	2.78	0.46
1:D:169:VAL:O	1:D:170:TYR:C	2.54	0.46
1:F:120:PRO:HB2	1:F:122:TYR:CE2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:HIS:CD2	1:A:247:ASN:HD22	2.33	0.46
1:D:218:TRP:CD1	1:D:218:TRP:C	2.89	0.46
1:H:28:GLN:NE2	1:H:28:GLN:HA	2.31	0.46
1:H:67:SER:OG	1:H:95:THR:HG21	2.15	0.46
1:H:142:ASP:N	1:H:142:ASP:OD1	2.49	0.46
1:E:251:THR:HG21	1:F:226:TYR:CD2	2.49	0.46
1:H:11:LEU:HD21	1:H:72:VAL:HG11	1.98	0.46
1:A:169:VAL:O	1:A:170:TYR:C	2.54	0.46
1:D:29:GLU:HB2	1:D:57:GLU:CD	2.36	0.46
1:F:99:LEU:O	1:F:103:SER:OG	2.21	0.46
1:B:114:GLY:HA2	1:B:124:LEU:HD11	1.97	0.45
1:C:246:GLY:HA3	1:C:268:ARG:HG2	1.97	0.45
1:G:87:ASN:ND2	1:G:278:THR:HB	2.32	0.45
1:G:176:LEU:O	1:G:180:VAL:HG23	2.15	0.45
1:B:39:ARG:HD2	1:B:41:PHE:CE2	2.52	0.45
1:B:136:ALA:HA	1:B:323:GLN:O	2.17	0.45
1:D:360:TRP:HA	1:D:363:VAL:HG12	1.97	0.45
1:G:228:PHE:CD2	1:G:263:MSE:HE1	2.51	0.45
1:B:8:ARG:HD3	1:B:41:PHE:CD2	2.51	0.45
1:H:133:LYS:HE3	1:H:345:TYR:CZ	2.52	0.45
1:B:264:TRP:HB3	1:B:266:ASP:O	2.16	0.45
1:E:26:ASP:HA	1:E:140:MSE:HE1	1.97	0.45
1:E:42:THR:OG1	1:E:46:THR:HB	2.17	0.45
1:B:124:LEU:HD22	1:C:124:LEU:HD22	1.99	0.45
1:E:53:MSE:HE3	1:E:55:TYR:HD1	1.81	0.45
1:G:227:ASP:OD2	1:G:230:THR:OG1	2.30	0.45
1:A:356:VAL:CG1	1:A:358:MSE:HE3	2.46	0.45
1:B:34:THR:HB	1:B:54:SER:HB2	1.98	0.45
1:C:321:PHE:CE2	1:C:323:GLN:HG2	2.52	0.45
1:G:325:TYR:CD1	1:G:326:PRO:HA	2.52	0.45
1:A:341:ASP:C	1:A:341:ASP:OD1	2.54	0.45
1:C:4:CYS:SG	1:C:116:LYS:NZ	2.88	0.45
1:E:62:ARG:HB2	1:F:66:GLU:CG	2.47	0.45
1:E:177:VAL:HG13	1:E:210:TRP:CZ3	2.52	0.45
1:E:327:TYR:O	1:E:328:GLU:C	2.55	0.45
1:H:140:MSE:HE3	1:H:167:TYR:HD1	1.82	0.45
1:C:72:VAL:N	1:C:73:PRO:CD	2.80	0.45
1:E:62:ARG:CB	1:F:66:GLU:HG2	2.47	0.45
1:F:103:SER:N	1:F:104:PRO:HD2	2.32	0.45
1:A:2:GLU:O	1:A:3:ASP:HB2	2.17	0.44
1:B:169:VAL:O	1:B:169:VAL:CG1	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:SER:O	1:C:374:GLU:HG3	2.16	0.44
1:D:327:TYR:O	1:D:328:GLU:C	2.55	0.44
1:H:332:LEU:O	1:H:333:ALA:HB3	2.17	0.44
1:D:14:LEU:HA	1:D:367:SER:HA	1.98	0.44
1:D:271:ALA:HB2	1:D:280:LEU:CD2	2.47	0.44
1:H:56:THR:HG21	1:H:61:ASP:HB2	1.98	0.44
1:H:261:THR:OG1	1:H:263:MSE:HE3	2.18	0.44
1:H:321:PHE:CE1	1:H:323:GLN:HG2	2.51	0.44
1:H:293:ASN:HA	1:H:317:ASN:HB2	2.00	0.44
1:C:247:ASN:HD21	1:C:297:GLN:HE22	1.65	0.44
1:E:49:LEU:HD21	1:E:360:TRP:HZ2	1.81	0.44
1:H:156:GLU:OE1	1:H:156:GLU:HA	2.18	0.44
1:A:66:GLU:HG3	1:B:62:ARG:HB2	1.99	0.44
1:A:103:SER:N	1:A:104:PRO:CD	2.80	0.44
1:C:148:PHE:HB2	1:C:149:PRO:HD3	2.00	0.44
1:D:52:THR:HG22	1:D:104:PRO:HG3	1.99	0.44
1:A:271:ALA:HB2	1:A:280:LEU:HD22	2.00	0.44
1:E:228:PHE:HB3	1:E:263:MSE:HE2	1.99	0.44
1:E:328:GLU:O	1:E:329:ALA:C	2.56	0.44
1:F:237:ASN:O	1:F:238:THR:HG22	2.18	0.44
1:F:247:ASN:HD21	1:F:297:GLN:NE2	2.16	0.44
1:A:93:ARG:NH1	1:B:57:GLU:OE2	2.51	0.44
1:D:166:CYS:HB2	1:D:173:ASP:OD1	2.18	0.44
1:F:249:LEU:HD12	1:F:249:LEU:N	2.33	0.44
1:B:98:GLY:O	1:B:102:LYS:HG3	2.18	0.44
1:G:15:ALA:HB1	1:G:60:PHE:CE1	2.53	0.44
1:C:129:ARG:NH1	1:C:312:ALA:O	2.51	0.43
1:E:44:ASP:OD2	1:E:116:LYS:CE	2.65	0.43
1:E:280:LEU:HG	1:E:311:VAL:HG11	2.00	0.43
1:F:118:GLY:HA2	1:F:352:ASN:ND2	2.33	0.43
1:G:9:VAL:HG12	1:G:40:LEU:HD23	1.99	0.43
1:G:194:ASP:OD1	1:G:194:ASP:C	2.56	0.43
1:C:94:CYS:O	1:C:95:THR:HB	2.18	0.43
1:F:192:MSE:HG3	1:F:217:GLU:HB3	2.00	0.43
1:F:293:ASN:HA	1:F:317:ASN:HB2	2.00	0.43
1:F:264:TRP:HB3	1:F:266:ASP:O	2.17	0.43
1:G:62:ARG:HB2	1:H:66:GLU:CG	2.48	0.43
1:G:135:TYR:CE1	1:G:322:GLU:HG3	2.53	0.43
1:E:138:THR:HG22	1:E:150:TYR:HE1	1.83	0.43
1:E:267:VAL:HG22	1:E:294:LEU:HG	2.00	0.43
1:C:37:ILE:CD1	1:C:358:MSE:HE2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TRP:CE2	1:C:214:HIS:CE1	3.06	0.43
1:E:19:ALA:O	1:E:21:PRO:HD3	2.18	0.43
1:A:280:LEU:HD23	1:A:311:VAL:HG21	2.00	0.43
1:C:218:TRP:CD1	1:C:218:TRP:C	2.92	0.43
1:C:332:LEU:O	1:C:333:ALA:HB3	2.18	0.43
1:D:83:THR:HG23	1:D:113:LYS:HD2	2.01	0.43
1:F:169:VAL:O	1:F:170:TYR:C	2.57	0.43
1:H:360:TRP:CE3	1:H:363:VAL:HG11	2.54	0.43
1:B:167:TYR:CG	1:B:172:LYS:HE3	2.54	0.43
1:E:267:VAL:HG13	1:E:294:LEU:HA	2.00	0.43
1:G:8:ARG:HD3	1:G:41:PHE:CD2	2.54	0.43
1:A:36:ASN:O	1:A:51:ALA:HA	2.19	0.43
1:A:218:TRP:CD1	1:A:218:TRP:C	2.92	0.43
1:C:163:LYS:HB2	1:C:192:MSE:HB2	2.01	0.43
1:G:140:MSE:HE3	1:G:167:TYR:CD2	2.54	0.43
1:D:163:LYS:NZ	1:D:220:GLU:OE1	2.42	0.43
1:B:177:VAL:HG11	1:B:210:TRP:CZ3	2.52	0.42
1:F:120:PRO:HB2	1:F:122:TYR:CD2	2.54	0.42
1:G:66:GLU:CG	1:H:62:ARG:HB2	2.42	0.42
1:C:49:LEU:HD21	1:C:360:TRP:HZ2	1.84	0.42
1:H:66:GLU:OE2	1:H:66:GLU:HA	2.19	0.42
1:H:177:VAL:HG12	1:H:210:TRP:CH2	2.54	0.42
1:H:218:TRP:CD1	1:H:218:TRP:C	2.93	0.42
1:A:121:LEU:HD12	1:A:124:LEU:HD12	2.01	0.42
1:C:140:MSE:HE3	1:C:167:TYR:CD2	2.54	0.42
1:C:221:ALA:N	1:C:222:PRO:CD	2.83	0.42
1:E:70:THR:O	1:F:58:ASN:ND2	2.50	0.42
1:E:218:TRP:CD1	1:E:218:TRP:C	2.92	0.42
1:A:128:ALA:HB1	1:A:316:ASP:OD1	2.20	0.42
1:C:181:GLU:HG2	1:C:214:HIS:CD2	2.55	0.42
1:A:66:GLU:HG2	1:B:62:ARG:CB	2.49	0.42
1:B:338:ILE:CG2	1:B:346:VAL:CG2	2.97	0.42
1:C:294:LEU:HD23	1:C:295:GLU:N	2.34	0.42
1:D:40:LEU:O	1:D:47:GLU:HA	2.19	0.42
1:D:260:SER:O	1:F:229:LYS:NZ	2.53	0.42
1:A:184:TYR:C	1:A:187:SER:HG	2.20	0.42
1:E:52:THR:HB	1:E:104:PRO:HG3	2.01	0.42
1:H:6:ILE:HD11	1:H:80:PRO:HB3	2.01	0.42
1:H:267:VAL:HG13	1:H:294:LEU:HA	2.01	0.42
1:A:99:LEU:N	1:A:100:PRO:HD2	2.35	0.42
1:C:26:ASP:OD2	1:C:172:LYS:HE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:LEU:CD2	1:D:348:ALA:HB2	2.49	0.42
1:H:119:MSE:HE2	1:H:123:MSE:SE	2.69	0.42
1:A:62:ARG:O	1:A:66:GLU:HB2	2.20	0.42
1:C:247:ASN:ND2	1:C:297:GLN:HE22	2.18	0.42
1:F:349:PRO:HB2	1:F:355:GLY:HA3	2.02	0.42
1:H:120:PRO:HB2	1:H:122:TYR:CE2	2.54	0.42
1:H:321:PHE:HE1	1:H:323:GLN:HG2	1.85	0.42
1:E:103:SER:HB2	1:E:104:PRO:HD3	2.02	0.41
1:F:124:LEU:HD22	1:G:124:LEU:HD22	2.02	0.41
1:G:42:THR:OG1	1:G:46:THR:HB	2.20	0.41
1:A:282:LYS:HB3	1:H:285:ALA:HB1	2.01	0.41
1:C:214:HIS:O	1:C:215:ASN:HB2	2.21	0.41
1:E:3:ASP:OD1	1:E:3:ASP:N	2.53	0.41
1:E:148:PHE:HB2	1:E:149:PRO:HD3	2.01	0.41
1:E:229:LYS:NZ	1:G:260:SER:O	2.49	0.41
1:E:359:ASP:O	1:E:363:VAL:HG12	2.19	0.41
1:B:48:GLY:HA3	1:B:112:ILE:HG13	2.02	0.41
1:F:261:THR:OG1	1:F:263:MSE:HE3	2.19	0.41
1:G:150:TYR:CE1	1:G:154:CYS:SG	3.14	0.41
1:D:113:LYS:CE	1:E:123:MSE:O	2.68	0.41
1:G:48:GLY:HA3	1:G:112:ILE:HG13	2.02	0.41
1:A:18:ASN:N	1:A:18:ASN:ND2	2.67	0.41
1:D:55:TYR:CD1	1:D:55:TYR:N	2.88	0.41
1:D:184:TYR:C	1:D:187:SER:HG	2.23	0.41
1:F:218:TRP:CD1	1:F:218:TRP:C	2.93	0.41
1:G:267:VAL:HG11	1:G:287:ALA:HB2	2.02	0.41
1:H:120:PRO:HB2	1:H:122:TYR:CD2	2.55	0.41
1:G:253:GLN:OE1	1:G:253:GLN:N	2.51	0.41
1:B:95:THR:HG23	1:B:95:THR:O	2.21	0.41
1:B:147:TYR:O	1:B:151:ILE:HG13	2.21	0.41
1:C:138:THR:HG21	1:C:162:ILE:HD11	2.03	0.41
1:D:26:ASP:O	1:D:27:ASN:C	2.59	0.41
1:H:72:VAL:CG2	1:H:73:PRO:HD3	2.51	0.41
1:F:135:TYR:CD1	1:F:135:TYR:C	2.94	0.41
1:G:264:TRP:HB3	1:G:266:ASP:O	2.21	0.41
1:H:35:ASN:HB2	1:H:301:TYR:CE1	2.56	0.41
1:B:28:GLN:HA	1:B:28:GLN:NE2	2.35	0.41
1:C:39:ARG:HD2	1:C:41:PHE:CZ	2.56	0.41
1:D:117:ALA:HB1	1:E:117:ALA:HB1	2.03	0.41
1:E:14:LEU:HD21	1:E:37:ILE:HD12	2.03	0.41
1:E:169:VAL:O	1:E:170:TYR:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:TRP:HB2	1:E:241:GLU:O	2.20	0.41
1:G:103:SER:N	1:G:104:PRO:CD	2.83	0.41
1:G:237:ASN:N	1:G:237:ASN:ND2	2.66	0.41
1:D:65:ILE:HG23	1:D:66:GLU:N	2.36	0.41
1:F:338:ILE:CG2	1:F:346:VAL:CG2	2.99	0.41
1:A:117:ALA:HB1	1:H:117:ALA:HB1	2.03	0.40
1:A:301:TYR:HA	1:A:330:PHE:HB3	2.02	0.40
1:C:267:VAL:HG13	1:C:294:LEU:HA	2.01	0.40
1:D:22:ILE:HG13	1:D:33:TYR:CE1	2.56	0.40
1:B:360:TRP:O	1:B:364:LYS:CG	2.70	0.40
1:G:28:GLN:O	1:G:29:GLU:C	2.59	0.40
1:A:107:ILE:HG12	1:A:277:ILE:HG12	2.02	0.40
1:C:8:ARG:HD3	1:C:41:PHE:CE1	2.55	0.40
1:C:264:TRP:HB3	1:C:266:ASP:O	2.21	0.40
1:D:29:GLU:HB2	1:D:57:GLU:OE2	2.21	0.40
1:F:39:ARG:HG3	1:F:360:TRP:CH2	2.55	0.40
1:F:363:VAL:CG2	1:F:364:LYS:N	2.84	0.40
1:G:82:MSE:HA	1:G:82:MSE:HE2	2.02	0.40
1:G:218:TRP:CZ2	1:G:268:ARG:NH2	2.89	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	373/384 (97%)	353 (95%)	18 (5%)	2 (0%)	29 61
1	B	373/384 (97%)	359 (96%)	14 (4%)	0	100 100
1	C	372/384 (97%)	351 (94%)	19 (5%)	2 (0%)	29 61
1	D	373/384 (97%)	348 (93%)	22 (6%)	3 (1%)	19 49
1	E	373/384 (97%)	353 (95%)	18 (5%)	2 (0%)	29 61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	373/384 (97%)	352 (94%)	21 (6%)	0	100 100
1	G	373/384 (97%)	355 (95%)	17 (5%)	1 (0%)	41 72
1	H	372/384 (97%)	357 (96%)	15 (4%)	0	100 100
All	All	2982/3072 (97%)	2828 (95%)	144 (5%)	10 (0%)	41 72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	328	GLU
1	D	170	TYR
1	E	328	GLU
1	C	95	THR
1	D	196	ALA
1	G	375	GLU
1	A	170	TYR
1	C	24	TRP
1	A	76	ILE
1	E	126	GLY

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	309/307 (101%)	291 (94%)	18 (6%)	20 50
1	B	312/307 (102%)	298 (96%)	14 (4%)	27 60
1	C	309/307 (101%)	295 (96%)	14 (4%)	27 60
1	D	308/307 (100%)	296 (96%)	12 (4%)	32 66
1	E	310/307 (101%)	297 (96%)	13 (4%)	30 63
1	F	308/307 (100%)	293 (95%)	15 (5%)	25 57
1	G	309/307 (101%)	293 (95%)	16 (5%)	23 55
1	H	307/307 (100%)	294 (96%)	13 (4%)	30 63
All	All	2472/2456 (101%)	2357 (95%)	115 (5%)	27 59

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	18	ASN
1	A	22	ILE
1	A	24	TRP
1	A	28	GLN
1	A	39	ARG
1	A	55	TYR
1	A	129	ARG
1	A	142	ASP
1	A	156	GLU
1	A	187	SER
1	A	192	MSE
1	A	206	LYS
1	A	218	TRP
1	A	253	GLN
1	A	267	VAL
1	A	299	MSE
1	A	302	THR
1	B	5	ARG
1	B	9	VAL
1	B	14	LEU
1	B	17	GLU
1	B	39	ARG
1	B	85	GLU
1	B	93	ARG
1	B	129	ARG
1	B	137	SER
1	B	192	MSE
1	B	263	MSE
1	B	267	VAL
1	B	302	THR
1	B	363	VAL
1	C	7	SER
1	C	9	VAL
1	C	14	LEU
1	C	53	MSE
1	C	55	TYR
1	C	85	GLU
1	C	93	ARG
1	C	129	ARG
1	C	137	SER
1	C	162	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	163	LYS
1	C	192	MSE
1	C	267	VAL
1	C	269	GLN
1	D	14	LEU
1	D	28	GLN
1	D	55	TYR
1	D	66	GLU
1	D	85	GLU
1	D	93	ARG
1	D	119	MSE
1	D	129	ARG
1	D	192	MSE
1	D	218	TRP
1	D	267	VAL
1	D	363	VAL
1	E	2[A]	GLU
1	E	2[B]	GLU
1	E	14	LEU
1	E	24	TRP
1	E	32	LEU
1	E	93	ARG
1	E	95	THR
1	E	129	ARG
1	E	130	THR
1	E	192	MSE
1	E	218	TRP
1	E	267	VAL
1	E	363	VAL
1	F	14	LEU
1	F	22	ILE
1	F	24	TRP
1	F	39	ARG
1	F	53	MSE
1	F	55	TYR
1	F	88	ASN
1	F	93	ARG
1	F	95	THR
1	F	129	ARG
1	F	162	ILE
1	F	192	MSE
1	F	207	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	213	ARG
1	F	218	TRP
1	G	2	GLU
1	G	3	ASP
1	G	14	LEU
1	G	24	TRP
1	G	28	GLN
1	G	32	LEU
1	G	53	MSE
1	G	55	TYR
1	G	63	CYS
1	G	88	ASN
1	G	93	ARG
1	G	129	ARG
1	G	192	MSE
1	G	213	ARG
1	G	218	TRP
1	G	237	ASN
1	H	14	LEU
1	H	28	GLN
1	H	39	ARG
1	H	44	ASP
1	H	85	GLU
1	H	119	MSE
1	H	129	ARG
1	H	142	ASP
1	H	192	MSE
1	H	206	LYS
1	H	218	TRP
1	H	265	SER
1	H	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	28	GLN
1	A	87	ASN
1	A	88	ASN
1	A	245	HIS
1	A	247	ASN
1	A	297	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	27	ASN
1	B	28	GLN
1	B	215	ASN
1	B	290	HIS
1	C	28	GLN
1	C	36	ASN
1	C	58	ASN
1	C	165	HIS
1	C	247	ASN
1	C	290	HIS
1	C	297	GLN
1	D	323	GLN
1	E	36	ASN
1	F	18	ASN
1	F	36	ASN
1	F	88	ASN
1	F	247	ASN
1	F	297	GLN
1	G	237	ASN
1	G	247	ASN
1	G	257	HIS
1	G	279	GLN
1	G	297	GLN
1	G	323	GLN
1	H	27	ASN
1	H	297	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 monosaccharides 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	363/384 (94%)	-0.36	1 (0%) 94 93	50, 78, 108, 151	0
1	B	363/384 (94%)	-0.42	0 100 100	47, 68, 101, 145	0
1	C	362/384 (94%)	-0.41	2 (0%) 89 86	48, 74, 109, 159	0
1	D	363/384 (94%)	-0.18	4 (1%) 80 75	53, 89, 122, 155	0
1	E	362/384 (94%)	-0.13	5 (1%) 75 70	57, 92, 116, 152	0
1	F	363/384 (94%)	-0.36	0 100 100	56, 87, 115, 146	0
1	G	363/384 (94%)	-0.15	5 (1%) 75 70	56, 87, 113, 146	0
1	H	362/384 (94%)	-0.11	10 (2%) 53 43	58, 92, 118, 155	0
All	All	2901/3072 (94%)	-0.27	27 (0%) 84 80	47, 84, 116, 159	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	27	ASN	5.0
1	A	27	ASN	3.9
1	H	186	THR	3.4
1	E	28[A]	GLN	3.1
1	H	248	CYS	3.0
1	G	6	ILE	3.0
1	H	372	VAL	3.0
1	H	60	PHE	2.8
1	C	27	ASN	2.7
1	E	60	PHE	2.7
1	D	27	ASN	2.6
1	E	325	TYR	2.5
1	H	184	TYR	2.5
1	G	248	CYS	2.5
1	D	40	LEU	2.5
1	C	29	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	95	THR	2.4
1	G	76	ILE	2.3
1	H	187	SER	2.3
1	G	27	ASN	2.2
1	D	159	PHE	2.2
1	D	149	PRO	2.1
1	H	12	TYR	2.1
1	G	75	LEU	2.1
1	H	327	TYR	2.1
1	H	167	TYR	2.1
1	H	27	ASN	2.1

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 monosaccharides 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.