



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:06 AM UTC

PDB ID : 4BAX / pdb_00004bax
Title : Crystal structure of glutamine synthetase from *Streptomyces coelicolor*
Authors : Zeth, K.
Deposited on : 2012-09-16
Resolution : 2.55 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

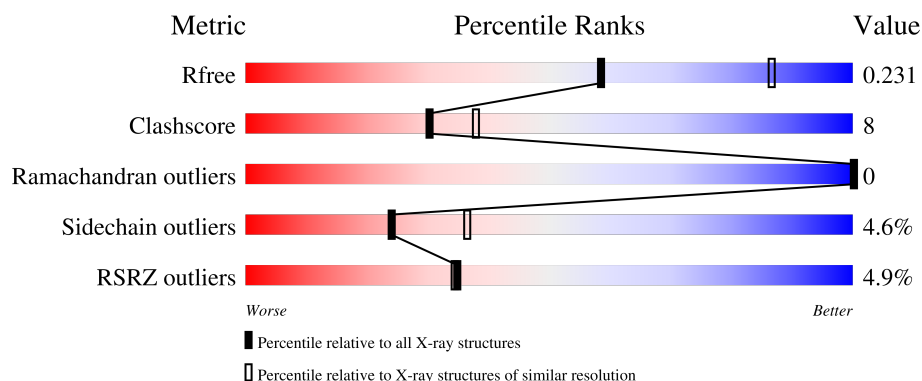
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.



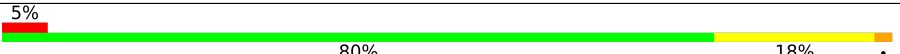
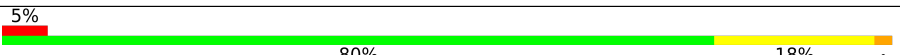
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	344	5% 78% 20% .
1	B	344	3% 80% 17% .
1	C	344	6% 81% 18% .
1	D	344	5% 75% 23% .
1	E	344	6% 81% 16% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	344	 5%78%21%.
1	G	344	 5%81%18%.
1	H	344	 5%78%22%.
1	I	344	 5%80%18%.
1	J	344	 5%80%18%.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27354 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	B	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	C	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	D	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	E	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	F	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	G	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	H	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	I	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			
1	J	344	Total	C	N	O	S	0	0	0
			2627	1658	443	514	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	HIS	-	expression tag	UNP Q9X958
B	6	HIS	-	expression tag	UNP Q9X958
C	6	HIS	-	expression tag	UNP Q9X958
D	6	HIS	-	expression tag	UNP Q9X958
E	6	HIS	-	expression tag	UNP Q9X958
F	6	HIS	-	expression tag	UNP Q9X958
G	6	HIS	-	expression tag	UNP Q9X958
H	6	HIS	-	expression tag	UNP Q9X958
I	6	HIS	-	expression tag	UNP Q9X958

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	6	HIS	-	expression tag	UNP Q9X958

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	B	1	Total Na 1 1	0	0
2	D	2	Total Na 2 2	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0

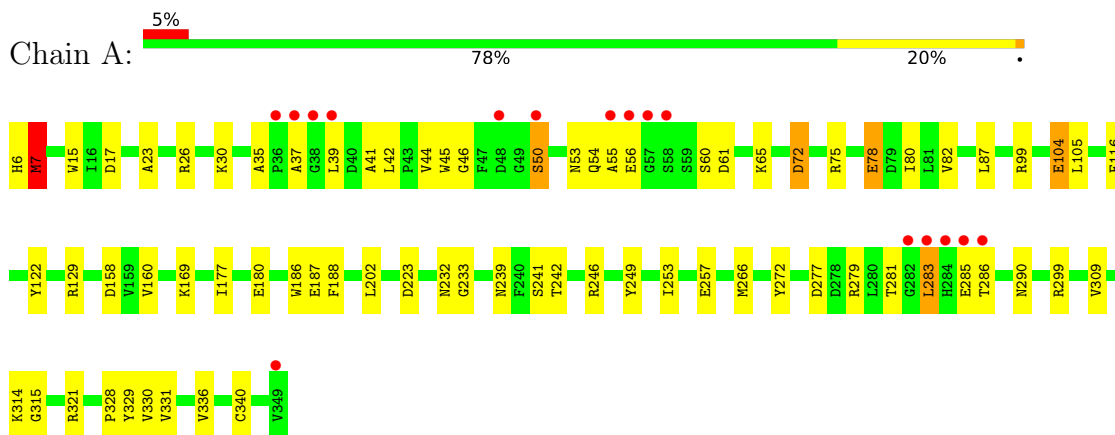
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	120	Total O 120 120	0	0
3	B	95	Total O 95 95	0	0
3	C	127	Total O 127 127	0	0
3	D	107	Total O 107 107	0	0
3	E	91	Total O 91 91	0	0
3	F	114	Total O 114 114	0	0
3	G	116	Total O 116 116	0	0
3	H	95	Total O 95 95	0	0
3	I	106	Total O 106 106	0	0
3	J	105	Total O 105 105	0	0

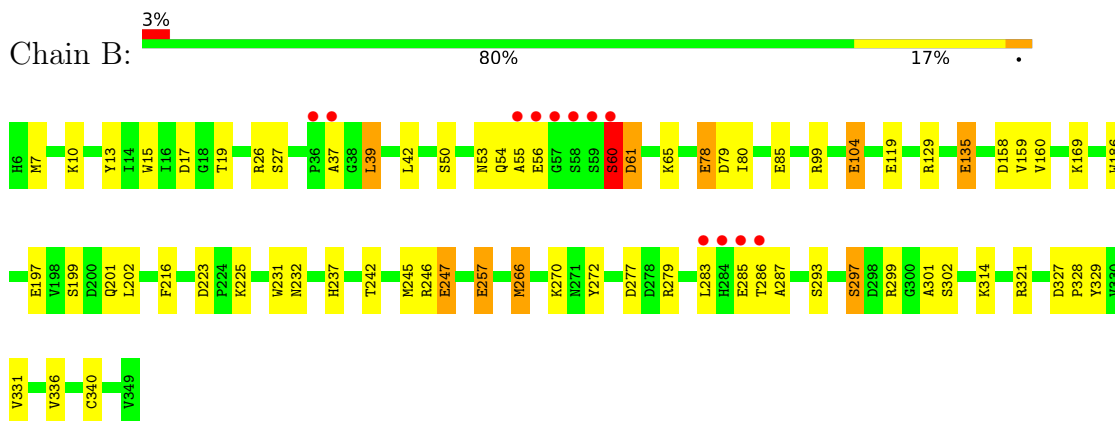
3 Residue-property plots [i](#)

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.

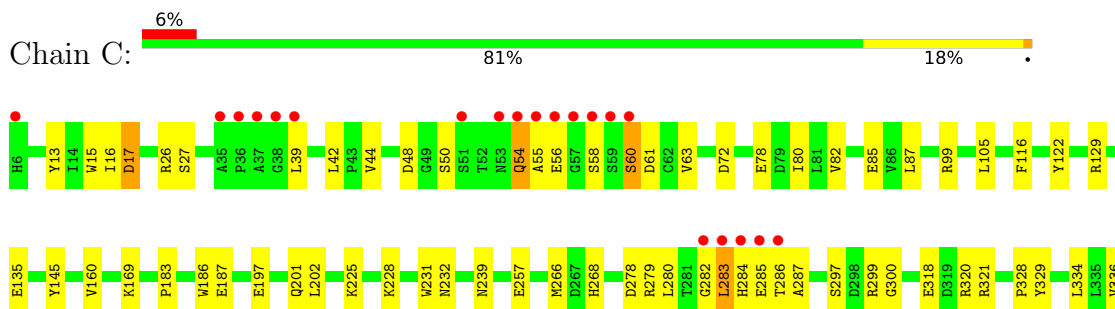
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE

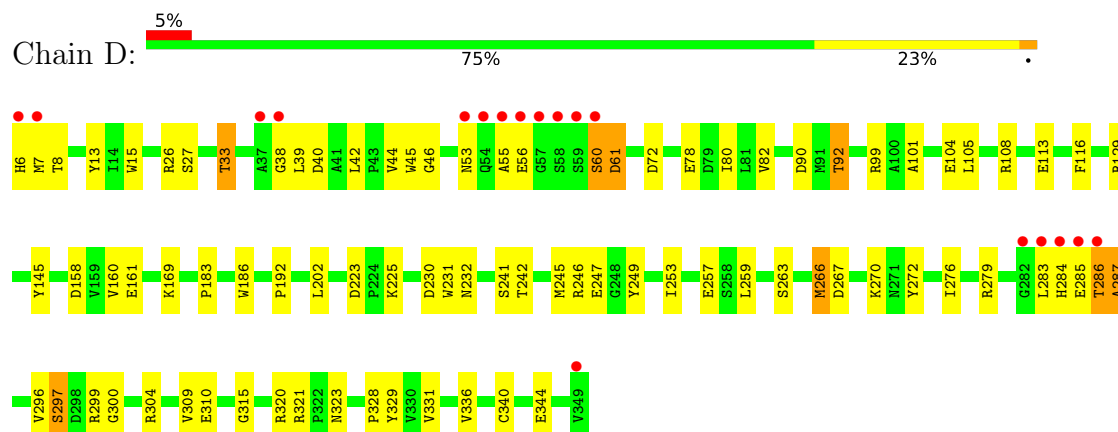


• Molecule 1: GLUTAMINE SYNTHETASE

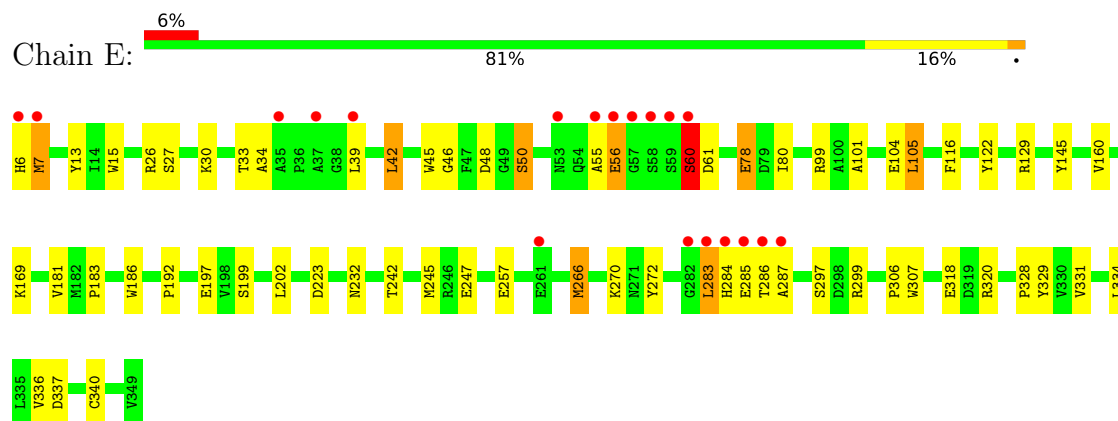




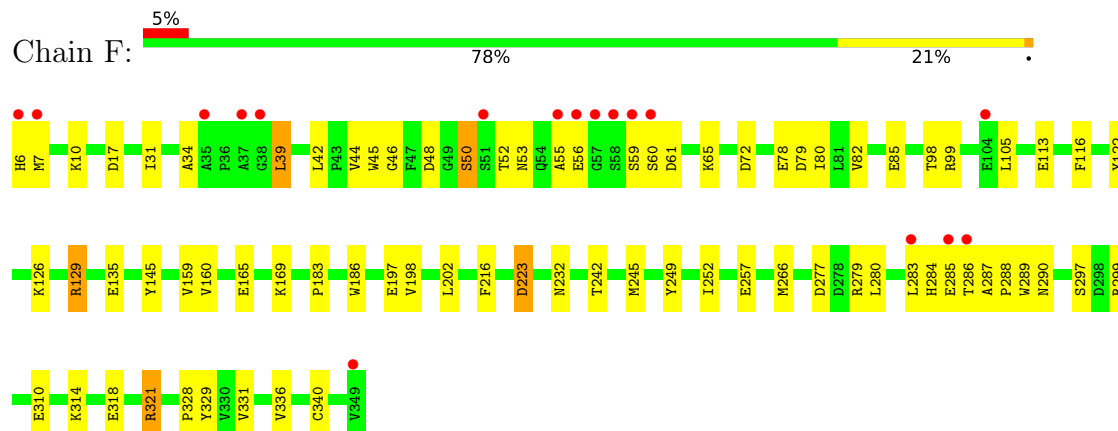
- Molecule 1: GLUTAMINE SYNTHETASE



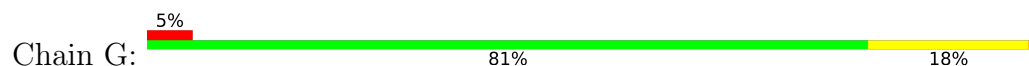
- Molecule 1: GLUTAMINE SYNTHETASE

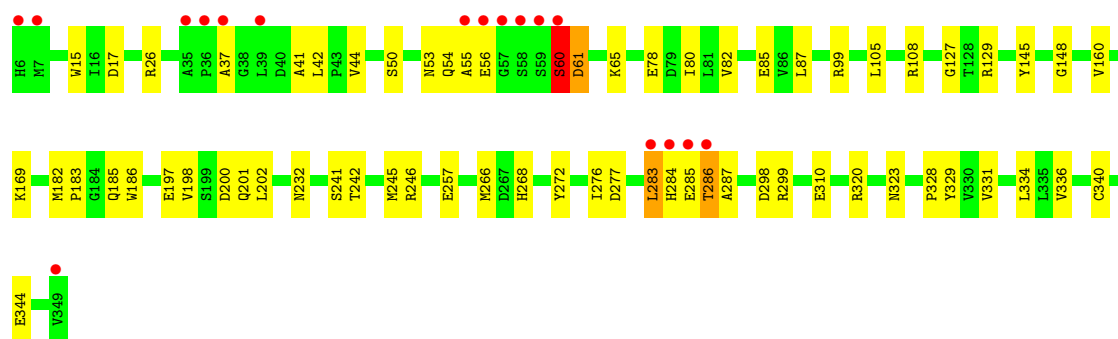


- Molecule 1: GLUTAMINE SYNTHETASE

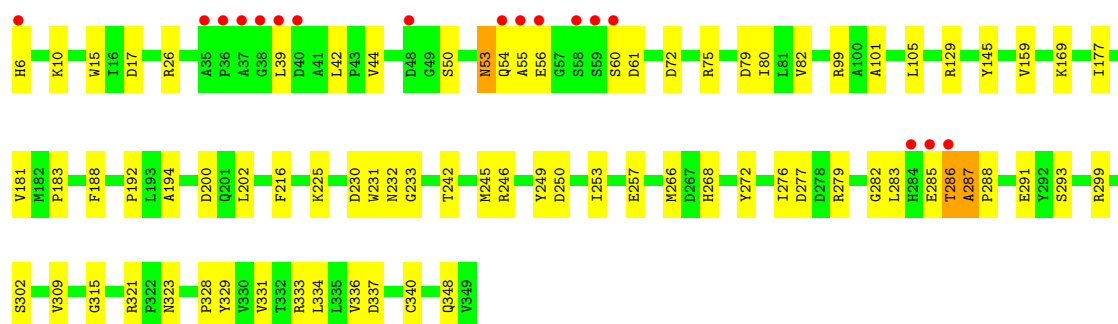
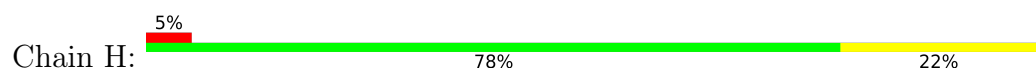


- Molecule 1: GLUTAMINE SYNTHETASE

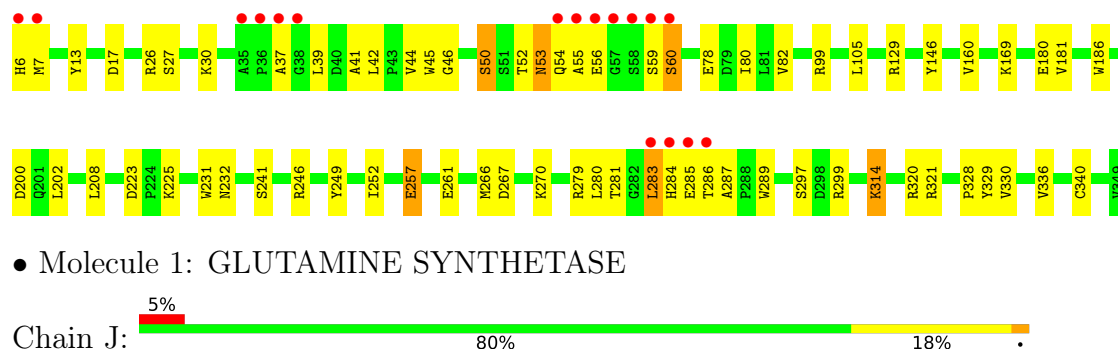
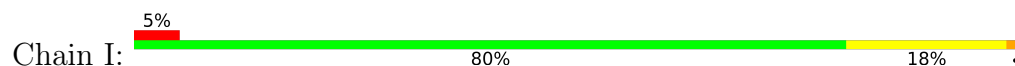




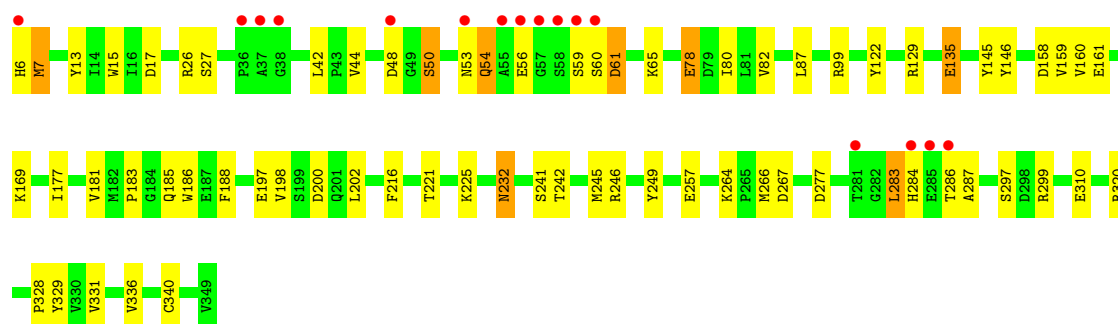
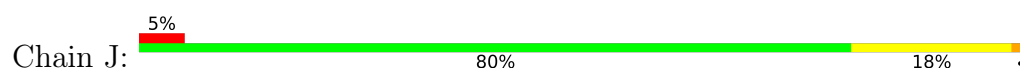
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.12Å 113.00Å 194.44Å 90.00° 98.55° 90.00°	Depositor
Resolution (Å)	25.00 – 2.55 25.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.55) 99.5 (25.00-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.206 , 0.236 0.201 , 0.231	Depositor DCC
R_{free} test set	6745 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27354	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 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

Bond lengths and bond angles in the following residue types are not validated in this section:
NA

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	0.58	0/2694	0.93	9/3667 (0.2%)
1	B	0.56	0/2694	0.97	9/3667 (0.2%)
1	C	0.59	0/2694	0.96	6/3667 (0.2%)
1	D	0.58	0/2694	0.95	8/3667 (0.2%)
1	E	0.59	0/2694	1.00	11/3667 (0.3%)
1	F	0.55	0/2694	0.95	8/3667 (0.2%)
1	G	0.60	0/2694	0.96	4/3667 (0.1%)
1	H	0.56	0/2694	0.94	5/3667 (0.1%)
1	I	0.57	0/2694	0.97	9/3667 (0.2%)
1	J	0.55	0/2694	0.95	7/3667 (0.2%)
All	All	0.57	0/26940	0.96	76/36670 (0.2%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	60	SER	N-CA-C	8.21	122.12	108.73
1	E	42	LEU	CA-C-N	7.61	127.61	119.78
1	E	42	LEU	C-N-CA	7.61	127.61	119.78
1	H	61	ASP	N-CA-C	-7.51	97.15	109.40
1	E	61	ASP	N-CA-C	-7.44	97.27	109.40
1	B	223	ASP	CA-C-N	6.94	126.55	119.19
1	B	223	ASP	C-N-CA	6.94	126.55	119.19
1	D	60	SER	N-CA-C	6.86	119.69	108.52
1	A	61	ASP	N-CA-C	-6.76	98.39	109.40
1	A	7	MET	N-CA-C	6.74	120.59	110.14
1	G	61	ASP	N-CA-C	-6.73	98.44	109.40
1	E	56	GLU	CA-CB-CG	6.61	127.32	114.10
1	E	223	ASP	CA-C-N	6.52	126.10	119.19
1	E	223	ASP	C-N-CA	6.52	126.10	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	194	ALA	CA-C-N	6.33	125.56	118.97
1	H	194	ALA	C-N-CA	6.33	125.56	118.97
1	B	42	LEU	CA-C-N	6.32	126.24	119.85
1	B	42	LEU	C-N-CA	6.32	126.24	119.85
1	D	223	ASP	CA-C-N	6.22	125.78	119.19
1	D	223	ASP	C-N-CA	6.22	125.78	119.19
1	A	72	ASP	CA-C-N	6.20	125.76	119.19
1	A	72	ASP	C-N-CA	6.20	125.76	119.19
1	I	54	GLN	N-CA-C	-6.11	105.14	112.59
1	B	65	LYS	CA-C-N	6.09	126.41	119.83
1	B	65	LYS	C-N-CA	6.09	126.41	119.83
1	F	321	ARG	CA-C-N	-6.03	113.73	119.76
1	F	321	ARG	C-N-CA	-6.03	113.73	119.76
1	J	61	ASP	N-CA-C	-5.99	99.63	109.40
1	F	72	ASP	CA-C-N	5.99	125.54	119.19
1	F	72	ASP	C-N-CA	5.99	125.54	119.19
1	C	61	ASP	N-CA-C	-5.98	99.65	109.40
1	B	60	SER	N-CA-C	5.97	118.26	108.52
1	E	287	ALA	CA-C-N	-5.93	113.86	119.85
1	E	287	ALA	C-N-CA	-5.93	113.86	119.85
1	B	247	GLU	N-CA-C	5.92	118.97	111.69
1	D	247	GLU	N-CA-C	5.86	118.89	111.69
1	F	65	LYS	CA-C-N	5.83	126.12	119.83
1	F	65	LYS	C-N-CA	5.83	126.12	119.83
1	E	56	GLU	N-CA-C	-5.82	103.63	111.54
1	B	61	ASP	N-CA-C	-5.80	99.94	109.40
1	H	287	ALA	N-CA-C	-5.79	101.54	110.58
1	I	59	SER	N-CA-C	5.73	122.94	113.89
1	J	42	LEU	CA-C-N	5.71	125.47	119.76
1	J	42	LEU	C-N-CA	5.71	125.47	119.76
1	J	7	MET	N-CA-C	5.64	118.88	110.14
1	I	330	VAL	N-CA-C	5.47	115.67	110.53
1	D	61	ASP	N-CA-C	-5.46	100.49	109.40
1	E	60	SER	N-CA-C	5.46	117.63	108.73
1	A	223	ASP	CA-C-N	5.43	124.95	119.19
1	A	223	ASP	C-N-CA	5.43	124.95	119.19
1	C	60	SER	N-CA-C	5.38	117.28	108.52
1	D	287	ALA	N-CA-C	-5.36	97.95	109.81
1	D	72	ASP	CA-C-N	5.35	124.86	119.19
1	D	72	ASP	C-N-CA	5.35	124.86	119.19
1	F	223	ASP	CA-C-N	5.33	124.84	119.19
1	F	223	ASP	C-N-CA	5.33	124.84	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	223	ASP	CA-C-N	5.32	124.83	119.19
1	I	223	ASP	C-N-CA	5.32	124.83	119.19
1	H	286	THR	CA-CB-CG2	5.32	119.54	110.50
1	A	281	THR	N-CA-C	-5.29	101.94	110.14
1	J	225	LYS	CA-C-N	5.23	124.86	119.05
1	J	225	LYS	C-N-CA	5.23	124.86	119.05
1	E	247	GLU	N-CA-C	5.22	118.11	111.69
1	I	287	ALA	CA-C-N	-5.21	114.58	119.85
1	I	287	ALA	C-N-CA	-5.21	114.58	119.85
1	G	60	SER	N-CA-C	5.18	117.18	108.73
1	C	72	ASP	CA-C-N	5.17	124.67	119.19
1	C	72	ASP	C-N-CA	5.17	124.67	119.19
1	A	283	LEU	N-CA-C	5.16	116.59	111.07
1	J	54	GLN	N-CA-C	-5.16	106.30	112.59
1	C	54	GLN	N-CA-C	-5.14	106.32	112.59
1	C	17	ASP	N-CA-C	5.14	117.83	109.86
1	G	42	LEU	N-CA-C	5.08	116.06	109.65
1	A	330	VAL	N-CA-C	5.06	115.29	110.53
1	I	281	THR	N-CA-C	-5.01	102.37	110.14
1	G	287	ALA	N-CA-C	-5.00	98.76	109.81

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	2627	0	2511	42	0
1	B	2627	0	2511	48	0
1	C	2627	0	2511	39	0
1	D	2627	0	2511	54	0
1	E	2627	0	2511	33	0
1	F	2627	0	2511	52	0
1	G	2627	0	2511	41	0
1	H	2627	0	2511	51	0
1	I	2627	0	2511	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2627	0	2511	43	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
3	A	120	0	0	10	0
3	B	95	0	0	15	0
3	C	127	0	0	11	0
3	D	107	0	0	8	0
3	E	91	0	0	4	0
3	F	114	0	0	15	0
3	G	116	0	0	9	0
3	H	95	0	0	11	0
3	I	106	0	0	7	0
3	J	105	0	0	8	0
All	All	27354	0	25110	431	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 8.

All (431) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASN:ND2	3:D:2006:HOH:O	1.94	1.00
1:F:98:THR:O	3:F:2040:HOH:O	1.83	0.95
1:G:284:HIS:O	3:G:2105:HOH:O	1.85	0.94
1:I:53:ASN:OD1	3:I:2008:HOH:O	1.85	0.93
1:J:53:ASN:ND2	3:J:2005:HOH:O	2.04	0.90
1:A:55:ALA:O	3:A:2016:HOH:O	1.90	0.89
1:H:192:PRO:O	3:H:2060:HOH:O	1.92	0.88
3:C:2034:HOH:O	1:D:161:GLU:OE1	1.89	0.88
1:F:197:GLU:OE1	3:F:2084:HOH:O	1.93	0.87
1:G:127:GLY:O	3:G:2043:HOH:O	1.94	0.86
1:F:318:GLU:OE2	3:F:2046:HOH:O	1.95	0.85
3:C:2024:HOH:O	1:D:297:SER:O	1.93	0.84
1:F:85:GLU:OE1	3:F:2036:HOH:O	1.95	0.83
1:C:286:THR:HG23	1:C:287:ALA:H	1.42	0.83
1:J:197:GLU:OE1	3:J:2073:HOH:O	1.96	0.83
1:B:257:GLU:OE2	3:B:2081:HOH:O	1.97	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLU:OE1	3:B:2026:HOH:O	1.97	0.81
1:A:7:MET:HE1	1:A:78:GLU:HG2	1.60	0.81
1:I:55:ALA:HB2	1:I:60:SER:HB3	1.63	0.81
1:G:285:GLU:OE2	1:G:320:ARG:NH2	2.13	0.80
1:A:72:ASP:OD2	3:A:2022:HOH:O	1.98	0.80
1:B:60:SER:O	3:B:2013:HOH:O	2.01	0.78
1:E:7:MET:HE1	1:E:78:GLU:HG2	1.66	0.78
1:G:85:GLU:OE1	3:G:2026:HOH:O	2.02	0.77
1:E:285:GLU:OE2	1:E:320:ARG:NH2	2.17	0.76
1:B:135:GLU:O	3:B:2041:HOH:O	2.04	0.76
1:B:135:GLU:OE2	3:B:2042:HOH:O	2.03	0.76
1:B:301:ALA:O	3:B:2091:HOH:O	2.02	0.75
1:H:286:THR:O	3:H:2086:HOH:O	2.05	0.74
1:A:56:GLU:O	3:A:2017:HOH:O	2.05	0.74
1:C:187:GLU:OE1	3:C:2059:HOH:O	2.04	0.74
1:F:135:GLU:OE2	3:F:2058:HOH:O	2.06	0.74
1:G:53:ASN:OD1	3:G:2017:HOH:O	2.06	0.74
1:F:113:GLU:OE1	3:F:2045:HOH:O	2.04	0.74
1:I:50:SER:HA	1:I:56:GLU:H	1.53	0.73
1:G:284:HIS:CG	1:G:285:GLU:H	2.07	0.72
3:F:2015:HOH:O	1:G:148:GLY:O	2.06	0.72
1:F:53:ASN:ND2	3:F:2021:HOH:O	2.17	0.71
1:C:285:GLU:OE2	1:C:320:ARG:NH2	2.18	0.71
1:F:99:ARG:HG3	1:F:329:TYR:CE1	2.26	0.71
1:G:298:ASP:OD2	3:G:2109:HOH:O	2.09	0.70
1:I:279:ARG:NH2	1:I:321:ARG:O	2.24	0.70
1:D:259:LEU:O	3:D:2096:HOH:O	2.08	0.70
1:D:158:ASP:O	3:D:2071:HOH:O	2.08	0.70
1:C:99:ARG:HG3	1:C:329:TYR:CE1	2.27	0.70
1:I:180:GLU:OE1	3:I:2046:HOH:O	2.09	0.70
1:E:181:VAL:O	3:E:2051:HOH:O	2.10	0.69
1:G:53:ASN:HA	1:G:56:GLU:HG2	1.73	0.69
1:C:58:SER:O	3:C:2023:HOH:O	2.11	0.69
1:I:99:ARG:HG3	1:I:329:TYR:CE1	2.28	0.69
1:B:297:SER:O	3:B:2090:HOH:O	2.10	0.68
1:J:329:TYR:O	3:J:2037:HOH:O	2.11	0.68
1:A:180:GLU:O	3:A:2060:HOH:O	2.11	0.68
1:B:237:HIS:HD2	3:B:2033:HOH:O	1.77	0.68
1:H:181:VAL:O	3:H:2049:HOH:O	2.12	0.68
1:E:50:SER:HA	1:E:56:GLU:H	1.57	0.68
1:A:23:ALA:O	3:A:2006:HOH:O	2.12	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:GLY:O	3:H:2086:HOH:O	2.13	0.67
1:F:59:SER:O	3:F:2025:HOH:O	2.10	0.67
1:A:187:GLU:OE1	3:A:2042:HOH:O	2.12	0.67
1:C:16:ILE:O	3:C:2006:HOH:O	2.11	0.67
1:F:299:ARG:NH2	1:J:61:ASP:OD1	2.24	0.67
1:C:135:GLU:O	3:C:2066:HOH:O	2.13	0.67
1:C:286:THR:CG2	1:C:287:ALA:H	2.06	0.67
1:D:284:HIS:CG	1:D:285:GLU:H	2.11	0.67
1:C:282:GLY:O	3:C:2118:HOH:O	2.12	0.67
1:A:99:ARG:HG3	1:A:329:TYR:CE1	2.30	0.67
1:E:306:PRO:HA	3:E:2088:HOH:O	1.96	0.66
1:F:126:LYS:NZ	3:F:2052:HOH:O	2.29	0.66
1:G:197:GLU:OE1	3:G:2067:HOH:O	2.13	0.66
1:H:286:THR:HG23	1:H:287:ALA:H	1.60	0.66
1:D:101:ALA:O	1:D:104:GLU:HG2	1.95	0.66
1:I:225:LYS:NZ	1:I:231:TRP:O	2.28	0.66
1:G:310:GLU:OE2	3:G:2112:HOH:O	2.13	0.65
1:I:50:SER:HA	1:I:55:ALA:HB3	1.78	0.65
1:F:165:GLU:OE2	3:F:2076:HOH:O	2.14	0.65
1:C:286:THR:HG23	1:C:287:ALA:N	2.12	0.64
1:I:286:THR:OG1	3:I:2085:HOH:O	2.11	0.64
1:B:286:THR:HB	3:B:2091:HOH:O	1.96	0.64
1:H:39:LEU:HA	1:H:42:LEU:HD12	1.80	0.64
1:H:55:ALA:HB2	1:H:60:SER:HB3	1.79	0.64
1:J:185:GLN:OE1	3:J:2071:HOH:O	2.15	0.64
1:B:119:GLU:HG2	3:B:2035:HOH:O	1.97	0.64
1:I:6:HIS:CD2	1:I:7:MET:H	2.15	0.64
1:F:288:PRO:HB2	1:F:290:ASN:OD1	1.99	0.63
1:C:48:ASP:OD1	1:D:299:ARG:NH1	2.32	0.63
1:E:99:ARG:HG3	1:E:329:TYR:CE1	2.33	0.63
1:G:53:ASN:ND2	3:G:2005:HOH:O	2.33	0.62
1:J:99:ARG:HG3	1:J:329:TYR:CE1	2.34	0.62
1:C:279:ARG:NH2	1:C:321:ARG:O	2.33	0.62
1:A:233:GLY:O	3:A:2043:HOH:O	2.16	0.61
1:H:99:ARG:HG3	1:H:329:TYR:CE1	2.35	0.61
1:I:26:ARG:NH1	1:J:146:TYR:O	2.32	0.61
1:I:202:LEU:HD23	1:I:328:PRO:HB3	1.82	0.61
1:C:39:LEU:HA	1:C:42:LEU:HD12	1.82	0.61
1:B:99:ARG:HG3	1:B:329:TYR:CE1	2.35	0.60
1:E:202:LEU:HD23	1:E:328:PRO:HB3	1.83	0.60
1:I:53:ASN:HA	1:I:56:GLU:HG3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:O	1:D:33:THR:OG1	2.18	0.59
3:G:2020:HOH:O	1:H:299:ARG:NH2	2.24	0.59
1:H:230:ASP:OD1	3:H:2075:HOH:O	2.16	0.59
1:H:286:THR:CG2	1:H:287:ALA:H	2.16	0.59
1:D:230:ASP:OD1	3:D:2092:HOH:O	2.16	0.59
1:A:53:ASN:HA	1:A:56:GLU:HG2	1.85	0.59
1:H:145:TYR:CD2	1:H:183:PRO:HD3	2.38	0.59
1:C:286:THR:O	3:C:2118:HOH:O	2.16	0.58
1:G:99:ARG:HG3	1:G:329:TYR:CE1	2.38	0.58
1:I:241:SER:OG	1:I:246:ARG:NH1	2.35	0.58
1:C:201:GLN:NE2	3:C:2090:HOH:O	2.29	0.58
1:C:50:SER:HA	1:C:55:ALA:HB3	1.85	0.58
3:A:2014:HOH:O	1:B:299:ARG:NH1	2.37	0.58
1:B:286:THR:OG1	1:B:287:ALA:N	2.35	0.58
1:E:39:LEU:HA	1:E:42:LEU:HD12	1.85	0.58
1:C:85:GLU:OE1	3:C:2040:HOH:O	2.17	0.58
1:H:105:LEU:HD22	1:H:333:ARG:HG2	1.84	0.58
1:J:221:THR:O	3:J:2048:HOH:O	2.18	0.58
1:D:53:ASN:HA	1:D:56:GLU:HG2	1.85	0.57
1:E:45:TRP:CD1	1:E:46:GLY:H	2.22	0.57
1:D:55:ALA:HA	3:D:2023:HOH:O	2.03	0.57
1:F:6:HIS:HE1	1:F:34:ALA:C	2.13	0.56
1:D:99:ARG:HG3	1:D:329:TYR:CE1	2.41	0.56
1:F:284:HIS:N	3:F:2112:HOH:O	2.21	0.56
1:H:233:GLY:O	3:H:2034:HOH:O	2.18	0.56
1:D:61:ASP:OD1	1:E:299:ARG:NH2	2.32	0.56
1:A:299:ARG:NE	1:E:48:ASP:OD1	2.39	0.56
1:J:336:VAL:O	1:J:340:CYS:HB2	2.06	0.56
1:F:53:ASN:HA	1:F:56:GLU:HG3	1.88	0.56
1:B:50:SER:HA	1:B:56:GLU:H	1.71	0.55
1:B:321:ARG:NH1	3:B:2082:HOH:O	2.17	0.55
1:I:60:SER:O	1:J:299:ARG:NH2	2.40	0.55
1:B:19:THR:HA	1:B:53:ASN:HD22	1.72	0.55
1:F:6:HIS:CE1	1:F:34:ALA:C	2.84	0.55
1:F:286:THR:OG1	1:F:287:ALA:N	2.27	0.55
1:A:17:ASP:HA	1:A:54:GLN:NE2	2.22	0.55
1:C:336:VAL:O	1:C:340:CYS:HB2	2.07	0.55
1:C:197:GLU:N	1:C:197:GLU:OE1	2.40	0.54
1:H:50:SER:HA	1:H:56:GLU:H	1.72	0.54
1:F:249:TYR:HA	1:F:252:ILE:HD12	1.89	0.54
1:H:79:ASP:OD2	3:H:2002:HOH:O	2.18	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:LEU:HA	1:I:42:LEU:HD12	1.90	0.53
1:A:6:HIS:CE1	1:A:35:ALA:HB2	2.43	0.53
1:G:284:HIS:CG	1:G:285:GLU:N	2.77	0.53
1:C:145:TYR:CD2	1:C:183:PRO:HD3	2.43	0.53
1:J:50:SER:HA	1:J:56:GLU:H	1.72	0.53
1:J:160:VAL:HG21	1:J:186:TRP:CD2	2.44	0.53
1:G:160:VAL:HG21	1:G:186:TRP:CD2	2.44	0.53
1:G:200:ASP:OD1	1:G:329:TYR:OH	2.23	0.53
1:A:50:SER:HA	1:A:55:ALA:HB3	1.89	0.53
1:D:160:VAL:HG21	1:D:186:TRP:CD2	2.44	0.53
1:H:10:LYS:HE2	1:H:79:ASP:OD2	2.08	0.53
1:D:15:TRP:CE2	1:D:26:ARG:HB2	2.43	0.53
1:C:160:VAL:HG21	1:C:186:TRP:CD2	2.44	0.53
1:E:283:LEU:HD12	1:E:284:HIS:ND1	2.24	0.52
1:G:241:SER:OG	1:G:246:ARG:NH1	2.36	0.52
1:F:50:SER:HA	1:F:55:ALA:HB3	1.90	0.52
1:J:200:ASP:OD1	1:J:329:TYR:OH	2.23	0.52
1:J:146:TYR:HB2	1:J:181:VAL:HA	1.91	0.52
1:F:223:ASP:O	3:F:2050:HOH:O	2.19	0.52
1:B:61:ASP:OD1	1:C:299:ARG:NH2	2.39	0.52
1:C:280:LEU:HD22	1:C:286:THR:HG22	1.91	0.52
1:F:129:ARG:HG3	3:F:2058:HOH:O	2.09	0.52
1:I:200:ASP:OD1	1:I:329:TYR:OH	2.26	0.51
1:I:249:TYR:HA	1:I:252:ILE:HD12	1.91	0.51
1:E:307:TRP:N	3:E:2088:HOH:O	2.26	0.51
1:H:279:ARG:NH2	1:H:321:ARG:O	2.44	0.51
1:G:15:TRP:CE2	1:G:26:ARG:HB2	2.45	0.51
1:H:276:ILE:HA	1:H:323:ASN:HD21	1.75	0.51
1:A:314:LYS:NZ	3:A:2117:HOH:O	2.37	0.51
1:G:108:ARG:NH2	1:G:344:GLU:OE1	2.37	0.51
1:C:287:ALA:HB2	1:C:300:GLY:O	2.10	0.51
1:E:6:HIS:HE1	1:E:34:ALA:C	2.18	0.51
1:F:242:THR:H	1:F:245:MET:HB2	1.76	0.51
1:J:59:SER:HA	3:J:2019:HOH:O	2.10	0.51
1:J:283:LEU:HD12	1:J:284:HIS:CD2	2.45	0.51
1:B:336:VAL:O	1:B:340:CYS:HB2	2.11	0.51
1:D:279:ARG:NH2	1:D:321:ARG:O	2.44	0.51
1:A:6:HIS:CD2	1:A:7:MET:H	2.29	0.51
1:D:113:GLU:O	1:D:246:ARG:NH2	2.29	0.51
1:E:318:GLU:OE1	1:E:320:ARG:NH1	2.40	0.50
1:D:202:LEU:HD23	1:D:328:PRO:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:MET:O	1:D:270:LYS:HG2	2.10	0.50
1:H:17:ASP:HA	1:H:54:GLN:NE2	2.27	0.50
1:J:145:TYR:CD2	1:J:183:PRO:HD3	2.47	0.50
1:C:318:GLU:OE2	3:C:2055:HOH:O	2.20	0.49
1:A:39:LEU:HA	1:A:42:LEU:HD12	1.95	0.49
1:F:48:ASP:OD1	1:G:299:ARG:NE	2.45	0.49
1:B:39:LEU:N	3:B:2011:HOH:O	2.46	0.49
1:D:90:ASP:OD1	1:D:92:THR:OG1	2.29	0.49
1:D:242:THR:H	1:D:245:MET:HB2	1.78	0.49
1:D:6:HIS:CD2	1:D:7:MET:H	2.30	0.49
1:I:314:LYS:O	3:I:2102:HOH:O	2.18	0.49
1:J:15:TRP:CE2	1:J:26:ARG:HB2	2.47	0.49
1:C:283:LEU:HD12	1:C:284:HIS:CD2	2.48	0.49
1:C:63:VAL:HB	1:C:87:LEU:HB2	1.95	0.49
1:B:160:VAL:HG21	1:B:186:TRP:CD2	2.48	0.48
1:G:242:THR:H	1:G:245:MET:HB2	1.78	0.48
1:B:242:THR:O	1:B:246:ARG:HG3	2.13	0.48
1:F:99:ARG:HG3	1:F:329:TYR:CZ	2.48	0.48
1:G:145:TYR:CD2	1:G:183:PRO:HD3	2.48	0.48
1:D:39:LEU:HA	1:D:42:LEU:HD12	1.95	0.48
1:D:263:SER:N	3:D:2098:HOH:O	1.91	0.48
1:F:48:ASP:OD1	1:F:50:SER:OG	2.31	0.48
1:F:122:TYR:CZ	1:F:186:TRP:HB2	2.48	0.48
1:B:242:THR:H	1:B:245:MET:HB2	1.79	0.48
1:I:13:TYR:O	1:I:27:SER:HA	2.13	0.48
1:I:267:ASP:HA	1:I:270:LYS:HE2	1.95	0.48
1:I:336:VAL:O	1:I:340:CYS:HB2	2.13	0.48
1:B:285:GLU:CD	1:B:285:GLU:H	2.22	0.48
1:C:202:LEU:HD23	1:C:328:PRO:HB3	1.95	0.48
1:D:284:HIS:CG	1:D:285:GLU:N	2.80	0.48
1:D:13:TYR:O	1:D:27:SER:HA	2.13	0.48
1:H:53:ASN:HA	1:H:56:GLU:HG2	1.96	0.48
1:I:280:LEU:HB2	1:I:289:TRP:HB3	1.96	0.48
1:D:45:TRP:CD1	1:D:46:GLY:H	2.31	0.48
1:G:61:ASP:OD1	1:H:299:ARG:NH2	2.46	0.48
1:G:277:ASP:N	1:G:277:ASP:OD1	2.47	0.48
1:A:290:ASN:ND2	3:A:2108:HOH:O	2.45	0.48
1:F:285:GLU:HA	1:F:286:THR:HA	1.50	0.48
1:A:37:ALA:HB3	1:A:41:ALA:CB	2.44	0.47
1:F:202:LEU:HD23	1:F:328:PRO:HB3	1.96	0.47
1:I:257:GLU:OE2	3:I:2088:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:285:GLU:HA	1:I:286:THR:HA	1.50	0.47
1:E:242:THR:H	1:E:245:MET:HB2	1.79	0.47
1:A:277:ASP:OD1	1:A:277:ASP:N	2.45	0.47
1:E:197:GLU:HG3	3:E:2066:HOH:O	2.14	0.47
1:J:6:HIS:HD1	1:J:6:HIS:N	2.13	0.47
1:C:15:TRP:CE2	1:C:26:ARG:HB2	2.50	0.47
1:D:108:ARG:NH2	1:D:344:GLU:OE1	2.38	0.47
1:H:336:VAL:O	1:H:340:CYS:HB2	2.15	0.47
1:J:249:TYR:CE1	1:J:310:GLU:HA	2.50	0.47
1:A:160:VAL:HG21	1:A:186:TRP:CD2	2.49	0.47
1:C:80:ILE:HD12	1:C:82:VAL:HG22	1.97	0.47
1:B:135:GLU:HA	1:B:135:GLU:OE1	2.15	0.47
1:F:6:HIS:HE1	1:F:34:ALA:O	1.98	0.47
1:G:268:HIS:HA	1:G:334:LEU:HD13	1.95	0.47
1:D:296:VAL:HG21	1:D:310:GLU:HG3	1.97	0.47
1:F:45:TRP:CD1	1:F:46:GLY:H	2.32	0.47
1:A:65:LYS:HD2	1:A:87:LEU:HD11	1.97	0.47
1:C:122:TYR:CZ	1:C:186:TRP:HB2	2.50	0.47
1:C:13:TYR:O	1:C:27:SER:HA	2.15	0.46
1:E:199:SER:HB3	1:E:329:TYR:CD1	2.50	0.46
1:H:72:ASP:OD2	1:H:75:ARG:HD2	2.15	0.46
1:H:286:THR:HG23	1:H:287:ALA:N	2.28	0.46
1:I:160:VAL:HG21	1:I:186:TRP:CD2	2.49	0.46
1:D:287:ALA:HB2	1:D:300:GLY:O	2.15	0.46
1:E:160:VAL:HG21	1:E:186:TRP:CD2	2.51	0.46
1:G:272:TYR:CE1	1:G:331:VAL:HG23	2.51	0.46
1:B:197:GLU:OE1	1:B:197:GLU:N	2.47	0.46
1:F:50:SER:HA	1:F:56:GLU:H	1.80	0.46
1:J:48:ASP:CG	1:J:50:SER:HG	2.22	0.46
1:A:45:TRP:CD1	1:A:46:GLY:H	2.33	0.46
1:J:7:MET:SD	1:J:78:GLU:HG2	2.56	0.46
1:H:50:SER:OG	1:I:299:ARG:NH2	2.48	0.46
1:B:202:LEU:HD23	1:B:328:PRO:HB3	1.97	0.46
1:A:80:ILE:HD12	1:A:82:VAL:HG22	1.97	0.46
1:F:279:ARG:NH2	1:F:321:ARG:O	2.49	0.46
1:E:101:ALA:O	1:E:104:GLU:HG2	2.14	0.46
1:D:80:ILE:HD12	1:D:82:VAL:HG22	1.98	0.46
1:D:285:GLU:HA	1:D:286:THR:HA	1.56	0.45
1:E:55:ALA:HB2	1:E:60:SER:HB2	1.99	0.45
1:G:37:ALA:HB3	1:G:41:ALA:CB	2.47	0.45
1:G:283:LEU:HD12	1:G:284:HIS:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:GLU:HA	1:E:286:THR:HA	1.60	0.45
1:E:334:LEU:HD23	1:E:334:LEU:HA	1.77	0.45
1:J:232:ASN:HB3	3:J:2071:HOH:O	2.15	0.45
1:B:199:SER:HB3	1:B:329:TYR:CD1	2.51	0.45
1:D:299:ARG:NH2	3:D:2105:HOH:O	2.41	0.45
1:G:202:LEU:HD23	1:G:328:PRO:HB3	1.98	0.45
1:H:242:THR:H	1:H:245:MET:HB2	1.81	0.45
1:J:277:ASP:N	1:J:277:ASP:OD1	2.50	0.45
1:H:159:VAL:HG22	1:H:216:PHE:CG	2.52	0.45
1:H:202:LEU:HD23	1:H:328:PRO:HB3	1.97	0.45
1:I:146:TYR:HB2	1:I:181:VAL:HA	1.99	0.45
1:B:7:MET:SD	1:B:78:GLU:HG2	2.57	0.45
1:J:80:ILE:HD12	1:J:82:VAL:HG22	1.98	0.45
1:B:15:TRP:CE2	1:B:26:ARG:HB2	2.51	0.45
1:B:37:ALA:O	3:B:2011:HOH:O	2.21	0.45
1:J:17:ASP:HA	1:J:54:GLN:NE2	2.31	0.45
1:J:65:LYS:HD2	1:J:87:LEU:HD11	1.99	0.44
1:J:328:PRO:HA	1:J:331:VAL:HG12	1.99	0.44
1:I:208:LEU:HD23	1:I:208:LEU:HA	1.87	0.44
1:I:283:LEU:HD12	1:I:284:HIS:CD2	2.53	0.44
1:G:285:GLU:HA	1:G:286:THR:HA	1.49	0.44
1:C:50:SER:HA	1:C:56:GLU:H	1.82	0.44
1:H:285:GLU:HA	1:H:286:THR:HA	1.53	0.44
1:F:336:VAL:O	1:F:340:CYS:HB2	2.18	0.44
1:J:159:VAL:HG22	1:J:216:PHE:CG	2.52	0.44
1:E:336:VAL:O	1:E:340:CYS:HB2	2.18	0.44
1:H:293:SER:O	1:H:302:SER:HB2	2.17	0.44
1:J:135:GLU:HA	1:J:135:GLU:OE1	2.18	0.44
1:J:241:SER:OG	1:J:246:ARG:NH1	2.47	0.44
1:A:336:VAL:O	1:A:340:CYS:HB2	2.18	0.44
1:D:336:VAL:O	1:D:340:CYS:HB2	2.18	0.44
1:E:122:TYR:CZ	1:E:186:TRP:HB2	2.52	0.44
1:F:280:LEU:HB2	1:F:289:TRP:HB3	2.00	0.44
1:A:241:SER:OG	1:A:246:ARG:NH1	2.45	0.43
1:D:272:TYR:CE1	1:D:331:VAL:HG23	2.53	0.43
1:G:17:ASP:HA	1:G:54:GLN:NE2	2.32	0.43
3:I:2030:HOH:O	1:J:161:GLU:OE1	2.21	0.43
1:D:304:ARG:NH1	3:D:2105:HOH:O	2.16	0.43
1:F:48:ASP:OD1	1:G:299:ARG:NH2	2.51	0.43
1:I:37:ALA:HB3	1:I:41:ALA:CB	2.48	0.43
1:H:105:LEU:HD11	1:H:337:ASP:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ALA:HB2	1:B:60:SER:OG	2.18	0.43
1:G:55:ALA:HB2	1:G:60:SER:HB2	2.00	0.43
1:I:45:TRP:CD1	1:I:46:GLY:H	2.36	0.43
1:I:286:THR:CG2	1:I:320:ARG:HE	2.32	0.43
1:E:13:TYR:O	1:E:27:SER:HA	2.18	0.43
1:F:17:ASP:HB2	1:F:52:THR:O	2.18	0.43
1:J:242:THR:H	1:J:245:MET:HB2	1.83	0.43
1:D:242:THR:O	1:D:246:ARG:HG3	2.19	0.43
1:D:309:VAL:HG22	1:D:315:GLY:HA3	2.00	0.43
1:F:61:ASP:OD1	1:G:299:ARG:NH2	2.52	0.43
1:A:72:ASP:OD2	1:A:75:ARG:HD2	2.19	0.43
1:D:284:HIS:CD2	1:D:285:GLU:H	2.37	0.43
1:H:192:PRO:HD2	3:H:2060:HOH:O	2.18	0.43
1:I:286:THR:HG23	1:I:320:ARG:HE	1.83	0.43
1:D:284:HIS:CD2	1:D:285:GLU:HG2	2.54	0.43
1:A:30:LYS:HB2	1:A:45:TRP:CZ3	2.54	0.42
1:F:328:PRO:HA	1:F:331:VAL:HG12	2.01	0.42
1:H:55:ALA:CB	1:H:60:SER:HB3	2.49	0.42
1:H:225:LYS:NZ	1:H:231:TRP:O	2.46	0.42
1:I:50:SER:CA	1:I:55:ALA:HB3	2.47	0.42
1:J:48:ASP:OD1	1:J:50:SER:OG	2.36	0.42
1:F:48:ASP:CG	1:F:50:SER:HG	2.26	0.42
1:H:291:GLU:CD	3:H:2088:HOH:O	2.62	0.42
1:I:17:ASP:HB2	1:I:52:THR:O	2.19	0.42
1:I:241:SER:HG	1:I:246:ARG:HH11	1.63	0.42
1:J:13:TYR:O	1:J:27:SER:HA	2.19	0.42
1:A:249:TYR:CE2	1:A:253:ILE:HD11	2.54	0.42
1:E:15:TRP:CE2	1:E:26:ARG:HB2	2.55	0.42
1:F:116:PHE:HB2	1:F:198:VAL:HG11	2.01	0.42
1:H:15:TRP:CE2	1:H:26:ARG:HB2	2.54	0.42
1:I:261:GLU:HB2	3:I:2089:HOH:O	2.18	0.42
1:A:15:TRP:CE2	1:A:26:ARG:HB2	2.55	0.42
1:B:225:LYS:NZ	1:B:231:TRP:O	2.43	0.42
1:B:272:TYR:CE1	1:B:331:VAL:HG23	2.54	0.42
1:D:145:TYR:CD2	1:D:183:PRO:HD3	2.54	0.42
1:E:272:TYR:CE1	1:E:331:VAL:HG23	2.53	0.42
1:I:30:LYS:HB2	1:I:45:TRP:CZ3	2.55	0.42
1:G:336:VAL:O	1:G:340:CYS:HB2	2.19	0.42
1:H:200:ASP:OD1	1:H:329:TYR:OH	2.34	0.42
1:E:145:TYR:CD2	1:E:183:PRO:HD3	2.54	0.42
1:J:202:LEU:HD23	1:J:328:PRO:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ALA:CB	1:D:60:SER:OG	2.67	0.42
1:D:249:TYR:CE1	1:D:310:GLU:HA	2.55	0.42
1:E:266:MET:O	1:E:270:LYS:HG2	2.20	0.42
1:G:182:MET:HB3	1:G:185:GLN:HB2	2.01	0.42
1:J:264:LYS:HA	1:J:267:ASP:HB2	2.02	0.42
1:C:285:GLU:HA	1:C:286:THR:HA	1.64	0.42
1:H:39:LEU:HA	1:H:39:LEU:HD12	1.83	0.42
1:C:225:LYS:NZ	1:C:231:TRP:O	2.45	0.42
1:F:10:LYS:HG2	1:F:31:ILE:CD1	2.50	0.42
1:G:80:ILE:HD12	1:G:82:VAL:HG22	2.02	0.42
1:H:80:ILE:HD12	1:H:82:VAL:HG22	2.01	0.42
1:H:177:ILE:HG22	1:H:188:PHE:CB	2.50	0.42
1:J:177:ILE:HG22	1:J:188:PHE:CB	2.49	0.42
1:C:17:ASP:HA	1:C:54:GLN:NE2	2.34	0.42
1:E:30:LYS:HB2	1:E:45:TRP:CZ3	2.55	0.42
1:G:65:LYS:HD2	1:G:87:LEU:HD11	2.02	0.42
1:G:283:LEU:HD12	1:G:284:HIS:HB2	2.01	0.42
1:J:286:THR:HG23	1:J:320:ARG:HE	1.85	0.42
1:A:177:ILE:HG22	1:A:188:PHE:CB	2.50	0.41
1:B:266:MET:O	1:B:270:LYS:HG2	2.20	0.41
1:C:228:LYS:NZ	1:C:278:ASP:HB3	2.34	0.41
1:F:159:VAL:HG22	1:F:216:PHE:CG	2.55	0.41
1:F:277:ASP:OD1	1:F:277:ASP:N	2.51	0.41
1:I:80:ILE:HD12	1:I:82:VAL:HG22	2.02	0.41
1:B:159:VAL:HG22	1:B:216:PHE:CG	2.55	0.41
1:B:279:ARG:NH2	1:B:321:ARG:O	2.52	0.41
1:D:241:SER:OG	1:D:246:ARG:NH1	2.48	0.41
1:H:242:THR:O	1:H:246:ARG:HG3	2.19	0.41
1:J:264:LYS:NZ	3:J:2092:HOH:O	2.50	0.41
1:A:285:GLU:HA	1:A:286:THR:HA	1.48	0.41
1:A:309:VAL:HG22	1:A:315:GLY:HA3	2.01	0.41
1:H:101:ALA:N	3:H:2029:HOH:O	2.43	0.41
1:D:225:LYS:NZ	1:D:231:TRP:O	2.46	0.41
1:E:105:LEU:HD21	1:E:337:ASP:OD1	2.20	0.41
1:B:246:ARG:O	1:B:314:LYS:HB2	2.20	0.41
1:B:247:GLU:CD	3:B:2078:HOH:O	2.64	0.41
1:H:309:VAL:HG22	1:H:315:GLY:HA3	2.02	0.41
1:A:122:TYR:CZ	1:A:186:TRP:HB2	2.56	0.41
1:B:17:ASP:HA	1:B:54:GLN:NE2	2.35	0.41
1:B:13:TYR:O	1:B:27:SER:HA	2.21	0.41
1:D:249:TYR:CE2	1:D:253:ILE:HD11	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:TYR:CE1	1:F:310:GLU:HA	2.56	0.41
1:H:249:TYR:CE2	1:H:253:ILE:HD11	2.55	0.41
1:H:268:HIS:HA	1:H:334:LEU:HD13	2.03	0.41
1:D:38:GLY:O	1:D:40:ASP:N	2.46	0.41
1:F:80:ILE:HD12	1:F:82:VAL:HG22	2.03	0.41
1:F:286:THR:HG1	1:F:287:ALA:H	1.60	0.41
1:G:276:ILE:HA	1:G:323:ASN:HD21	1.85	0.41
1:J:122:TYR:CZ	1:J:186:TRP:HB2	2.56	0.41
1:B:10:LYS:HE2	1:B:79:ASP:OD2	2.21	0.41
1:B:119:GLU:OE2	3:B:2035:HOH:O	2.22	0.41
1:B:158:ASP:N	1:B:158:ASP:OD1	2.54	0.41
1:B:293:SER:O	1:B:302:SER:HB2	2.21	0.41
1:D:116:PHE:O	1:D:192:PRO:HA	2.21	0.41
1:D:299:ARG:HG3	1:D:320:ARG:NH2	2.35	0.41
1:F:145:TYR:CD2	1:F:183:PRO:HD3	2.55	0.41
1:H:288:PRO:O	3:H:2087:HOH:O	2.22	0.41
1:D:7:MET:HG2	1:D:8:THR:N	2.36	0.41
1:H:277:ASP:OD1	1:H:277:ASP:N	2.54	0.41
1:D:267:ASP:HA	1:D:270:LYS:HE2	2.02	0.40
1:D:286:THR:HB	1:D:287:ALA:H	1.71	0.40
1:F:39:LEU:HA	1:F:42:LEU:HD12	2.03	0.40
1:H:250:ASP:HB3	1:H:348:GLN:NE2	2.36	0.40
1:A:104:GLU:OE1	1:A:104:GLU:HA	2.21	0.40
1:A:158:ASP:OD1	1:A:158:ASP:N	2.52	0.40
1:B:197:GLU:O	1:B:201:GLN:HG3	2.22	0.40
1:E:116:PHE:O	1:E:192:PRO:HA	2.20	0.40
1:J:158:ASP:OD1	1:J:158:ASP:N	2.54	0.40
1:A:39:LEU:HA	1:A:39:LEU:HD12	1.86	0.40
1:A:242:THR:O	1:A:246:ARG:HG3	2.21	0.40
1:B:104:GLU:OE1	1:B:104:GLU:HA	2.21	0.40
1:F:10:LYS:HE2	1:F:79:ASP:OD2	2.21	0.40
1:F:99:ARG:HD3	3:F:2036:HOH:O	2.21	0.40
1:H:286:THR:CG2	1:H:287:ALA:N	2.84	0.40
1:A:116:PHE:HA	1:A:239:ASN:O	2.22	0.40
1:A:279:ARG:NH2	1:A:321:ARG:O	2.55	0.40
1:C:116:PHE:HA	1:C:239:ASN:O	2.22	0.40
1:C:268:HIS:HA	1:C:334:LEU:HD13	2.02	0.40
1:G:197:GLU:O	1:G:201:GLN:HG3	2.20	0.40
1:H:272:TYR:CE1	1:H:331:VAL:HG23	2.57	0.40
1:J:286:THR:HB	1:J:287:ALA:H	1.66	0.40
1:A:202:LEU:HD23	1:A:328:PRO:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TYR:CE1	1:A:331:VAL:HG23	2.56	0.40
1:B:277:ASP:OD1	1:B:277:ASP:N	2.54	0.40
1:B:327:ASP:HA	1:B:328:PRO:HD2	1.93	0.40
1:D:276:ILE:HA	1:D:323:ASN:HD21	1.86	0.40
1:F:160:VAL:HG21	1:F:186:TRP:CD2	2.56	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	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
1	B	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
1	C	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
1	D	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
1	E	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
1	F	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
1	G	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
1	H	342/344 (99%)	335 (98%)	7 (2%)	0	100	100
1	I	342/344 (99%)	335 (98%)	7 (2%)	0	100	100
1	J	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
All	All	3420/3440 (99%)	3342 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	274/275 (100%)	261 (95%)	13 (5%)	23	36
1	B	274/275 (100%)	261 (95%)	13 (5%)	23	36
1	C	274/275 (100%)	263 (96%)	11 (4%)	28	42
1	D	274/275 (100%)	261 (95%)	13 (5%)	23	36
1	E	274/275 (100%)	260 (95%)	14 (5%)	21	33
1	F	274/275 (100%)	259 (94%)	15 (6%)	19	29
1	G	274/275 (100%)	261 (95%)	13 (5%)	23	36
1	H	274/275 (100%)	265 (97%)	9 (3%)	33	50
1	I	274/275 (100%)	261 (95%)	13 (5%)	23	36
1	J	274/275 (100%)	261 (95%)	13 (5%)	23	36
All	All	2740/2750 (100%)	2613 (95%)	127 (5%)	24	36

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	44	VAL
1	A	50	SER
1	A	60	SER
1	A	78	GLU
1	A	104	GLU
1	A	105	LEU
1	A	129	ARG
1	A	169	LYS
1	A	232	ASN
1	A	257	GLU
1	A	266	MET
1	A	283	LEU
1	B	39	LEU
1	B	60	SER
1	B	78	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	80	ILE
1	B	104	GLU
1	B	129	ARG
1	B	135	GLU
1	B	169	LYS
1	B	232	ASN
1	B	257	GLU
1	B	266	MET
1	B	283	LEU
1	B	297	SER
1	C	44	VAL
1	C	60	SER
1	C	78	GLU
1	C	105	LEU
1	C	129	ARG
1	C	169	LYS
1	C	232	ASN
1	C	257	GLU
1	C	266	MET
1	C	283	LEU
1	C	297	SER
1	D	33	THR
1	D	44	VAL
1	D	78	GLU
1	D	92	THR
1	D	105	LEU
1	D	129	ARG
1	D	169	LYS
1	D	232	ASN
1	D	257	GLU
1	D	266	MET
1	D	283	LEU
1	D	286	THR
1	D	297	SER
1	E	7	MET
1	E	33	THR
1	E	50	SER
1	E	60	SER
1	E	78	GLU
1	E	80	ILE
1	E	105	LEU
1	E	129	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	169	LYS
1	E	232	ASN
1	E	257	GLU
1	E	266	MET
1	E	283	LEU
1	E	297	SER
1	F	7	MET
1	F	39	LEU
1	F	44	VAL
1	F	50	SER
1	F	60	SER
1	F	78	GLU
1	F	105	LEU
1	F	129	ARG
1	F	169	LYS
1	F	232	ASN
1	F	257	GLU
1	F	266	MET
1	F	283	LEU
1	F	297	SER
1	F	314	LYS
1	G	44	VAL
1	G	50	SER
1	G	60	SER
1	G	78	GLU
1	G	105	LEU
1	G	129	ARG
1	G	169	LYS
1	G	198	VAL
1	G	232	ASN
1	G	257	GLU
1	G	266	MET
1	G	283	LEU
1	G	286	THR
1	H	6	HIS
1	H	44	VAL
1	H	53	ASN
1	H	129	ARG
1	H	169	LYS
1	H	232	ASN
1	H	257	GLU
1	H	266	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	283	LEU
1	I	44	VAL
1	I	50	SER
1	I	53	ASN
1	I	78	GLU
1	I	105	LEU
1	I	129	ARG
1	I	169	LYS
1	I	232	ASN
1	I	257	GLU
1	I	266	MET
1	I	283	LEU
1	I	297	SER
1	I	314	LYS
1	J	44	VAL
1	J	50	SER
1	J	60	SER
1	J	78	GLU
1	J	129	ARG
1	J	135	GLU
1	J	169	LYS
1	J	198	VAL
1	J	232	ASN
1	J	257	GLU
1	J	266	MET
1	J	283	LEU
1	J	297	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	B	53	ASN
1	B	232	ASN
1	B	239	ASN
1	C	239	ASN
1	D	6	HIS
1	D	239	ASN
1	D	284	HIS
1	E	53	ASN
1	F	6	HIS
1	F	239	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	239	ASN
1	H	112	GLN
1	H	185	GLN
1	I	6	HIS
1	I	112	GLN
1	I	185	GLN
1	I	239	ASN
1	I	284	HIS
1	J	232	ASN
1	J	239	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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, 95th 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	344/344 (100%)	-0.06	16 (4%)	36 36	21, 35, 73, 105	0
1	B	344/344 (100%)	-0.03	12 (3%)	47 48	21, 35, 70, 109	0
1	C	344/344 (100%)	-0.11	20 (5%)	29 28	21, 32, 77, 110	0
1	D	344/344 (100%)	0.03	18 (5%)	33 32	23, 38, 71, 117	0
1	E	344/344 (100%)	0.03	19 (5%)	30 30	20, 37, 80, 116	0
1	F	344/344 (100%)	0.15	17 (4%)	35 34	23, 40, 69, 109	0
1	G	344/344 (100%)	0.02	17 (4%)	35 34	23, 36, 80, 107	0
1	H	344/344 (100%)	0.12	17 (4%)	35 34	23, 41, 78, 110	0
1	I	344/344 (100%)	0.03	17 (4%)	35 34	23, 36, 78, 131	0
1	J	344/344 (100%)	0.04	16 (4%)	36 36	23, 37, 73, 114	0
All	All	3440/3440 (100%)	0.02	169 (4%)	35 34	20, 36, 77, 131	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	THR	7.1
1	F	57	GLY	6.5
1	C	55	ALA	6.5
1	G	286	THR	6.2
1	D	286	THR	5.9
1	I	55	ALA	5.9
1	C	285	GLU	5.8
1	A	57	GLY	5.7
1	E	285	GLU	5.7
1	A	55	ALA	5.6
1	A	286	THR	5.6
1	G	57	GLY	5.3
1	E	55	ALA	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	57	GLY	5.2
1	F	286	THR	5.1
1	G	37	ALA	5.0
1	F	55	ALA	5.0
1	D	285	GLU	4.9
1	H	285	GLU	4.9
1	J	286	THR	4.8
1	J	57	GLY	4.7
1	C	286	THR	4.7
1	C	58	SER	4.7
1	C	60	SER	4.6
1	G	285	GLU	4.6
1	J	55	ALA	4.5
1	F	58	SER	4.5
1	H	60	SER	4.5
1	J	60	SER	4.5
1	B	60	SER	4.4
1	H	286	THR	4.4
1	I	285	GLU	4.4
1	F	6	HIS	4.4
1	C	283	LEU	4.4
1	F	285	GLU	4.4
1	I	286	THR	4.2
1	I	58	SER	4.1
1	E	56	GLU	4.1
1	E	57	GLY	4.1
1	J	285	GLU	4.0
1	E	6	HIS	4.0
1	D	60	SER	4.0
1	C	57	GLY	4.0
1	E	286	THR	4.0
1	D	37	ALA	4.0
1	B	285	GLU	3.9
1	H	37	ALA	3.8
1	G	55	ALA	3.8
1	H	58	SER	3.7
1	D	349	VAL	3.7
1	D	55	ALA	3.7
1	A	285	GLU	3.7
1	B	56	GLU	3.7
1	J	284	HIS	3.7
1	H	55	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	284	HIS	3.6
1	G	36	PRO	3.5
1	A	284	HIS	3.5
1	I	35	ALA	3.4
1	I	284	HIS	3.4
1	F	7	MET	3.3
1	B	37	ALA	3.3
1	E	60	SER	3.3
1	C	54	GLN	3.3
1	C	284	HIS	3.3
1	E	35	ALA	3.3
1	E	37	ALA	3.3
1	E	287	ALA	3.3
1	J	59	SER	3.2
1	D	59	SER	3.2
1	B	284	HIS	3.2
1	H	56	GLU	3.2
1	I	60	SER	3.2
1	E	284	HIS	3.2
1	G	35	ALA	3.1
1	A	56	GLU	3.1
1	G	6	HIS	3.1
1	J	37	ALA	3.1
1	D	56	GLU	3.1
1	A	36	PRO	3.1
1	I	59	SER	3.1
1	F	35	ALA	3.1
1	J	58	SER	3.1
1	H	6	HIS	3.1
1	I	56	GLU	3.0
1	C	59	SER	3.0
1	A	282	GLY	3.0
1	C	36	PRO	3.0
1	E	59	SER	2.9
1	H	38	GLY	2.9
1	I	36	PRO	2.9
1	D	282	GLY	2.9
1	C	37	ALA	2.8
1	G	7	MET	2.8
1	H	54	GLN	2.8
1	F	37	ALA	2.8
1	C	38	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	284	HIS	2.8
1	H	284	HIS	2.8
1	G	349	VAL	2.8
1	D	57	GLY	2.7
1	D	6	HIS	2.7
1	E	53	ASN	2.7
1	C	56	GLU	2.7
1	J	56	GLU	2.7
1	A	58	SER	2.7
1	B	59	SER	2.7
1	F	60	SER	2.7
1	G	59	SER	2.7
1	G	283	LEU	2.7
1	H	59	SER	2.7
1	B	55	ALA	2.7
1	F	56	GLU	2.7
1	H	40	ASP	2.6
1	A	283	LEU	2.6
1	H	39	LEU	2.6
1	J	38	GLY	2.6
1	G	39	LEU	2.6
1	F	283	LEU	2.5
1	E	58	SER	2.5
1	F	59	SER	2.5
1	C	282	GLY	2.5
1	E	283	LEU	2.5
1	E	282	GLY	2.5
1	I	37	ALA	2.5
1	G	58	SER	2.5
1	J	53	ASN	2.5
1	B	36	PRO	2.4
1	F	38	GLY	2.4
1	B	58	SER	2.4
1	A	38	GLY	2.4
1	B	57	GLY	2.4
1	A	39	LEU	2.4
1	C	51	SER	2.3
1	D	54	GLN	2.3
1	D	38	GLY	2.3
1	B	283	LEU	2.3
1	C	6	HIS	2.3
1	E	7	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	60	SER	2.3
1	A	48	ASP	2.3
1	J	6	HIS	2.3
1	C	39	LEU	2.3
1	H	35	ALA	2.2
1	A	349	VAL	2.2
1	J	281	THR	2.2
1	F	104	GLU	2.2
1	F	349	VAL	2.2
1	I	54	GLN	2.2
1	D	7	MET	2.2
1	A	50	SER	2.2
1	H	48	ASP	2.2
1	J	48	ASP	2.2
1	D	283	LEU	2.2
1	I	7	MET	2.1
1	H	36	PRO	2.1
1	A	37	ALA	2.1
1	C	35	ALA	2.1
1	D	53	ASN	2.1
1	I	6	HIS	2.1
1	C	53	ASN	2.1
1	I	38	GLY	2.1
1	E	261	GLU	2.1
1	D	58	SER	2.1
1	F	51	SER	2.1
1	E	39	LEU	2.0
1	G	56	GLU	2.0
1	I	283	LEU	2.0
1	J	36	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	A	1350	1/1	0.67	0.18	42,42,42,42	0
2	NA	G	1000	1/1	0.88	0.30	44,44,44,44	0
2	NA	A	1351	1/1	0.89	0.25	45,45,45,45	0
2	NA	D	1350	1/1	0.90	0.16	35,35,35,35	0
2	NA	F	1000	1/1	0.94	0.32	43,43,43,43	0
2	NA	D	1000	1/1	0.95	0.21	34,34,34,34	0
2	NA	E	1350	1/1	0.95	0.19	39,39,39,39	0
2	NA	B	1350	1/1	0.96	0.23	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.