



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:47 AM UTC

PDB ID : 6RCV / pdb_00006rcv
Title : PfRH5 bound to monoclonal antibodies R5.011 and R5.016
Authors : Alanine, D.W.G.; Draper, S.J.; Higgins, M.K.
Deposited on : 2019-04-11
Resolution : 3.58 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

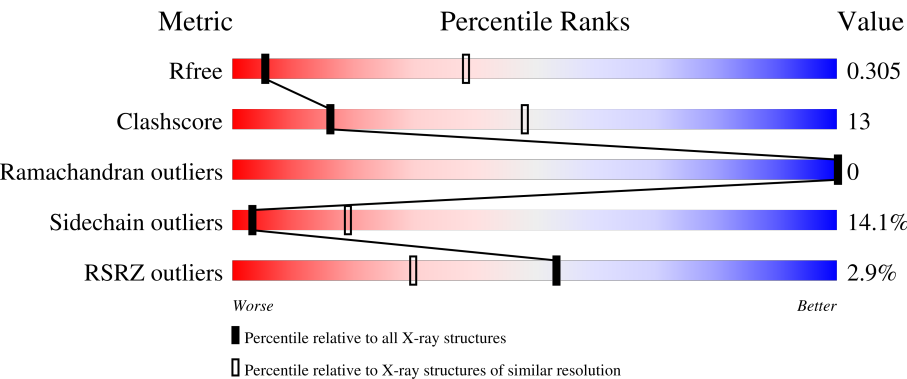
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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	501	42%14%•40%
1	F	501	41%15%•40%
2	B	217	66%26%6%•
2	G	217	63%30%••
3	C	240	2%66%26%•7%

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Mol	Chain	Length	Quality of chain
3	H	240	2% 61% 28% • 7%
4	D	219	% 62% 26% 8% •
4	I	219	3% 53% 36% 7% •
5	E	464	4% 34% 14% • 50%
5	J	464	3% 35% 12% • 52%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18311 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 Reticulocyte binding protein homologue 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2540	1640	426	459	15			
1	F	299	Total	C	N	O	S	0	0	0
			2540	1640	426	459	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	ASN	conflict	UNP Q8IFM5
A	216	ALA	THR	conflict	UNP Q8IFM5
F	38	GLN	ASN	conflict	UNP Q8IFM5
F	216	ALA	THR	conflict	UNP Q8IFM5

- Molecule 2 is a protein called R5.011 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1579	985	267	323	4			
2	G	210	Total	C	N	O	S	0	0	0
			1574	982	266	322	4			

- Molecule 3 is a protein called R5.011 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	224	Total	C	N	O	S	0	0	0
			1695	1081	272	336	6			
3	H	223	Total	C	N	O	S	0	0	0
			1691	1079	271	335	6			

- Molecule 4 is a protein called R5.016 light chain.

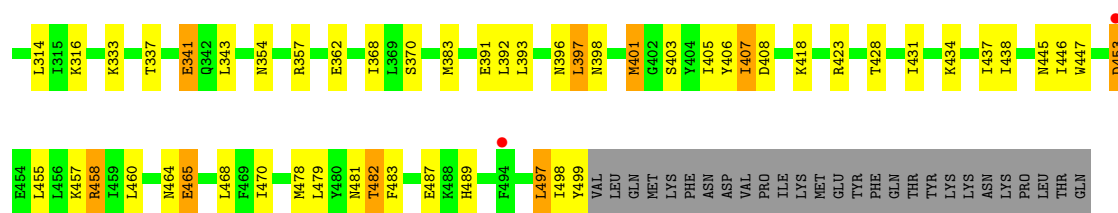
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	210	Total	C	N	O	S	0	0	0
			1624	1017	275	327	5			
4	I	210	Total	C	N	O	S	0	0	0
			1624	1017	275	327	5			

- Molecule 5 is a protein called R5.016 heavy chain.

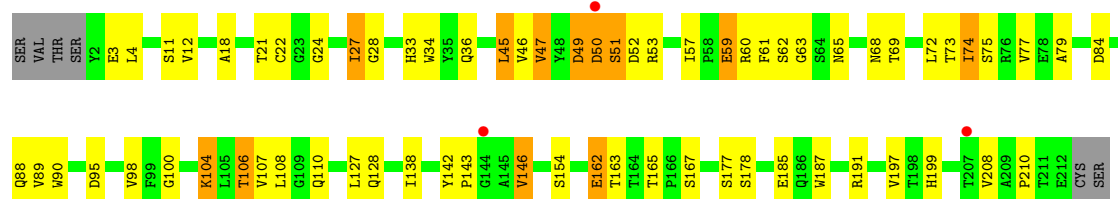
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	232	Total	C	N	O	S	0	0	0
			1746	1098	290	349	9			
5	J	224	Total	C	N	O	S	0	0	0
			1698	1072	281	336	9			

- Molecule 1: Reticulocyte binding protein homologue 5

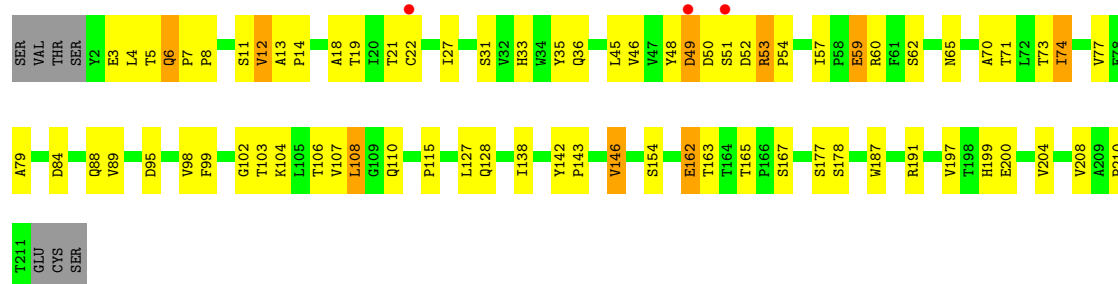




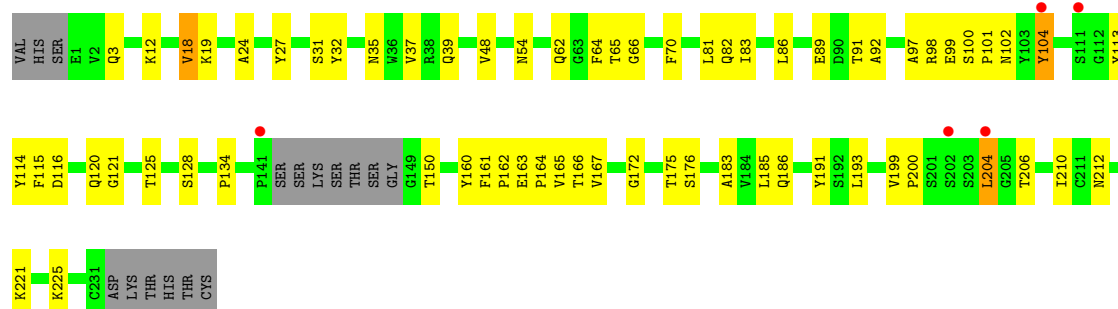
• Molecule 2: R5.011 light chain



• Molecule 2: R5.011 light chain

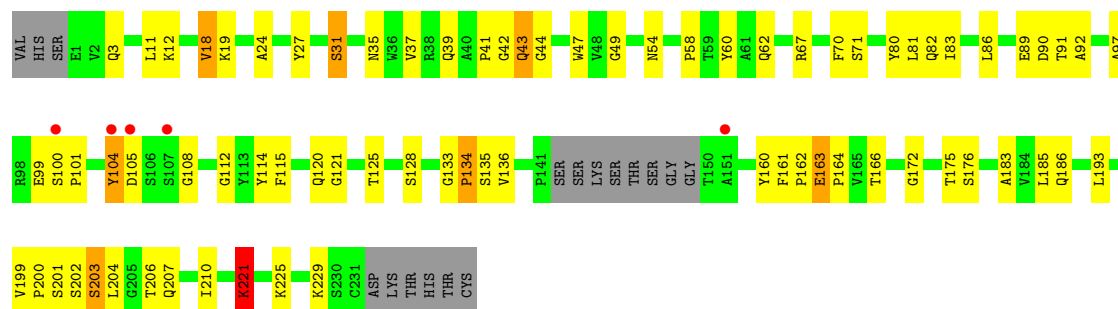


• Molecule 3: R5.011 heavy chain

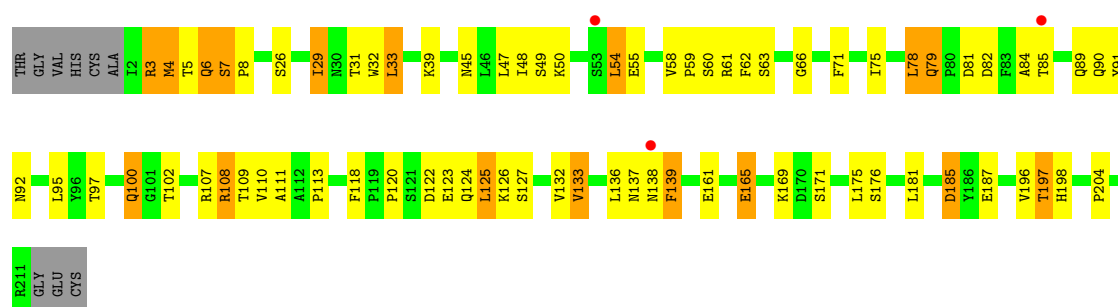


• Molecule 3: R5.011 heavy chain

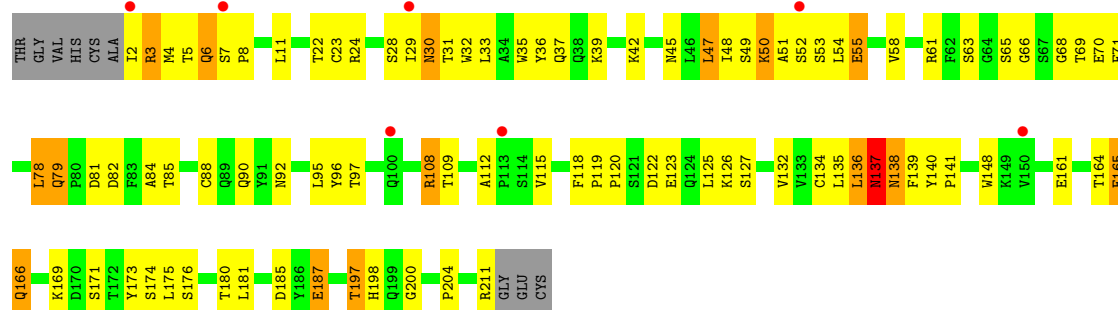




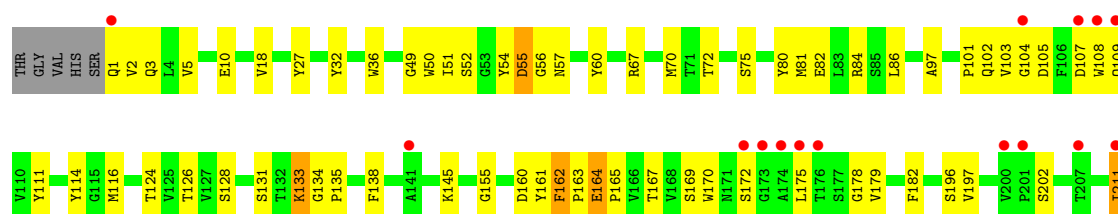
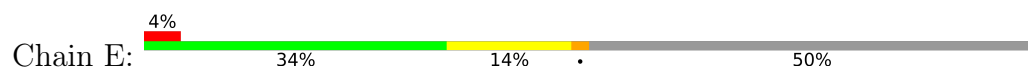
• Molecule 4: R5.016 light chain

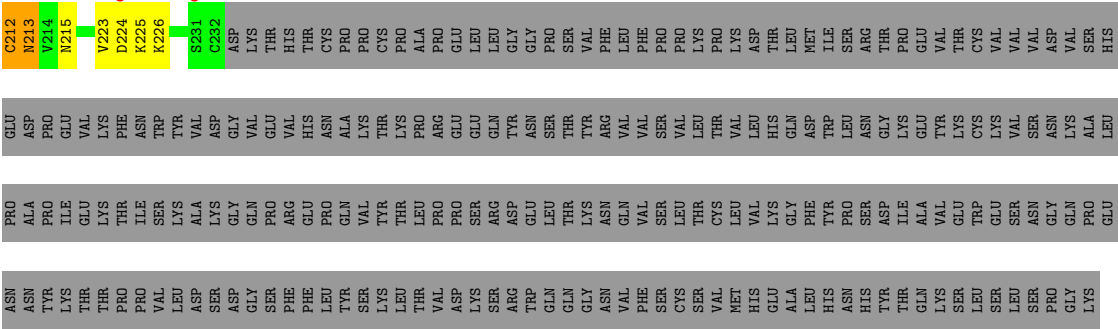


• Molecule 4: R5.016 light chain

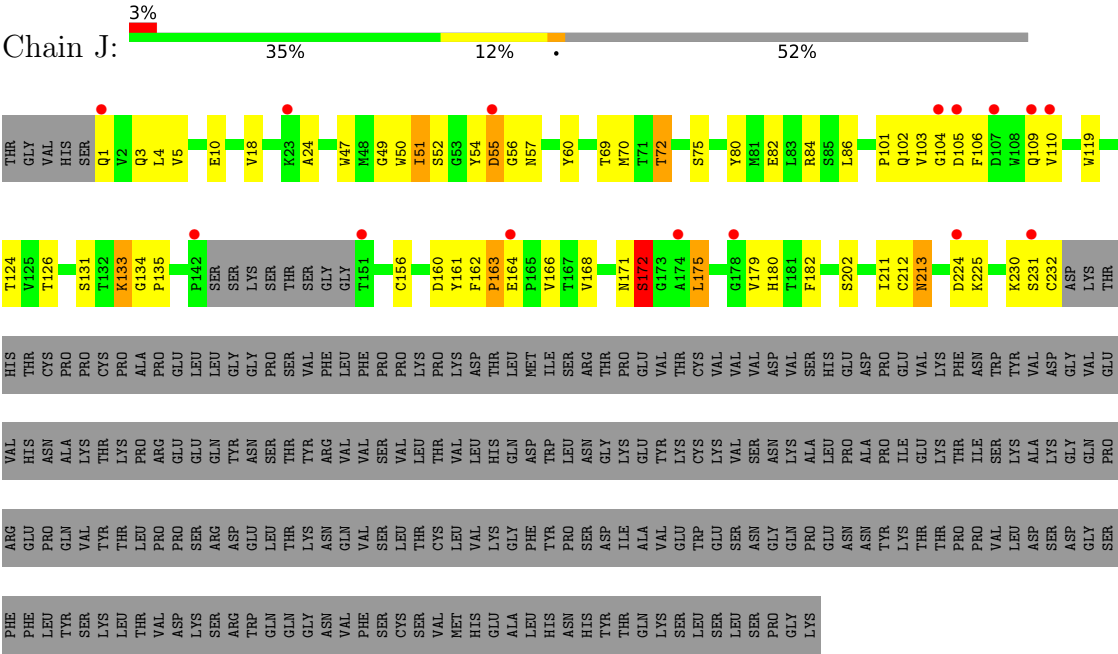


• Molecule 5: R5.016 heavy chain





• Molecule 5: R5.016 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.99Å 150.99Å 163.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 3.58 49.16 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.16-3.58) 97.1 (49.16-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.57Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.280 , 0.305 0.280 , 0.305	Depositor DCC
R_{free} test set	2052 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtrriage
Anisotropy	0.707	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18311	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4904e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.23	0/2594	0.65	1/3479 (0.0%)
1	F	0.28	0/2595	0.70	2/3481 (0.1%)
2	B	0.27	0/1619	0.78	1/2214 (0.0%)
2	G	0.43	1/1614 (0.1%)	0.81	3/2207 (0.1%)
3	C	0.27	0/1742	0.71	0/2380
3	H	0.48	4/1738 (0.2%)	0.90	7/2375 (0.3%)
4	D	0.33	0/1659	0.82	3/2253 (0.1%)
4	I	0.51	2/1659 (0.1%)	0.91	9/2253 (0.4%)
5	E	0.46	2/1790 (0.1%)	0.87	9/2442 (0.4%)
5	J	0.43	2/1741 (0.1%)	0.89	8/2376 (0.3%)
All	All	0.37	11/18751 (0.1%)	0.80	43/25460 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	11	LEU	CA-C	-9.24	1.41	1.52
2	G	53	ARG	CA-C	8.73	1.63	1.52
4	I	115	VAL	CA-C	-8.30	1.42	1.52
5	E	213	ASN	CA-C	7.55	1.62	1.53
3	H	136	VAL	CA-C	-6.91	1.44	1.52
5	J	166	VAL	CA-C	6.61	1.60	1.52
5	J	164	GLU	C-N	6.42	1.40	1.33
3	H	44	GLY	CA-C	-6.39	1.44	1.52
3	H	166	THR	CA-C	-6.11	1.45	1.52
5	E	178	GLY	CA-C	-5.56	1.44	1.51
3	H	221	LYS	CA-C	5.28	1.58	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	223	VAL	N-CA-C	8.75	120.36	108.11
4	I	138	ASN	N-CA-C	8.12	121.17	111.02
4	D	139	PHE	N-CA-C	8.06	120.23	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	30	ASN	N-CA-C	7.95	120.59	109.15
3	H	163	GLU	C-N-CD	7.63	137.38	120.60
5	E	164	GLU	C-N-CD	7.60	137.32	120.60
1	F	401	MET	N-CA-C	7.39	119.97	108.96
5	E	162	PHE	C-N-CD	7.31	136.67	120.60
4	I	137	ASN	N-CA-C	7.12	121.45	110.20
4	I	115	VAL	N-CA-C	6.74	118.28	108.58
5	J	160	ASP	N-CA-C	6.62	120.38	111.24
3	H	44	GLY	CA-C-N	-6.55	112.95	122.19
3	H	44	GLY	C-N-CA	-6.55	112.95	122.19
4	I	50	LYS	N-CA-C	-6.48	99.95	110.20
2	G	12	VAL	N-CA-C	6.24	118.12	108.44
5	E	212	CYS	N-CA-C	6.12	118.50	108.52
5	J	164	GLU	N-CA-C	6.07	121.78	113.16
4	I	6	GLN	N-CA-C	-6.06	101.03	110.42
5	J	56	GLY	N-CA-C	-6.04	105.78	115.08
3	H	203	SER	N-CA-C	-5.97	106.64	112.97
5	E	56	GLY	N-CA-C	-5.79	106.17	115.08
5	E	178	GLY	N-CA-C	5.77	123.57	115.43
1	A	405	ILE	N-CA-C	5.75	121.29	109.34
5	E	108	TRP	N-CA-C	5.71	117.91	110.43
4	D	137	ASN	N-CA-C	5.65	118.60	109.40
1	F	498	ILE	N-CA-C	5.51	116.24	108.36
4	I	169	LYS	N-CA-C	5.48	119.94	111.56
5	J	164	GLU	CA-C-N	-5.46	113.51	120.23
5	J	164	GLU	C-N-CA	-5.46	113.51	120.23
4	I	53	SER	N-CA-C	5.44	118.05	107.71
3	H	133	GLY	CA-C-N	-5.41	115.17	120.52
3	H	133	GLY	C-N-CA	-5.41	115.17	120.52
5	J	172	SER	N-CA-C	5.23	121.45	113.51
4	I	28	SER	N-CA-C	5.20	117.14	107.99
2	B	47	VAL	N-CA-C	-5.20	100.64	108.12
3	H	43	GLN	N-CA-C	5.19	115.23	108.07
2	G	6	GLN	CA-C-N	-5.18	115.05	120.38
2	G	6	GLN	C-N-CA	-5.18	115.05	120.38
5	E	160	ASP	N-CA-C	5.15	118.73	111.52
4	D	169	LYS	N-CA-C	5.11	119.38	111.56
5	E	178	GLY	CA-C-O	5.08	124.90	119.06
5	J	163	PRO	CA-C-N	5.02	126.36	120.09
5	J	163	PRO	C-N-CA	5.02	126.36	120.09

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	2540	0	2554	53	0
1	F	2540	0	2552	54	0
2	B	1579	0	1515	40	0
2	G	1574	0	1513	57	0
3	C	1695	0	1627	44	0
3	H	1691	0	1624	44	0
4	D	1624	0	1581	50	0
4	I	1624	0	1581	71	0
5	E	1746	0	1685	52	0
5	J	1698	0	1640	48	0
All	All	18311	0	17872	472	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 13.

All (472) 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:A:446:ILE:HG23	1:A:447:TRP:CD1	1.93	1.04
3:H:163:GLU:HG2	3:H:164:PRO:HA	1.42	0.98
3:H:134:PRO:HB3	3:H:160:TYR:HB3	1.54	0.90
2:G:6:GLN:NE2	2:G:102:GLY:C	2.30	0.90
1:F:434:LYS:HA	1:F:437:ILE:HG22	1.54	0.89
5:E:164:GLU:HB2	5:E:165:PRO:HA	1.58	0.84
4:D:113:PRO:HB3	4:D:139:PHE:CD2	2.19	0.78
1:F:238:LEU:O	1:F:238:LEU:HD23	1.84	0.78
1:F:434:LYS:O	1:F:437:ILE:HG22	1.84	0.77
3:H:163:GLU:CG	3:H:164:PRO:HA	2.14	0.77
5:J:156:CYS:HG	5:J:212:CYS:HG	1.16	0.76
2:B:12:VAL:HG21	2:B:18:ALA:HB2	1.67	0.75
1:F:434:LYS:HA	1:F:437:ILE:CG2	2.17	0.75
2:G:4:LEU:HD21	2:G:89:VAL:CG2	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:GLN:NE2	2:G:103:THR:N	2.37	0.73
1:F:235:ILE:O	1:F:239:GLU:HG3	1.89	0.73
1:F:316:LYS:HE2	2:G:49:ASP:OD2	1.89	0.73
4:D:109:THR:HG22	4:D:110:VAL:N	2.05	0.72
3:C:134:PRO:HB3	3:C:160:TYR:HB3	1.70	0.72
4:D:109:THR:HG22	4:D:110:VAL:H	1.55	0.72
3:H:221:LYS:O	3:H:221:LYS:HG3	1.88	0.72
5:E:164:GLU:CB	5:E:165:PRO:HA	2.19	0.71
2:G:6:GLN:NE2	2:G:103:THR:OG1	2.23	0.71
1:A:186:LYS:HG3	1:A:210:ILE:HD13	1.73	0.71
1:F:434:LYS:CA	1:F:437:ILE:HG22	2.20	0.71
2:G:18:ALA:HB3	2:G:74:ILE:HG23	1.73	0.70
5:J:230:LYS:HG3	5:J:232:CYS:H	1.56	0.70
4:I:136:LEU:N	4:I:136:LEU:HD12	2.06	0.70
3:C:91:THR:HG23	3:C:125:THR:HA	1.73	0.70
4:I:61:ARG:HH22	4:I:79:GLN:H	1.40	0.70
4:D:118:PHE:HB2	4:D:133:VAL:HG23	1.72	0.70
3:C:160:TYR:CZ	3:C:165:VAL:HG11	2.26	0.69
1:A:434:LYS:HE3	1:A:468:LEU:HD12	1.72	0.69
1:A:446:ILE:CG2	1:A:447:TRP:CD1	2.75	0.69
2:G:6:GLN:HE21	2:G:102:GLY:C	1.98	0.69
4:I:135:LEU:C	4:I:136:LEU:HD12	2.18	0.68
4:D:90:GLN:HE21	4:D:97:THR:HG22	1.59	0.68
1:F:354:ASN:OD1	1:F:357:ARG:NH1	2.26	0.68
3:C:163:GLU:HB3	3:C:164:PRO:HA	1.75	0.67
2:B:18:ALA:HB3	2:B:74:ILE:HG23	1.74	0.67
3:H:105:ASP:HB3	3:H:108:GLY:H	1.60	0.67
1:A:197:SER:HA	1:A:200:TYR:HD1	1.60	0.67
1:A:188:LEU:HD11	1:A:460:LEU:HD23	1.77	0.67
4:I:140:TYR:CG	4:I:141:PRO:HA	2.29	0.67
2:G:4:LEU:HD21	2:G:89:VAL:HG22	1.77	0.67
3:H:91:THR:HG23	3:H:125:THR:HA	1.77	0.66
5:J:102:GLN:HB3	5:J:105:ASP:HB2	1.76	0.66
4:I:61:ARG:HH22	4:I:79:GLN:N	1.93	0.66
5:J:213:ASN:N	5:J:213:ASN:HD22	1.91	0.66
2:G:4:LEU:CD1	2:G:98:VAL:HG12	2.24	0.66
4:I:2:ILE:O	4:I:97:THR:HG21	1.96	0.66
4:I:112:ALA:HB2	4:I:200:GLY:O	1.96	0.66
2:B:34:TRP:HB2	2:B:47:VAL:HB	1.78	0.66
4:I:137:ASN:HD22	4:I:138:ASN:H	1.45	0.65
1:F:188:LEU:HD11	1:F:460:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LYS:HG3	1:F:210:ILE:HD13	1.79	0.64
5:J:175:LEU:HD22	5:J:179:VAL:HB	1.78	0.64
3:H:18:VAL:HG22	3:H:86:LEU:HD11	1.80	0.64
2:G:6:GLN:HE21	2:G:103:THR:N	1.96	0.64
2:G:35:TYR:CE1	2:G:45:LEU:HD13	2.33	0.63
4:I:54:LEU:HD23	4:I:54:LEU:N	2.13	0.63
5:J:82:GLU:OE2	5:J:84:ARG:NH1	2.32	0.63
2:B:4:LEU:HB2	2:B:100:GLY:HA2	1.80	0.63
5:E:67:ARG:O	5:E:84:ARG:HG2	1.99	0.63
1:F:434:LYS:HD3	1:F:437:ILE:HG21	1.79	0.63
1:F:195:HIS:HB3	1:F:343:LEU:HD11	1.80	0.63
4:I:66:GLY:HA3	4:I:71:PHE:HD1	1.64	0.62
3:C:163:GLU:CB	3:C:164:PRO:HA	2.27	0.62
5:J:171:ASN:O	5:J:172:SER:HB2	1.99	0.62
1:A:195:HIS:HB3	1:A:343:LEU:HD11	1.80	0.62
2:G:6:GLN:NE2	2:G:102:GLY:CA	2.63	0.62
3:C:97:ALA:HB1	3:C:115:PHE:HB3	1.82	0.62
2:G:4:LEU:HD11	2:G:98:VAL:HG12	1.80	0.62
5:E:102:GLN:HB3	5:E:105:ASP:HB2	1.82	0.62
1:F:434:LYS:C	1:F:437:ILE:HG22	2.25	0.62
1:A:393:LEU:O	1:A:397:LEU:HB2	1.98	0.61
3:H:200:PRO:HG2	3:H:203:SER:HB2	1.80	0.61
4:I:140:TYR:CD2	4:I:141:PRO:HA	2.35	0.61
3:C:160:TYR:CZ	3:C:165:VAL:CG1	2.83	0.61
2:B:79:ALA:HA	2:B:107:VAL:HG21	1.83	0.61
5:J:105:ASP:CG	5:J:106:PHE:N	2.59	0.61
4:D:7:SER:HB3	4:D:8:PRO:HD3	1.81	0.61
5:E:175:LEU:HD12	5:E:179:VAL:HG21	1.81	0.61
1:F:204:ILE:HG12	5:J:54:TYR:CD2	2.36	0.61
4:D:61:ARG:HH22	4:D:79:GLN:HB2	1.66	0.60
1:F:154:ASN:HD22	3:H:31:SER:HA	1.67	0.60
5:E:175:LEU:O	5:E:175:LEU:HG	2.00	0.60
5:J:49:GLY:HA3	5:J:70:MET:HE1	1.84	0.60
4:I:137:ASN:ND2	4:I:174:SER:OG	2.35	0.60
3:H:67:ARG:HH12	3:H:90:ASP:CG	2.10	0.59
1:A:204:ILE:HG12	5:E:54:TYR:CD2	2.37	0.59
3:H:58:PRO:HB2	3:H:60:TYR:CZ	2.38	0.59
4:I:7:SER:HB3	4:I:8:PRO:HD3	1.83	0.59
1:A:204:ILE:HG12	5:E:54:TYR:CE2	2.37	0.59
3:C:18:VAL:HG22	3:C:86:LEU:HD11	1.85	0.58
4:I:54:LEU:HD23	4:I:54:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:HG23	1:A:406:TYR:CD2	2.39	0.58
1:F:434:LYS:NZ	1:F:465:GLU:OE2	2.36	0.58
2:G:4:LEU:HD21	2:G:89:VAL:HG21	1.84	0.58
2:B:45:LEU:HD12	3:C:116:ASP:HA	1.86	0.58
3:C:210:ILE:HG22	3:C:225:LYS:HG2	1.85	0.58
2:G:6:GLN:HE22	2:G:102:GLY:HA2	1.69	0.58
5:E:49:GLY:HA3	5:E:70:MET:HE1	1.85	0.58
1:F:164:LEU:HD22	1:F:478:MET:HB3	1.86	0.58
4:I:29:ILE:HG23	4:I:90:GLN:HG2	1.86	0.58
5:J:60:TYR:CE1	5:J:70:MET:HE2	2.39	0.57
2:G:142:TYR:HA	2:G:143:PRO:C	2.28	0.57
2:G:142:TYR:CD1	2:G:143:PRO:HA	2.39	0.57
2:B:24:GLY:HA3	2:B:27:ILE:HD12	1.85	0.57
4:I:135:LEU:CD1	5:J:182:PHE:HZ	2.18	0.57
1:F:204:ILE:HG12	5:J:54:TYR:CE2	2.40	0.57
4:I:31:THR:HG22	4:I:31:THR:O	2.04	0.57
3:C:163:GLU:HB3	3:C:164:PRO:CA	2.36	0.56
4:D:47:LEU:HB3	4:D:48:ILE:HD12	1.87	0.56
2:G:6:GLN:HG2	2:G:103:THR:OG1	2.05	0.56
1:A:230:ASP:HB3	1:A:310:LYS:HD2	1.87	0.56
4:D:4:MET:HE2	4:D:90:GLN:HB2	1.86	0.56
1:F:230:ASP:HB3	1:F:310:LYS:HD2	1.87	0.56
1:F:437:ILE:HG23	1:F:438:ILE:N	2.20	0.56
1:A:164:LEU:HD22	1:A:478:MET:HB3	1.86	0.56
3:H:71:SER:OG	3:H:80:TYR:HB2	2.06	0.56
5:E:60:TYR:CE1	5:E:70:MET:HE2	2.41	0.56
3:H:97:ALA:HB1	3:H:115:PHE:HB3	1.87	0.56
3:C:66:GLY:HA2	1:F:447:TRP:CZ3	2.41	0.55
5:J:60:TYR:HE1	5:J:70:MET:HG2	1.71	0.55
4:D:4:MET:HE3	4:D:33:LEU:CD1	2.36	0.55
1:F:398:ASN:OD1	1:F:407:ILE:HG12	2.06	0.55
4:I:54:LEU:H	4:I:54:LEU:CD2	2.19	0.55
4:I:140:TYR:CD2	4:I:141:PRO:CA	2.88	0.55
1:F:145:LEU:HD22	1:F:145:LEU:H	1.72	0.55
3:H:112:GLY:HA2	3:H:114:TYR:CE1	2.40	0.55
4:D:78:LEU:HD13	4:D:82:ASP:HB2	1.89	0.55
4:I:51:ALA:O	4:I:52:SER:CB	2.55	0.55
4:I:137:ASN:HD22	4:I:138:ASN:N	2.03	0.55
2:G:6:GLN:HG2	2:G:7:PRO:HD2	1.89	0.55
2:B:51:SER:HB3	2:B:63:GLY:O	2.07	0.54
2:B:4:LEU:HD11	2:B:89:VAL:HG22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:446:ILE:HG23	1:F:447:TRP:CD1	2.42	0.54
5:J:60:TYR:CD1	5:J:70:MET:HE2	2.41	0.54
2:B:59:GLU:H	2:B:59:GLU:CD	2.15	0.54
5:E:60:TYR:HE1	5:E:70:MET:HG2	1.73	0.54
4:I:29:ILE:O	4:I:71:PHE:HZ	1.90	0.54
5:J:105:ASP:CG	5:J:106:PHE:H	2.16	0.54
5:J:82:GLU:CD	5:J:84:ARG:HH11	2.16	0.54
4:D:48:ILE:HA	4:D:54:LEU:HA	1.90	0.54
5:E:50:TRP:CE3	5:E:103:VAL:HG22	2.43	0.54
5:E:162:PHE:C	5:E:162:PHE:CD2	2.86	0.54
3:H:163:GLU:CB	3:H:164:PRO:HA	2.34	0.54
1:F:155:TYR:CD1	3:H:101:PRO:HB3	2.43	0.53
2:G:12:VAL:HG12	2:G:13:ALA:N	2.23	0.53
3:H:161:PHE:C	3:H:161:PHE:CD2	2.86	0.53
1:A:316:LYS:HE2	2:B:49:ASP:OD2	2.08	0.53
1:A:337:THR:O	1:A:341:GLU:HB2	2.09	0.53
4:I:24:ARG:HG2	4:I:70:GLU:HB3	1.91	0.53
5:J:55:ASP:HB3	5:J:57:ASN:HB2	1.90	0.53
2:G:6:GLN:HE22	2:G:102:GLY:CA	2.21	0.53
5:J:50:TRP:CE3	5:J:103:VAL:HG22	2.44	0.53
2:G:33:HIS:ND1	3:H:114:TYR:HB3	2.23	0.53
4:I:69:THR:HG23	4:I:70:GLU:HG2	1.91	0.53
2:G:65:ASN:HA	2:G:70:ALA:HA	1.90	0.53
5:J:212:CYS:C	5:J:213:ASN:HD22	2.16	0.53
3:H:35:ASN:ND2	3:H:99:GLU:HB2	2.23	0.52
1:A:197:SER:HA	1:A:200:TYR:CD1	2.42	0.52
2:G:142:TYR:HA	2:G:143:PRO:O	2.08	0.52
3:C:210:ILE:HD12	3:C:212:ASN:HD21	1.73	0.52
2:G:33:HIS:ND1	2:G:48:TYR:O	2.26	0.52
3:H:163:GLU:HG2	3:H:164:PRO:CA	2.27	0.52
5:E:128:SER:HB3	5:E:162:PHE:CZ	2.44	0.52
4:I:136:LEU:N	4:I:136:LEU:CD1	2.73	0.52
4:D:109:THR:CG2	4:D:110:VAL:H	2.22	0.52
5:E:211:ILE:HG23	5:E:226:LYS:HG3	1.92	0.52
1:F:160:SER:HA	3:H:104:TYR:HB3	1.91	0.52
1:F:337:THR:O	1:F:341:GLU:HB2	2.10	0.52
5:E:60:TYR:CD1	5:E:70:MET:HE2	2.45	0.52
4:D:4:MET:HE1	4:D:29:ILE:HD11	1.93	0.51
4:D:48:ILE:HG13	4:D:54:LEU:HB3	1.91	0.51
2:G:49:ASP:O	2:G:50:ASP:C	2.52	0.51
4:I:138:ASN:OD1	5:J:180:HIS:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ASP:HB3	5:E:57:ASN:HB2	1.92	0.51
4:I:30:ASN:HA	4:I:68:GLY:HA2	1.92	0.51
1:A:145:LEU:HD22	1:A:145:LEU:H	1.75	0.51
3:C:39:GLN:O	3:C:92:ALA:HB1	2.11	0.51
2:G:60:ARG:NH1	2:G:74:ILE:HD11	2.26	0.51
4:I:39:LYS:HG3	4:I:84:ALA:HB2	1.91	0.51
4:I:61:ARG:NH1	4:I:82:ASP:OD1	2.43	0.51
4:D:90:GLN:HB3	4:D:97:THR:HG22	1.93	0.51
4:I:90:GLN:HE21	4:I:92:ASN:H	1.58	0.51
1:A:145:LEU:HG	1:A:340:PHE:HE2	1.75	0.51
4:D:29:ILE:HG22	4:D:92:ASN:HB2	1.92	0.51
4:D:109:THR:CG2	4:D:110:VAL:N	2.73	0.51
4:I:120:PRO:HD3	4:I:132:VAL:HG22	1.93	0.51
2:B:163:THR:HG23	2:B:178:SER:HB2	1.93	0.51
4:D:165:GLU:HA	4:D:165:GLU:OE1	2.11	0.51
2:G:163:THR:HG23	2:G:178:SER:HB2	1.92	0.51
3:H:161:PHE:CE2	3:H:162:PRO:HB3	2.46	0.51
3:C:161:PHE:C	3:C:161:PHE:CD2	2.89	0.50
4:D:123:GLU:OE2	5:E:225:LYS:HE2	2.12	0.50
2:G:49:ASP:HB2	2:G:52:ASP:HB2	1.93	0.50
2:G:162:GLU:HG2	3:H:186:GLN:HA	1.93	0.50
4:I:61:ARG:NH1	4:I:79:GLN:HB2	2.26	0.50
5:J:50:TRP:CH2	5:J:52:SER:HB2	2.46	0.50
3:C:161:PHE:CD1	3:C:191:TYR:HE2	2.29	0.50
5:E:167:THR:HG1	5:E:215:ASN:HB3	1.76	0.50
1:F:241:PRO:HB3	1:F:405:ILE:CG2	2.41	0.50
2:G:31:SER:HA	2:G:50:ASP:OD1	2.12	0.50
3:H:210:ILE:HG22	3:H:225:LYS:HG2	1.93	0.50
3:C:35:ASN:ND2	3:C:99:GLU:HB2	2.26	0.50
1:A:146:GLN:O	1:A:146:GLN:HG3	2.12	0.50
3:C:48:VAL:HG13	3:C:64:PHE:CD1	2.47	0.50
4:D:29:ILE:HD12	4:D:71:PHE:CE1	2.45	0.50
4:I:29:ILE:CD1	4:I:90:GLN:HG3	2.41	0.50
1:F:406:TYR:HD1	1:F:497:LEU:HG	1.77	0.50
2:B:53:ARG:HD3	2:B:61:PHE:O	2.12	0.49
2:G:142:TYR:CG	2:G:143:PRO:HA	2.48	0.49
1:F:146:GLN:O	1:F:146:GLN:HG3	2.12	0.49
1:F:164:LEU:HD22	1:F:478:MET:CB	2.42	0.49
1:F:300:PHE:CZ	1:F:408:ASP:HB3	2.47	0.49
2:B:162:GLU:HG2	3:C:186:GLN:HG2	1.95	0.49
4:I:4:MET:HE3	4:I:23:CYS:SG	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:135:LEU:CD1	5:J:182:PHE:CZ	2.96	0.49
1:A:185:TYR:CZ	1:A:333:LYS:HG3	2.48	0.49
4:D:32:TRP:HB3	4:D:91:TYR:CD2	2.48	0.49
5:E:212:CYS:O	5:E:224:ASP:HA	2.12	0.49
3:H:161:PHE:CD2	3:H:162:PRO:N	2.81	0.49
1:A:478:MET:O	1:A:482:THR:HG23	2.13	0.49
4:D:4:MET:HG2	4:D:97:THR:HG23	1.94	0.49
4:D:107:ARG:HG3	4:D:107:ARG:O	2.13	0.49
5:E:84:ARG:HB3	5:E:84:ARG:HH11	1.77	0.49
1:F:478:MET:O	1:F:482:THR:HG23	2.12	0.49
3:H:202:SER:C	3:H:204:LEU:H	2.20	0.49
4:D:120:PRO:HD3	4:D:132:VAL:HG22	1.95	0.49
1:F:185:TYR:CZ	1:F:333:LYS:HG3	2.47	0.48
2:G:79:ALA:HA	2:G:107:VAL:HG21	1.94	0.48
4:I:3:ARG:HG3	4:I:4:MET:N	2.28	0.48
4:I:139:PHE:CD1	4:I:198:HIS:NE2	2.81	0.48
4:D:161:GLU:HG2	4:D:175:LEU:HD21	1.94	0.48
2:G:35:TYR:CZ	2:G:45:LEU:HD13	2.49	0.48
3:H:41:PRO:HD3	3:H:92:ALA:HA	1.94	0.48
5:E:135:PRO:HB3	5:E:161:TYR:HB3	1.94	0.48
1:A:147:TYR:CE2	1:A:337:THR:HG22	2.49	0.48
5:J:82:GLU:CD	5:J:84:ARG:NH1	2.72	0.48
4:I:135:LEU:HD12	4:I:175:LEU:O	2.13	0.48
1:A:164:LEU:HD22	1:A:478:MET:CB	2.43	0.48
1:A:383:MET:HG2	1:A:483:PHE:CE1	2.49	0.47
3:C:70:PHE:HE1	3:C:81:LEU:HD13	1.79	0.47
3:H:11:LEU:HD22	3:H:162:PRO:HG3	1.96	0.47
3:C:120:GLN:HG2	3:C:121:GLY:N	2.28	0.47
4:I:29:ILE:HD12	4:I:90:GLN:HG3	1.97	0.47
3:C:160:TYR:CE2	3:C:165:VAL:HG11	2.50	0.47
4:D:39:LYS:HG3	4:D:84:ALA:HB2	1.95	0.47
5:E:50:TRP:CH2	5:E:52:SER:HB2	2.49	0.47
5:E:97:ALA:HB1	5:E:116:MET:HB3	1.96	0.47
2:G:12:VAL:HG21	2:G:18:ALA:HB2	1.94	0.47
2:G:48:TYR:CE2	2:G:49:ASP:HB2	2.49	0.47
1:F:403:SER:HB2	1:F:407:ILE:HD13	1.97	0.47
1:F:428:THR:HA	1:F:431:ILE:HD12	1.96	0.47
4:I:187:GLU:HA	4:I:211:ARG:NH2	2.28	0.47
1:F:437:ILE:CG2	1:F:438:ILE:N	2.77	0.47
2:G:12:VAL:O	2:G:108:LEU:HB2	2.15	0.47
3:H:120:GLN:HG2	3:H:121:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:HA	3:C:104:TYR:HB3	1.97	0.47
1:A:202:LYS:HB3	5:E:111:TYR:CE1	2.49	0.47
5:E:49:GLY:C	5:E:70:MET:HE1	2.40	0.47
2:B:53:ARG:HD2	2:B:57:ILE:HG22	1.96	0.47
2:B:146:VAL:HG23	2:B:199:HIS:HB2	1.96	0.47
4:D:3:ARG:HB3	4:D:26:SER:HB3	1.96	0.47
4:D:6:GLN:HG2	4:D:102:THR:OG1	2.14	0.47
2:G:33:HIS:CE1	3:H:114:TYR:HB3	2.50	0.47
4:I:61:ARG:CZ	4:I:79:GLN:HB2	2.45	0.47
2:B:90:TRP:HB2	3:C:113:TYR:HB2	1.96	0.47
4:D:66:GLY:HA3	4:D:71:PHE:HA	1.97	0.47
4:I:78:LEU:HD13	4:I:82:ASP:HB2	1.96	0.47
1:A:300:PHE:CE1	1:A:408:ASP:HB3	2.49	0.47
5:E:167:THR:OG1	5:E:215:ASN:HB3	2.15	0.47
4:I:55:GLU:O	4:I:58:VAL:HG22	2.15	0.47
5:J:175:LEU:HD13	5:J:175:LEU:O	2.14	0.47
4:D:47:LEU:HD22	4:D:58:VAL:HG13	1.96	0.46
4:I:61:ARG:NH2	4:I:79:GLN:HB2	2.30	0.46
3:C:24:ALA:HB1	3:C:27:TYR:CE1	2.50	0.46
4:I:29:ILE:HG13	4:I:90:GLN:HG3	1.97	0.46
3:C:167:VAL:O	3:C:167:VAL:HG13	2.16	0.46
5:E:50:TRP:CD2	5:E:103:VAL:HG22	2.51	0.46
1:F:445:ASN:CG	1:F:458:ARG:HG3	2.40	0.46
1:A:400:LYS:O	1:A:401:MET:C	2.57	0.46
2:B:138:ILE:HG12	2:B:197:VAL:HG21	1.98	0.46
1:F:160:SER:HA	3:H:104:TYR:CB	2.44	0.46
1:F:383:MET:HG2	1:F:483:PHE:CE1	2.51	0.46
5:J:162:PHE:CG	5:J:163:PRO:HA	2.51	0.46
1:A:166:GLU:HG2	1:A:481:ASN:HB2	1.97	0.46
1:F:147:TYR:CE2	1:F:337:THR:HG22	2.51	0.46
4:I:54:LEU:N	4:I:54:LEU:CD2	2.77	0.46
5:J:18:VAL:O	5:J:82:GLU:HA	2.16	0.46
3:C:12:LYS:HG3	3:C:18:VAL:HG13	1.98	0.46
2:G:162:GLU:HG2	3:H:186:GLN:HG2	1.97	0.46
2:B:68:ASN:C	2:B:69:THR:CG2	2.89	0.46
4:I:96:TYR:HD2	5:J:47:TRP:CD1	2.33	0.46
1:A:428:THR:HA	1:A:431:ILE:HD12	1.96	0.46
1:A:498:ILE:H	1:A:498:ILE:HG13	1.60	0.45
5:E:84:ARG:HB3	5:E:84:ARG:NH1	2.31	0.45
1:F:166:GLU:HG2	1:F:481:ASN:HB2	1.98	0.45
1:A:300:PHE:CZ	1:A:408:ASP:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.81	0.45
3:H:42:GLY:O	3:H:43:GLN:CD	2.59	0.45
4:I:29:ILE:CG2	4:I:90:GLN:HG2	2.46	0.45
3:H:12:LYS:HG3	3:H:18:VAL:HG13	1.98	0.45
3:H:24:ALA:HB1	3:H:27:TYR:CE1	2.51	0.45
3:H:67:ARG:NH1	3:H:90:ASP:OD2	2.34	0.45
4:I:164:THR:HG23	4:I:164:THR:O	2.15	0.45
1:A:445:ASN:CG	1:A:458:ARG:HG3	2.42	0.45
2:G:138:ILE:HG12	2:G:197:VAL:HG21	1.99	0.45
5:J:50:TRP:CD2	5:J:103:VAL:HG22	2.51	0.45
3:C:183:ALA:HA	3:C:193:LEU:HB3	1.99	0.45
5:E:164:GLU:CB	5:E:165:PRO:CA	2.92	0.45
4:I:108:ARG:HA	4:I:108:ARG:HD2	1.72	0.45
1:A:165:GLN:HG3	1:A:171:LEU:HD23	1.99	0.45
2:B:142:TYR:CD1	2:B:143:PRO:HA	2.52	0.45
3:C:172:GLY:O	3:C:175:THR:HG23	2.17	0.45
5:E:103:VAL:HG23	5:E:104:GLY:N	2.32	0.45
5:E:170:TRP:HH2	5:E:196:SER:HG	1.64	0.45
2:G:4:LEU:HD12	2:G:98:VAL:HG12	1.98	0.45
2:B:60:ARG:HB3	2:B:75:SER:O	2.17	0.45
5:E:70:MET:HB2	5:E:80:TYR:O	2.17	0.45
4:D:32:TRP:HB3	4:D:91:TYR:CE2	2.52	0.44
5:J:50:TRP:N	5:J:70:MET:HE1	2.32	0.44
1:A:211:LYS:HB3	5:E:32:TYR:OH	2.16	0.44
2:B:33:HIS:CG	3:C:114:TYR:HB3	2.52	0.44
3:C:161:PHE:HD1	3:C:191:TYR:CE2	2.35	0.44
1:A:155:TYR:CD1	3:C:101:PRO:HB3	2.52	0.44
2:B:68:ASN:O	2:B:69:THR:HG22	2.17	0.44
5:E:170:TRP:HH2	5:E:196:SER:CB	2.31	0.44
1:F:453:ASP:OD1	1:F:457:LYS:HE3	2.18	0.44
4:I:90:GLN:HE21	4:I:92:ASN:N	2.15	0.44
2:G:14:PRO:HG3	2:G:107:VAL:CG1	2.47	0.44
4:I:4:MET:CG	4:I:97:THR:HG23	2.48	0.44
2:B:49:ASP:H	2:B:52:ASP:HB2	1.82	0.44
2:B:88:GLN:HA	2:B:98:VAL:O	2.17	0.44
4:I:36:TYR:CE2	5:J:119:TRP:HZ2	2.36	0.44
3:C:161:PHE:CD1	3:C:191:TYR:CE2	3.06	0.44
4:I:176:SER:HB3	5:J:182:PHE:CE2	2.52	0.44
1:A:371:VAL:HG11	1:A:435:THR:HG21	2.00	0.44
1:A:405:ILE:HG23	1:A:406:TYR:N	2.33	0.44
4:D:136:LEU:HD21	4:D:196:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:74:ILE:HG13	2:G:77:VAL:HG22	2.00	0.44
4:I:32:TRP:CZ2	5:J:110:VAL:HG12	2.52	0.44
5:E:49:GLY:CA	5:E:70:MET:HE1	2.47	0.44
5:E:50:TRP:N	5:E:70:MET:HE1	2.32	0.44
1:F:165:GLN:HG3	1:F:171:LEU:HD23	2.00	0.44
2:G:115:PRO:HG2	2:G:204:VAL:HG21	1.99	0.44
4:I:49:SER:HB2	4:I:50:LYS:H	1.63	0.44
4:I:164:THR:CG2	4:I:174:SER:HB2	2.48	0.44
2:B:33:HIS:CE1	3:C:114:TYR:HD1	2.36	0.43
4:D:61:ARG:HH12	4:D:79:GLN:HB2	1.82	0.43
4:D:139:PHE:HD1	4:D:198:HIS:NE2	2.16	0.43
2:G:146:VAL:HG23	2:G:199:HIS:HB2	2.00	0.43
1:A:160:SER:HA	3:C:104:TYR:CB	2.48	0.43
4:D:62:PHE:CE1	4:D:75:ILE:HG12	2.53	0.43
1:A:406:TYR:HD1	1:A:497:LEU:HD22	1.83	0.43
1:A:446:ILE:HG23	1:A:447:TRP:N	2.33	0.43
3:C:165:VAL:HG13	3:C:193:LEU:HD21	2.00	0.43
4:D:89:GLN:HG2	4:D:90:GLN:N	2.33	0.43
5:E:50:TRP:CZ2	5:E:52:SER:HB2	2.54	0.43
2:G:142:TYR:O	2:G:199:HIS:NE2	2.50	0.43
4:I:51:ALA:O	4:I:52:SER:HB3	2.18	0.43
5:J:50:TRP:CZ2	5:J:52:SER:HB2	2.53	0.43
1:A:157:ILE:H	1:A:157:ILE:HG13	1.67	0.43
4:I:165:GLU:H	4:I:165:GLU:HG2	1.53	0.43
5:J:49:GLY:C	5:J:70:MET:HE1	2.42	0.43
2:B:187:TRP:CZ2	2:B:210:PRO:HA	2.54	0.43
4:D:197:THR:HG23	4:D:204:PRO:HB3	2.01	0.43
4:I:197:THR:HG23	4:I:204:PRO:HB3	2.01	0.43
1:A:202:LYS:HB3	5:E:111:TYR:CD1	2.54	0.43
1:A:300:PHE:HA	1:A:303:MET:HB2	1.99	0.43
1:A:433:ASP:O	1:A:437:ILE:HG12	2.18	0.43
4:D:111:ALA:O	4:D:139:PHE:HB2	2.19	0.43
1:F:229:ASN:HA	1:F:232:ILE:HD12	2.00	0.43
2:G:36:GLN:HB2	2:G:46:VAL:HG11	2.01	0.43
2:G:46:VAL:O	2:G:57:ILE:HG21	2.19	0.43
5:J:4:LEU:HD23	5:J:24:ALA:HA	2.00	0.43
1:F:157:ILE:H	1:F:157:ILE:HG13	1.66	0.43
2:B:34:TRP:CD2	2:B:72:LEU:HB2	2.54	0.43
5:E:133:LYS:HD3	5:E:134:GLY:O	2.19	0.43
1:F:147:TYR:HE2	1:F:188:LEU:HD21	1.84	0.43
4:I:118:PHE:HA	4:I:119:PRO:HD3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:166:GLN:HG2	4:I:173:TYR:CZ	2.53	0.43
5:J:103:VAL:HG23	5:J:104:GLY:N	2.34	0.43
2:B:28:GLY:HA2	2:B:65:ASN:OD1	2.18	0.43
5:J:49:GLY:CA	5:J:70:MET:HE1	2.47	0.43
2:B:104:LYS:CE	2:B:106:THR:HG23	2.49	0.42
1:F:162:ASP:O	1:F:173:PHE:HA	2.19	0.42
3:C:70:PHE:CE1	3:C:81:LEU:HD13	2.54	0.42
3:C:19:LYS:HG3	3:C:82:GLN:HG2	2.00	0.42
5:E:128:SER:HB3	5:E:162:PHE:CE1	2.54	0.42
1:F:434:LYS:HD2	1:F:465:GLU:HG3	2.02	0.42
1:A:406:TYR:CD1	1:A:497:LEU:HD22	2.55	0.42
4:D:139:PHE:CD1	4:D:198:HIS:NE2	2.87	0.42
2:G:46:VAL:O	2:G:54:PRO:HD2	2.19	0.42
2:G:53:ARG:CZ	2:G:59:GLU:HA	2.49	0.42
4:I:37:GLN:HB2	4:I:47:LEU:CD2	2.49	0.42
4:D:7:SER:HB3	4:D:8:PRO:CD	2.48	0.42
3:H:58:PRO:HB2	3:H:60:TYR:CE2	2.54	0.42
4:I:4:MET:HG3	4:I:97:THR:HG23	2.02	0.42
1:A:204:ILE:HD13	5:E:101:PRO:HB2	2.01	0.42
2:B:12:VAL:HG21	2:B:18:ALA:CB	2.43	0.42
3:H:39:GLN:O	3:H:92:ALA:HB1	2.19	0.42
5:J:133:LYS:HD2	5:J:134:GLY:O	2.19	0.42
5:J:162:PHE:HA	5:J:163:PRO:C	2.43	0.42
2:B:104:LYS:HE2	2:B:106:THR:HG23	2.02	0.42
3:C:24:ALA:HB1	3:C:27:TYR:HE1	1.84	0.42
4:D:125:LEU:HD22	4:D:125:LEU:HA	1.82	0.42
1:F:183:ASP:O	1:F:186:LYS:HB3	2.20	0.42
3:H:183:ALA:HA	3:H:193:LEU:HB3	2.00	0.42
1:A:212:LYS:HG2	5:E:114:TYR:CE2	2.54	0.42
5:E:18:VAL:O	5:E:82:GLU:HA	2.19	0.42
4:I:140:TYR:CD2	4:I:141:PRO:N	2.88	0.42
4:D:59:PRO:HD2	4:D:62:PHE:CE2	2.55	0.42
4:I:7:SER:HB2	4:I:22:THR:HB	2.01	0.42
5:E:2:VAL:HG13	5:E:27:TYR:CD2	2.55	0.41
1:F:164:LEU:HD23	1:F:479:LEU:HG	2.02	0.41
3:H:70:PHE:HE1	3:H:81:LEU:HD13	1.84	0.41
4:I:134:CYS:HB2	4:I:148:TRP:CZ2	2.55	0.41
5:J:179:VAL:O	5:J:179:VAL:HG13	2.20	0.41
2:B:74:ILE:HG13	2:B:77:VAL:HG22	2.01	0.41
3:C:27:TYR:CE2	3:C:32:TYR:HB2	2.55	0.41
4:D:61:ARG:NH2	4:D:79:GLN:HB2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:LEU:HD12	1:F:397:LEU:HA	1.86	0.41
2:G:187:TRP:CZ2	2:G:210:PRO:HA	2.54	0.41
2:B:34:TRP:CE2	2:B:72:LEU:HB2	2.56	0.41
1:F:204:ILE:HD13	5:J:101:PRO:HB2	2.02	0.41
4:D:108:ARG:HD3	4:D:109:THR:H	1.85	0.41
4:D:176:SER:HB3	5:E:182:PHE:CE2	2.55	0.41
2:G:88:GLN:HG3	2:G:99:PHE:CE1	2.55	0.41
5:J:70:MET:HB2	5:J:80:TYR:O	2.20	0.41
2:G:19:THR:HG23	2:G:71:THR:CG2	2.51	0.41
3:H:172:GLY:O	3:H:175:THR:HG23	2.20	0.41
1:A:365:HIS:CD2	1:A:369:LEU:HD11	2.55	0.41
2:B:95:ASP:O	2:B:95:ASP:CG	2.63	0.41
4:D:4:MET:HE3	4:D:33:LEU:HD12	2.01	0.41
3:C:204:LEU:H	3:C:204:LEU:HD22	1.86	0.41
5:E:169:SER:O	5:E:213:ASN:HB2	2.20	0.41
3:H:210:ILE:HG13	3:H:210:ILE:O	2.21	0.41
4:I:123:GLU:OE2	5:J:225:LYS:HE2	2.21	0.41
1:A:163:ILE:C	1:A:164:LEU:HG	2.44	0.41
5:E:162:PHE:HA	5:E:163:PRO:HA	1.75	0.41
2:B:142:TYR:CG	2:B:143:PRO:HA	2.56	0.41
4:D:6:GLN:HB2	4:D:100:GLN:HG3	2.02	0.41
4:D:124:GLN:HG3	5:E:138:PHE:CE2	2.55	0.41
4:D:181:LEU:HD13	4:D:185:ASP:OD2	2.21	0.41
2:G:6:GLN:CG	2:G:7:PRO:HD2	2.51	0.41
2:G:7:PRO:HA	2:G:8:PRO:HD3	1.96	0.41
2:G:95:ASP:CG	2:G:95:ASP:O	2.63	0.41
5:J:69:THR:CB	5:J:84:ARG:HH22	2.33	0.41
5:J:175:LEU:HD22	5:J:175:LEU:HA	1.85	0.41
2:B:68:ASN:C	2:B:69:THR:HG23	2.45	0.41
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.56	0.41
4:I:35:TRP:CZ3	4:I:88:CYS:HB3	2.56	0.41
5:J:51:ILE:HD11	5:J:72:THR:HB	2.03	0.41
2:B:49:ASP:O	2:B:50:ASP:C	2.63	0.40
3:C:199:VAL:HA	3:C:200:PRO:HD3	1.96	0.40
3:H:19:LYS:HG3	3:H:82:GLN:HG2	2.03	0.40
5:J:135:PRO:HB3	5:J:161:TYR:HB3	2.02	0.40
1:A:195:HIS:CB	1:A:343:LEU:HD11	2.49	0.40
1:A:202:LYS:CB	5:E:111:TYR:CE1	3.04	0.40
2:B:36:GLN:HB2	2:B:46:VAL:HG11	2.03	0.40
2:B:142:TYR:HA	2:B:143:PRO:C	2.46	0.40
3:C:161:PHE:HA	3:C:162:PRO:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:TRP:CE2	5:E:81:MET:HB2	2.56	0.40
1:F:149:PHE:O	1:F:185:TYR:OH	2.34	0.40
2:G:6:GLN:HE22	2:G:102:GLY:C	2.24	0.40
4:I:161:GLU:HG2	4:I:175:LEU:HD21	2.03	0.40
4:I:180:THR:C	4:I:181:LEU:HD22	2.47	0.40
3:C:160:TYR:CZ	3:C:165:VAL:HG12	2.55	0.40
5:E:155:GLY:HA3	5:E:197:VAL:HG12	2.02	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	295/501 (59%)	280 (95%)	15 (5%)	0	100	100
1	F	295/501 (59%)	281 (95%)	14 (5%)	0	100	100
2	B	209/217 (96%)	197 (94%)	12 (6%)	0	100	100
2	G	208/217 (96%)	196 (94%)	12 (6%)	0	100	100
3	C	220/240 (92%)	204 (93%)	16 (7%)	0	100	100
3	H	219/240 (91%)	206 (94%)	13 (6%)	0	100	100
4	D	208/219 (95%)	192 (92%)	16 (8%)	0	100	100
4	I	208/219 (95%)	187 (90%)	21 (10%)	0	100	100
5	E	230/464 (50%)	215 (94%)	15 (6%)	0	100	100
5	J	220/464 (47%)	207 (94%)	13 (6%)	0	100	100
All	All	2312/3282 (70%)	2165 (94%)	147 (6%)	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	289/486 (60%)	246 (85%)	43 (15%)	3	17
1	F	289/486 (60%)	244 (84%)	45 (16%)	2	16
2	B	177/184 (96%)	148 (84%)	29 (16%)	2	14
2	G	177/184 (96%)	149 (84%)	28 (16%)	2	15
3	C	189/204 (93%)	168 (89%)	21 (11%)	6	27
3	H	189/204 (93%)	168 (89%)	21 (11%)	6	27
4	D	186/192 (97%)	153 (82%)	33 (18%)	2	11
4	I	186/192 (97%)	156 (84%)	30 (16%)	2	15
5	E	195/409 (48%)	176 (90%)	19 (10%)	8	31
5	J	189/409 (46%)	167 (88%)	22 (12%)	5	25
All	All	2066/2950 (70%)	1775 (86%)	291 (14%)	3	19

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LEU
1	A	146	GLN
1	A	148	HIS
1	A	151	GLU
1	A	152	LEU
1	A	153	SER
1	A	157	ILE
1	A	162	ASP
1	A	163	ILE
1	A	164	LEU
1	A	165	GLN
1	A	174	VAL
1	A	188	LEU
1	A	203	CYS
1	A	226	ASP
1	A	236	LYS

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	240	HIS
1	A	302	LYS
1	A	314	LEU
1	A	341	GLU
1	A	368	ILE
1	A	370	SER
1	A	392	LEU
1	A	393	LEU
1	A	396	ASN
1	A	397	LEU
1	A	401	MET
1	A	404	TYR
1	A	418	LYS
1	A	423	ARG
1	A	455	LEU
1	A	458	ARG
1	A	464	ASN
1	A	465	GLU
1	A	468	LEU
1	A	470	ILE
1	A	482	THR
1	A	487	GLU
1	A	489	HIS
1	A	497	LEU
1	A	498	ILE
1	A	499	TYR
2	B	3	GLU
2	B	11	SER
2	B	21	THR
2	B	22	CYS
2	B	27	ILE
2	B	45	LEU
2	B	49	ASP
2	B	50	ASP
2	B	51	SER
2	B	59	GLU
2	B	62	SER
2	B	73	THR
2	B	74	ILE
2	B	84	ASP
2	B	104	LYS

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Mol	Chain	Res	Type
2	B	106	THR
2	B	108	LEU
2	B	110	GLN
2	B	127	LEU
2	B	128	GLN
2	B	146	VAL
2	B	154	SER
2	B	162	GLU
2	B	165	THR
2	B	167	SER
2	B	177	SER
2	B	185	GLU
2	B	191	ARG
2	B	208	VAL
3	C	3	GLN
3	C	18	VAL
3	C	31	SER
3	C	37	VAL
3	C	54	ASN
3	C	62	GLN
3	C	65	THR
3	C	83	ILE
3	C	89	GLU
3	C	98	ARG
3	C	100	SER
3	C	102	ASN
3	C	104	TYR
3	C	128	SER
3	C	150	THR
3	C	166	THR
3	C	176	SER
3	C	185	LEU
3	C	204	LEU
3	C	206	THR
3	C	221	LYS
4	D	3	ARG
4	D	4	MET
4	D	5	THR
4	D	6	GLN
4	D	7	SER
4	D	29	ILE
4	D	31	THR

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Mol	Chain	Res	Type
4	D	33	LEU
4	D	45	ASN
4	D	49	SER
4	D	50	LYS
4	D	54	LEU
4	D	55	GLU
4	D	60	SER
4	D	63	SER
4	D	78	LEU
4	D	79	GLN
4	D	81	ASP
4	D	85	THR
4	D	95	LEU
4	D	100	GLN
4	D	108	ARG
4	D	122	ASP
4	D	125	LEU
4	D	126	LYS
4	D	127	SER
4	D	133	VAL
4	D	138	ASN
4	D	165	GLU
4	D	171	SER
4	D	185	ASP
4	D	187	GLU
4	D	197	THR
5	E	1	GLN
5	E	3	GLN
5	E	5	VAL
5	E	10	GLU
5	E	51	ILE
5	E	55	ASP
5	E	72	THR
5	E	75	SER
5	E	86	LEU
5	E	107	ASP
5	E	109	GLN
5	E	124	THR
5	E	126	THR
5	E	131	SER
5	E	133	LYS
5	E	145	LYS

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Mol	Chain	Res	Type
5	E	172	SER
5	E	202	SER
5	E	211	ILE
1	F	145	LEU
1	F	146	GLN
1	F	148	HIS
1	F	152	LEU
1	F	153	SER
1	F	157	ILE
1	F	162	ASP
1	F	163	ILE
1	F	164	LEU
1	F	165	GLN
1	F	174	VAL
1	F	188	LEU
1	F	200	TYR
1	F	203	CYS
1	F	211	LYS
1	F	226	ASP
1	F	236	LYS
1	F	238	LEU
1	F	301	LYS
1	F	314	LEU
1	F	341	GLU
1	F	362	GLU
1	F	368	ILE
1	F	370	SER
1	F	391	GLU
1	F	392	LEU
1	F	393	LEU
1	F	396	ASN
1	F	397	LEU
1	F	401	MET
1	F	407	ILE
1	F	418	LYS
1	F	423	ARG
1	F	453	ASP
1	F	455	LEU
1	F	458	ARG
1	F	464	ASN
1	F	465	GLU
1	F	468	LEU

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Mol	Chain	Res	Type
1	F	470	ILE
1	F	482	THR
1	F	487	GLU
1	F	489	HIS
1	F	497	LEU
1	F	499	TYR
2	G	3	GLU
2	G	5	THR
2	G	11	SER
2	G	21	THR
2	G	22	CYS
2	G	27	ILE
2	G	49	ASP
2	G	51	SER
2	G	59	GLU
2	G	62	SER
2	G	73	THR
2	G	74	ILE
2	G	84	ASP
2	G	104	LYS
2	G	106	THR
2	G	108	LEU
2	G	110	GLN
2	G	127	LEU
2	G	128	GLN
2	G	146	VAL
2	G	154	SER
2	G	162	GLU
2	G	165	THR
2	G	167	SER
2	G	177	SER
2	G	191	ARG
2	G	200	GLU
2	G	208	VAL
3	H	3	GLN
3	H	18	VAL
3	H	31	SER
3	H	37	VAL
3	H	54	ASN
3	H	62	GLN
3	H	83	ILE
3	H	89	GLU

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Mol	Chain	Res	Type
3	H	100	SER
3	H	104	TYR
3	H	128	SER
3	H	134	PRO
3	H	135	SER
3	H	176	SER
3	H	185	LEU
3	H	199	VAL
3	H	201	SER
3	H	206	THR
3	H	207	GLN
3	H	221	LYS
3	H	229	LYS
4	I	3	ARG
4	I	5	THR
4	I	6	GLN
4	I	33	LEU
4	I	42	LYS
4	I	45	ASN
4	I	47	LEU
4	I	48	ILE
4	I	55	GLU
4	I	63	SER
4	I	65	SER
4	I	78	LEU
4	I	79	GLN
4	I	81	ASP
4	I	85	THR
4	I	95	LEU
4	I	108	ARG
4	I	109	THR
4	I	122	ASP
4	I	125	LEU
4	I	126	LYS
4	I	127	SER
4	I	136	LEU
4	I	137	ASN
4	I	165	GLU
4	I	166	GLN
4	I	171	SER
4	I	185	ASP
4	I	187	GLU

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Mol	Chain	Res	Type
4	I	197	THR
5	J	1	GLN
5	J	3	GLN
5	J	5	VAL
5	J	10	GLU
5	J	51	ILE
5	J	55	ASP
5	J	72	THR
5	J	75	SER
5	J	86	LEU
5	J	109	GLN
5	J	124	THR
5	J	126	THR
5	J	131	SER
5	J	133	LYS
5	J	168	VAL
5	J	172	SER
5	J	175	LEU
5	J	202	SER
5	J	211	ILE
5	J	213	ASN
5	J	224	ASP
5	J	231	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	321	HIS
1	A	396	ASN
1	A	439	GLN
1	A	464	ASN
1	A	474	HIS
2	B	37	GLN
2	B	88	GLN
2	B	110	GLN
3	C	39	GLN
3	C	54	ASN
4	D	89	GLN
4	D	90	GLN
4	D	138	ASN
5	E	3	GLN

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Mol	Chain	Res	Type
5	E	43	GLN
5	E	59	ASN
5	E	180	HIS
5	E	208	GLN
1	F	154	ASN
1	F	195	HIS
1	F	321	HIS
1	F	396	ASN
1	F	464	ASN
1	F	474	HIS
1	F	496	HIS
2	G	6	GLN
2	G	37	GLN
3	H	39	GLN
3	H	54	ASN
4	I	6	GLN
4	I	90	GLN
4	I	92	ASN
4	I	100	GLN
4	I	137	ASN
4	I	138	ASN
4	I	160	GLN
5	J	43	GLN
5	J	59	ASN
5	J	213	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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, 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	299/501 (59%)	0.34	6 (2%) 65 37	37, 58, 108, 147	0
1	F	299/501 (59%)	0.45	5 (1%) 69 40	43, 62, 113, 143	0
2	B	211/217 (97%)	0.53	3 (1%) 73 45	45, 58, 112, 130	0
2	G	210/217 (96%)	0.43	3 (1%) 73 45	38, 58, 88, 102	0
3	C	224/240 (93%)	0.51	5 (2%) 62 35	45, 70, 126, 152	0
3	H	223/240 (92%)	0.47	5 (2%) 62 35	46, 65, 109, 140	0
4	D	210/219 (95%)	0.48	3 (1%) 73 45	49, 99, 135, 161	0
4	I	210/219 (95%)	0.55	7 (3%) 49 27	53, 96, 135, 148	0
5	E	232/464 (50%)	0.63	17 (7%) 21 13	48, 80, 137, 144	0
5	J	224/464 (48%)	0.70	15 (6%) 24 14	47, 73, 135, 148	0
All	All	2342/3282 (71%)	0.50	69 (2%) 53 30	37, 67, 129, 161	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	174	ALA	3.8
2	B	50	ASP	3.6
4	D	138	ASN	3.5
3	C	104	TYR	3.5
5	J	104	GLY	3.5
1	F	453	ASP	3.4
1	A	500	VAL	3.3
4	I	29	ILE	3.3
5	E	173	GLY	3.2
5	E	211	ILE	3.1
4	I	100	GLN	2.9
5	J	107	ASP	2.9
4	I	52	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	498	ILE	2.9
3	H	104	TYR	2.8
5	E	176	THR	2.8
5	J	174	ALA	2.7
2	G	49	ASP	2.7
3	H	100	SER	2.6
3	C	141	PRO	2.6
4	I	113	PRO	2.6
5	J	55	ASP	2.6
4	I	2	ILE	2.5
5	E	224	ASP	2.5
1	F	147	TYR	2.5
5	J	110	VAL	2.5
1	A	240	HIS	2.4
5	J	151	THR	2.4
1	A	403	SER	2.4
3	H	107	SER	2.4
5	J	224	ASP	2.4
5	E	109	GLN	2.4
5	E	104	GLY	2.3
5	E	207	THR	2.3
3	C	111	SER	2.3
5	J	178	GLY	2.3
3	H	105	ASP	2.3
5	E	1	GLN	2.3
1	A	405	ILE	2.3
5	J	142	PRO	2.3
5	E	172	SER	2.3
1	A	404	TYR	2.3
5	J	23	LYS	2.3
2	G	22	CYS	2.2
5	E	200	VAL	2.2
2	B	144	GLY	2.2
5	J	1	GLN	2.2
4	I	7	SER	2.2
5	J	164	GLU	2.2
5	E	231	SER	2.2
5	E	107	ASP	2.1
5	J	231	SER	2.1
5	E	141	ALA	2.1
3	C	202	SER	2.1
3	H	151	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	148	HIS	2.1
4	I	150	VAL	2.1
2	G	51	SER	2.1
2	B	207	THR	2.1
1	F	221	LYS	2.1
1	F	494	PHE	2.1
3	C	204	LEU	2.1
5	E	108	TRP	2.0
4	D	85	THR	2.0
4	D	53	SER	2.0
5	E	175	LEU	2.0
5	J	109	GLN	2.0
5	E	201	PRO	2.0
5	J	105	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.