



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 4U1G / pdb_00004u1g
Title : Plasmodium falciparum reticulocyte-binding protein homologue 5 (PfRH5)
bound to monoclonal antibody QA1
Authors : Wright, K.E.; Hjerrild, K.A.; Bartlett, J.; Douglas, A.D.; Jin, J.; Brown, R.E.;
Ashfield, R.; Clemmensen, S.B.; de Jongh, W.A.; Draper, S.J.; Higgins, M.K.
Deposited on : 2014-07-15
Resolution : 3.10 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

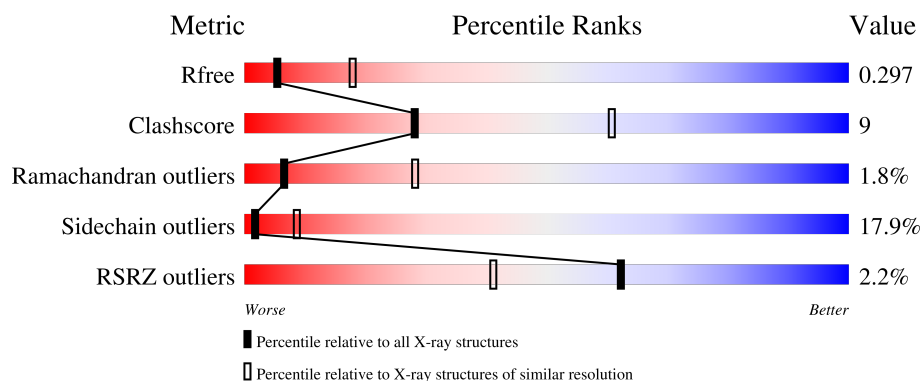
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	526	2% 33% 16% 5% 45%
1	D	526	% 36% 15% . . 45%
2	B	258	% 56% 20% 7% 17%
2	E	258	% 51% 25% 5% . 17%
3	C	238	2% 57% 28% 5% 10%

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Mol	Chain	Length	Quality of chain
3	F	238	2% 58% 27% • • 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11478 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 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2446	1579	411	441	15			
1	D	289	Total	C	N	O	S	0	0	0
			2458	1588	412	443	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	ALA	THR	engineered mutation	UNP B2L3N7
D	216	ALA	THR	engineered mutation	UNP B2L3N7

- Molecule 2 is a protein called QA1 monoclonal antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1611	1020	262	320	9			
2	E	213	Total	C	N	O	S	0	0	0
			1611	1020	262	320	9			

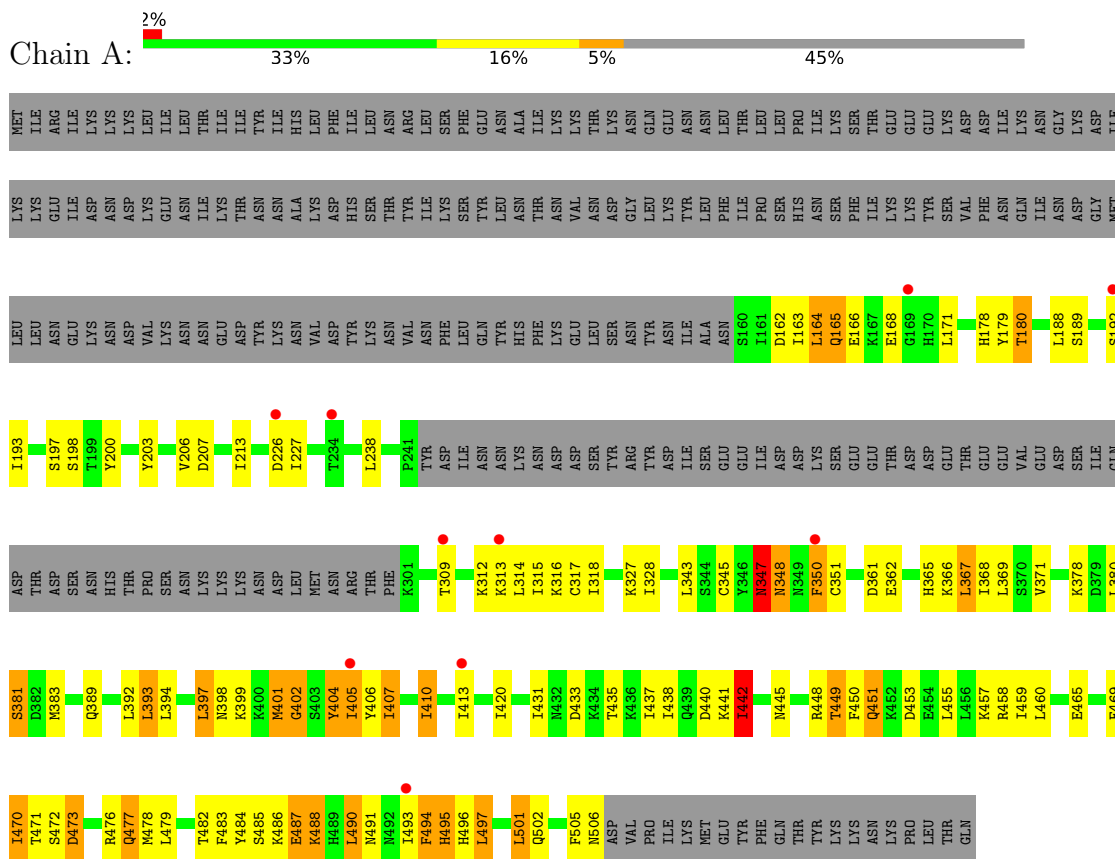
- Molecule 3 is a protein called QA1 monoclonal antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1676	1049	283	339	5			
3	F	215	Total	C	N	O	S	0	0	0
			1676	1049	283	339	5			

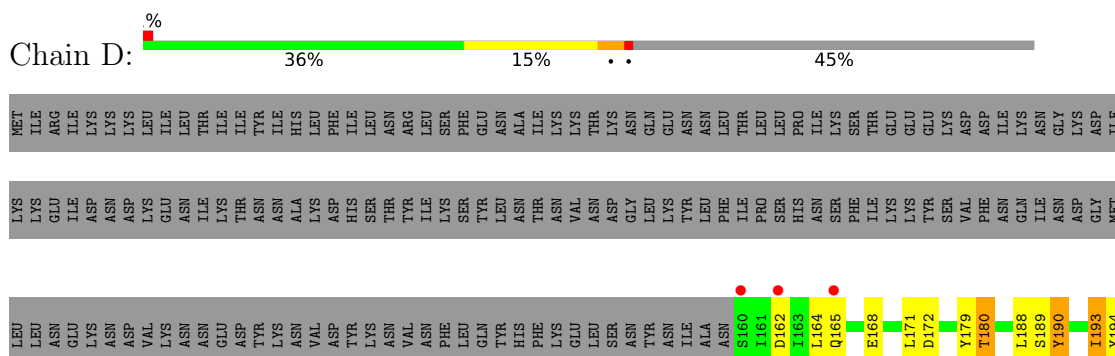
3 Residue-property plots

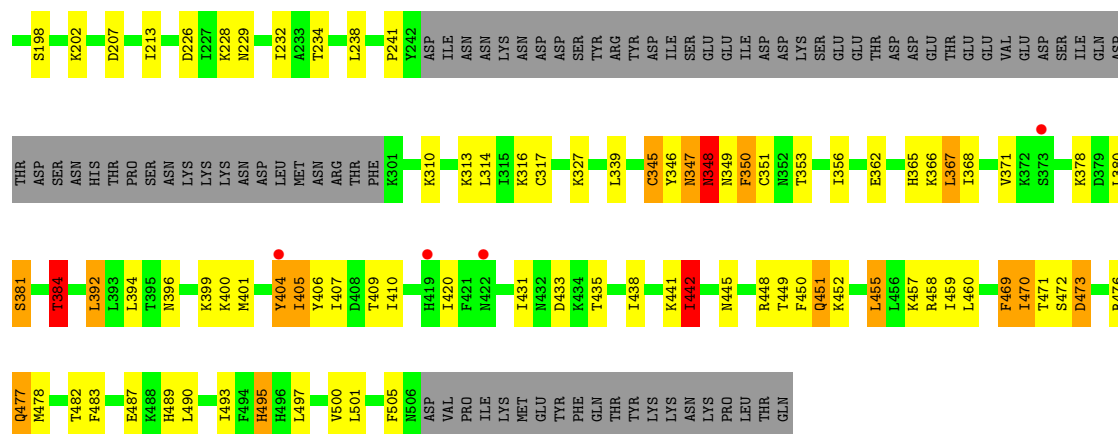
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reticulocyte binding protein 5

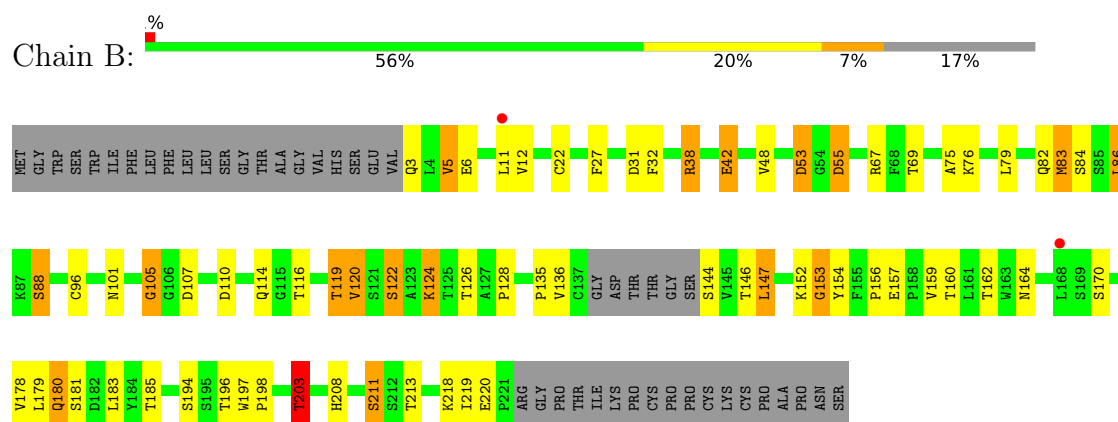


- Molecule 1: Reticulocyte binding protein 5

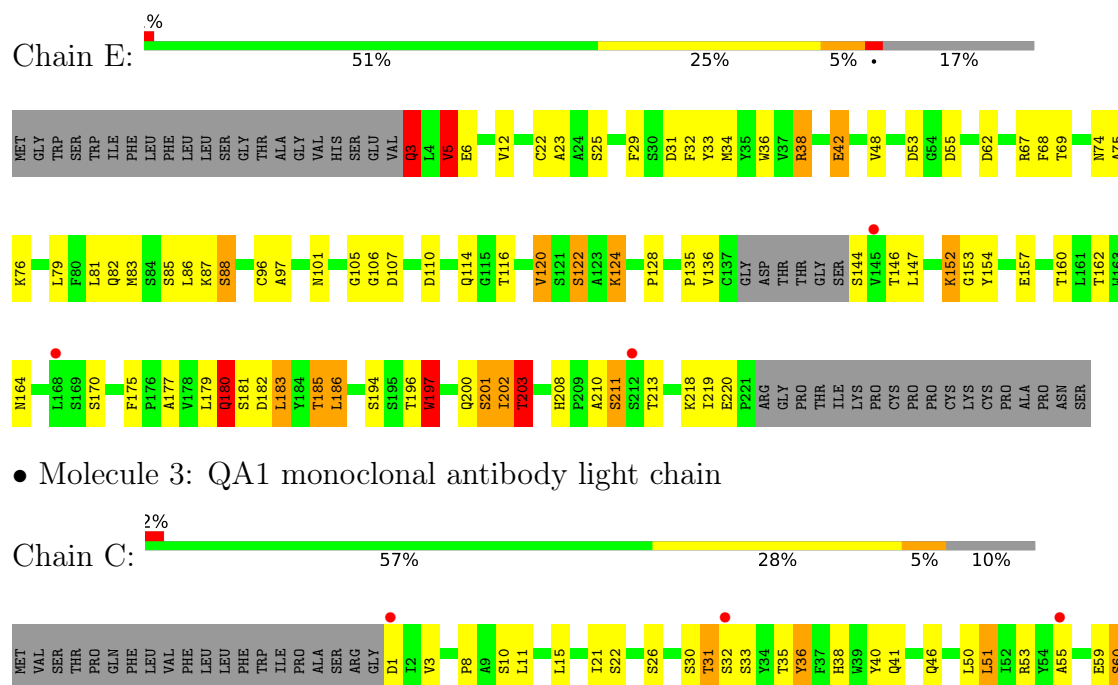


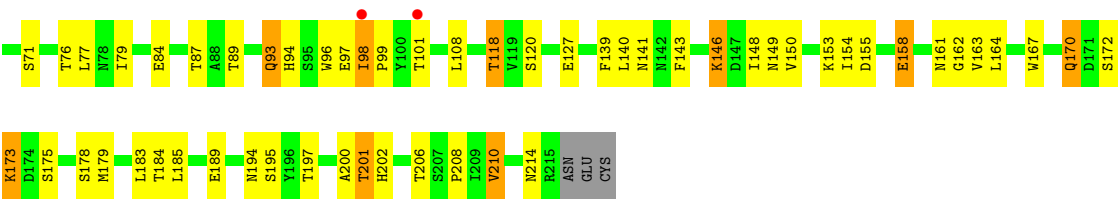


• Molecule 2: QA1 monoclonal antibody heavy chain

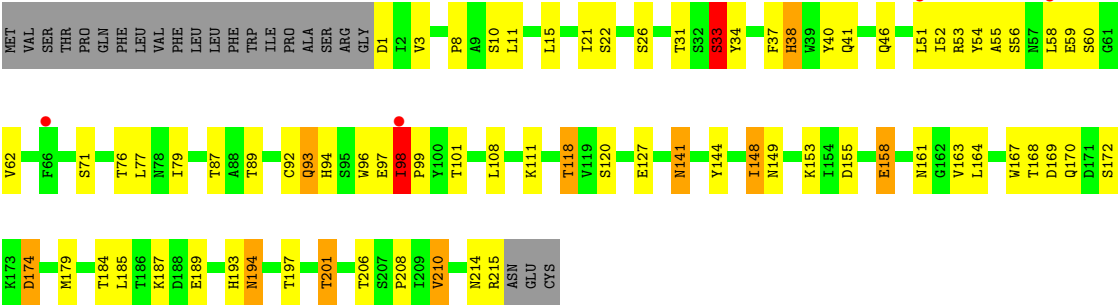


• Molecule 3: QA1 monoclonal antibody light chain





● Molecule 3: QA1 monoclonal antibody light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	65.12Å 137.30Å 228.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 3.10 46.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (46.57-3.10) 95.1 (46.57-3.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.236 , 0.281 0.253 , 0.297	Depositor DCC
R_{free} test set	1793 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 105.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11478	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

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	0.87	0/2497	1.59	31/3347 (0.9%)
1	D	0.89	1/2510 (0.0%)	1.57	20/3365 (0.6%)
2	B	0.91	1/1651 (0.1%)	1.46	19/2248 (0.8%)
2	E	0.99	4/1651 (0.2%)	1.49	23/2248 (1.0%)
3	C	0.91	0/1719	1.40	13/2340 (0.6%)
3	F	0.90	0/1719	1.35	10/2340 (0.4%)
All	All	0.91	6/11747 (0.1%)	1.49	116/15888 (0.7%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	180	GLN	CA-C	-6.64	1.50	1.53
2	B	181	SER	CA-C	-5.81	1.45	1.52
2	E	34	MET	SD-CE	-5.73	1.65	1.79
2	E	186	LEU	CA-C	-5.34	1.46	1.52
2	E	33	TYR	CA-C	5.05	1.59	1.52
1	D	451	GLN	CA-C	5.02	1.59	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	347	ASN	CA-CB-CG	9.46	122.06	112.60
2	B	159	VAL	N-CA-CB	9.22	124.97	111.52
3	C	141	ASN	N-CA-C	8.44	123.90	112.68
3	F	96	TRP	N-CA-C	8.29	120.01	110.97
3	C	96	TRP	N-CA-C	8.12	119.82	110.97
2	E	152	LYS	N-CA-C	7.79	121.21	108.52
3	C	35	THR	CB-CA-C	7.51	122.19	111.82
1	A	448	ARG	N-CA-C	7.21	117.79	108.34
2	B	105	GLY	N-CA-C	7.15	119.85	111.63
1	A	347	ASN	CA-CB-CG	7.03	119.63	112.60
2	B	5	VAL	N-CA-C	7.00	118.22	107.78
2	E	105	GLY	N-CA-C	7.00	119.68	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	SER	CA-C-N	6.88	131.56	121.31
2	B	122	SER	C-N-CA	6.88	131.56	121.31
2	E	122	SER	CA-C-N	6.83	131.48	121.31
2	E	122	SER	C-N-CA	6.83	131.48	121.31
2	E	114	GLN	N-CA-C	6.69	119.41	111.71
3	F	210	VAL	N-CA-C	6.69	117.48	108.11
3	F	98	ILE	N-CA-CB	6.57	120.40	111.21
1	A	164	LEU	N-CA-C	6.54	119.12	108.26
3	C	98	ILE	N-CA-CB	6.45	120.23	111.21
2	B	32	PHE	N-CA-C	6.41	120.27	109.76
2	E	5	VAL	N-CA-C	6.40	118.25	107.18
3	C	163	VAL	N-CA-C	6.38	117.31	108.89
3	C	143	PHE	N-CA-C	6.36	119.08	109.41
1	A	488	LYS	N-CA-C	-6.32	104.47	111.36
2	E	87	LYS	N-CA-C	-6.30	101.19	110.52
2	B	198	PRO	CA-C-N	6.29	128.95	120.65
2	B	198	PRO	C-N-CA	6.29	128.95	120.65
3	C	210	VAL	N-CA-C	6.28	116.91	107.75
2	E	32	PHE	N-CA-C	6.21	120.18	110.17
2	E	31	ASP	CA-CB-CG	6.16	118.76	112.60
1	D	442	ILE	N-CA-CB	6.14	118.43	110.57
2	E	3	GLN	CA-C-N	6.09	131.77	122.93
2	E	3	GLN	C-N-CA	6.09	131.77	122.93
1	A	442	ILE	N-CA-CB	6.09	118.37	110.57
1	A	206	VAL	N-CA-C	-6.00	104.89	110.53
1	D	489	HIS	CA-C-N	5.92	128.47	120.65
1	D	489	HIS	C-N-CA	5.92	128.47	120.65
1	D	495	HIS	N-CA-C	-5.92	104.91	111.36
2	B	135	PRO	N-CA-C	5.90	119.77	111.33
1	A	495	HIS	CA-C-N	5.85	128.05	120.44
1	A	495	HIS	C-N-CA	5.85	128.05	120.44
1	A	347	ASN	N-CA-C	-5.84	97.64	107.99
1	A	361	ASP	CA-CB-CG	5.83	118.43	112.60
3	C	118	THR	CB-CA-C	5.83	120.76	111.73
3	F	163	VAL	N-CA-C	5.81	116.56	108.89
3	C	30	SER	CA-C-N	5.81	132.16	121.94
3	C	30	SER	C-N-CA	5.81	132.16	121.94
1	A	404	TYR	N-CA-C	5.80	120.36	113.16
2	B	27	PHE	N-CA-C	5.76	117.54	108.96
1	A	494	PHE	N-CA-C	-5.75	106.42	113.50
1	D	365	HIS	N-CA-C	5.74	117.21	111.07
1	A	348	ASN	N-CA-C	-5.73	105.17	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	LYS	N-CA-C	5.73	118.30	111.71
1	D	384	THR	CA-C-N	5.70	128.18	120.38
1	D	384	THR	C-N-CA	5.70	128.18	120.38
2	B	5	VAL	N-CA-CB	5.65	120.35	111.99
2	E	68	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	207	ASP	CA-C-N	5.59	128.09	120.54
1	A	207	ASP	C-N-CA	5.59	128.09	120.54
2	E	110	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	365	HIS	N-CA-C	5.57	117.03	111.07
2	B	110	ASP	CA-CB-CG	5.56	118.16	112.60
1	D	441	LYS	N-CA-C	5.54	118.08	111.71
2	E	197	TRP	CA-C-O	-5.52	112.60	120.16
2	E	203	THR	CA-C-N	5.52	128.60	120.82
2	E	203	THR	C-N-CA	5.52	128.60	120.82
3	C	155	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	449	THR	N-CA-C	5.49	116.37	107.32
3	C	139	PHE	CA-CB-CG	5.48	119.28	113.80
3	F	187	LYS	N-CA-C	-5.46	105.41	111.36
3	F	118	THR	CB-CA-C	5.46	120.19	111.73
1	D	470	ILE	N-CA-C	5.46	115.66	110.42
2	B	31	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	448	ARG	N-CA-C	5.44	115.31	108.45
1	D	348	ASN	CA-CB-CG	5.42	118.02	112.60
1	D	452	LYS	CA-C-N	5.39	127.76	120.38
1	D	452	LYS	C-N-CA	5.39	127.76	120.38
2	E	97	ALA	N-CA-C	5.36	117.54	109.23
3	F	141	ASN	N-CA-C	5.35	122.20	110.80
2	E	182	ASP	N-CA-C	-5.35	105.03	112.30
1	A	350	PHE	CA-C-N	5.34	128.43	120.95
1	A	350	PHE	C-N-CA	5.34	128.43	120.95
2	B	126	THR	CA-C-N	5.33	128.76	120.60
2	B	126	THR	C-N-CA	5.33	128.76	120.60
3	F	174	ASP	CA-CB-CG	5.30	117.90	112.60
2	E	62	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	440	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	207	ASP	CA-CB-CG	5.29	117.89	112.60
2	E	202	ILE	CB-CA-C	5.26	118.19	110.98
2	B	203	THR	CA-C-N	5.26	129.98	122.72
2	B	203	THR	C-N-CA	5.26	129.98	122.72
1	D	392	LEU	CA-C-N	5.22	127.23	120.44
1	D	392	LEU	C-N-CA	5.22	127.23	120.44
2	B	114	GLN	N-CA-C	5.21	118.89	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	LEU	CA-C-N	5.20	127.50	120.38
1	A	380	LEU	C-N-CA	5.20	127.50	120.38
1	D	190	TYR	N-CA-C	5.18	116.92	111.28
2	E	135	PRO	N-CA-C	5.15	118.70	111.33
1	A	348	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	397	LEU	N-CA-C	-5.13	106.18	112.90
2	E	88	SER	CA-C-N	5.12	127.86	120.38
2	E	88	SER	C-N-CA	5.12	127.86	120.38
3	F	33	SER	N-CA-C	5.11	119.40	112.04
1	A	369	LEU	CA-C-N	5.11	127.38	120.38
1	A	369	LEU	C-N-CA	5.11	127.38	120.38
1	A	328	ILE	CA-C-N	5.10	127.07	120.44
1	A	328	ILE	C-N-CA	5.10	127.07	120.44
3	C	55	ALA	N-CA-C	-5.09	105.91	112.68
2	B	55	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	469	PHE	CA-C-N	5.07	126.95	120.56
1	D	469	PHE	C-N-CA	5.07	126.95	120.56
3	F	155	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	164	LEU	N-CA-C	5.06	116.66	108.26
1	A	470	ILE	N-CA-C	5.04	115.26	110.42

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	2446	0	2474	52	0
1	D	2458	0	2483	43	0
2	B	1611	0	1559	40	0
2	E	1611	0	1559	34	0
3	C	1676	0	1597	28	0
3	F	1676	0	1597	25	0
All	All	11478	0	11269	203	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 9.

All (203) 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)
2:B:75:ALA:HB1	2:E:75:ALA:HB1	1.51	0.92
1:D:179:TYR:HD2	1:D:471:THR:HG22	1.35	0.91
1:A:179:TYR:HD2	1:A:471:THR:HG22	1.34	0.90
2:B:11:LEU:HD11	2:B:156:PRO:HG3	1.53	0.90
2:B:153:GLY:HA2	2:B:183:LEU:HB3	1.60	0.81
1:A:192:SER:HA	1:A:343:LEU:HD12	1.61	0.80
3:C:38:HIS:ND1	3:C:53:ARG:O	2.13	0.79
1:D:347:ASN:HB3	1:D:350:PHE:HB2	1.65	0.78
2:B:152:LYS:HA	2:B:185:THR:HG22	1.65	0.77
2:B:11:LEU:HD11	2:B:156:PRO:CG	2.17	0.75
1:A:402:GLY:HA2	1:A:407:ILE:HD13	1.68	0.74
2:E:128:PRO:HB3	2:E:154:TYR:HB3	1.69	0.73
1:D:190:TYR:OH	1:D:207:ASP:OD1	2.06	0.73
2:E:208:HIS:ND1	2:E:211:SER:HB2	2.03	0.72
2:B:11:LEU:CD1	2:B:156:PRO:HG3	2.22	0.70
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.75	0.69
2:B:11:LEU:HD23	2:B:119:THR:HG23	1.74	0.68
2:E:153:GLY:HA2	2:E:183:LEU:HB3	1.73	0.68
2:E:208:HIS:CE1	2:E:210:ALA:HB3	2.29	0.67
1:A:405:ILE:HG12	1:A:497:LEU:HD23	1.75	0.67
1:A:179:TYR:CD2	1:A:471:THR:HG22	2.23	0.67
1:D:179:TYR:CD2	1:D:471:THR:HG22	2.24	0.66
2:B:153:GLY:CA	2:B:183:LEU:HB3	2.24	0.66
1:A:345:CYS:HB2	1:A:348:ASN:HD22	1.61	0.66
2:E:180:GLN:OE1	2:E:180:GLN:HA	1.95	0.65
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.79	0.64
2:B:180:GLN:HE22	2:B:185:THR:CG2	2.11	0.64
1:D:193:ILE:HD13	1:D:339:LEU:HD13	1.79	0.64
1:D:351:CYS:HB2	1:D:450:PHE:O	1.98	0.63
1:D:241:PRO:HG3	1:D:409:THR:HG21	1.80	0.63
1:A:348:ASN:HB2	3:C:36:TYR:OH	1.99	0.63
3:F:148:ILE:HG22	3:F:167:TRP:CH2	2.34	0.63
1:A:484:TYR:HD1	1:A:487:GLU:HG2	1.63	0.63
1:A:165:GLN:HE22	1:A:486:LYS:HZ2	1.45	0.62
1:A:501:LEU:HB3	1:D:501:LEU:HD22	1.81	0.62
2:E:6:GLU:HB3	2:E:116:THR:HG22	1.81	0.62
1:A:394:LEU:HD21	1:A:410:ILE:HB	1.83	0.61
1:A:478:MET:O	1:A:482:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:SER:N	2:E:194:SER:HG	1.99	0.60
3:F:194:ASN:O	3:F:214:ASN:HA	2.02	0.60
2:B:144:SER:N	2:B:194:SER:HG	1.99	0.60
1:D:349:ASN:ND2	3:F:34:TYR:OH	2.35	0.60
2:E:197:TRP:HH2	2:E:219:ILE:O	1.85	0.60
1:A:345:CYS:HB2	1:A:348:ASN:ND2	2.17	0.59
2:B:180:GLN:HB3	3:C:164:LEU:HD11	1.84	0.59
2:E:69:THR:HB	2:E:82:GLN:HB3	1.84	0.59
3:C:31:THR:C	3:C:33:SER:H	2.10	0.59
2:E:211:SER:HB3	2:E:213:THR:HG23	1.85	0.58
2:B:42:GLU:CD	2:B:42:GLU:H	2.11	0.58
3:C:31:THR:O	3:C:33:SER:N	2.36	0.58
3:C:31:THR:HG22	3:C:33:SER:H	1.69	0.58
1:A:476:ARG:HH11	1:A:477:GLN:HG2	1.69	0.57
2:E:42:GLU:CD	2:E:42:GLU:H	2.12	0.57
1:D:478:MET:O	1:D:482:THR:HG23	2.04	0.57
3:F:21:ILE:HD13	3:F:77:LEU:HD23	1.87	0.57
2:B:208:HIS:ND1	2:B:211:SER:HB2	2.20	0.56
1:D:347:ASN:C	1:D:349:ASN:H	2.13	0.56
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.87	0.56
2:E:124:LYS:HE2	2:E:124:LYS:H	1.71	0.56
2:B:124:LYS:HE2	2:B:124:LYS:H	1.70	0.56
2:E:88:SER:HA	2:E:120:VAL:HB	1.87	0.56
2:B:38:ARG:HG2	2:B:48:VAL:HG23	1.88	0.56
1:D:180:THR:HA	1:D:471:THR:HG21	1.88	0.56
2:E:5:VAL:HG23	2:E:23:ALA:HB3	1.88	0.56
1:A:431:ILE:HD11	1:A:473:ASP:HA	1.88	0.55
1:D:371:VAL:HG11	1:D:435:THR:HG21	1.89	0.55
3:C:21:ILE:HD13	3:C:77:LEU:HD23	1.88	0.55
1:D:431:ILE:HD11	1:D:473:ASP:HA	1.89	0.55
1:A:393:LEU:O	1:A:397:LEU:HB2	2.07	0.55
1:A:451:GLN:OE1	1:A:453:ASP:HB2	2.06	0.55
2:B:6:GLU:HB3	2:B:116:THR:HG22	1.88	0.54
1:A:505:PHE:CE2	1:D:501:LEU:HD23	2.42	0.54
2:B:105:GLY:HA2	3:C:36:TYR:OH	2.08	0.53
1:D:476:ARG:HH11	1:D:477:GLN:HG2	1.73	0.53
1:A:180:THR:HA	1:A:471:THR:HG21	1.91	0.53
2:E:38:ARG:HG2	2:E:48:VAL:HG23	1.90	0.53
1:A:371:VAL:HG11	1:A:435:THR:HG21	1.90	0.53
3:C:97:GLU:HB3	3:C:99:PRO:HD2	1.90	0.53
3:F:148:ILE:HG22	3:F:167:TRP:CZ3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:HE22	1:A:486:LYS:NZ	2.07	0.52
2:B:11:LEU:HD23	2:B:119:THR:CG2	2.39	0.52
3:F:31:THR:HG23	3:F:33:SER:H	1.74	0.52
3:F:52:ILE:HG22	3:F:54:TYR:O	2.09	0.52
1:A:197:SER:HB2	2:B:53:ASP:OD1	2.09	0.52
2:B:88:SER:HA	2:B:120:VAL:HB	1.90	0.52
2:B:180:GLN:NE2	2:B:185:THR:HG23	2.26	0.51
2:E:38:ARG:HG2	2:E:48:VAL:CG2	2.40	0.51
2:B:38:ARG:HG2	2:B:48:VAL:CG2	2.40	0.51
2:B:180:GLN:HE22	2:B:185:THR:HG23	1.76	0.51
1:D:396:ASN:O	1:D:399:LYS:HB3	2.11	0.51
1:D:350:PHE:CZ	3:F:98:ILE:HD12	2.46	0.51
2:B:11:LEU:HD21	2:B:156:PRO:HB3	1.93	0.51
3:F:97:GLU:HB3	3:F:99:PRO:HD2	1.91	0.51
2:E:180:GLN:HG2	3:F:164:LEU:HD11	1.93	0.51
1:A:163:ILE:C	1:A:164:LEU:HG	2.36	0.50
2:B:83:MET:HB3	2:B:86:LEU:HD23	1.92	0.50
1:A:491:ASN:HA	1:A:494:PHE:HB2	1.94	0.50
3:C:194:ASN:OD1	3:C:214:ASN:HB3	2.11	0.50
1:A:165:GLN:NE2	1:A:486:LYS:NZ	2.59	0.50
2:E:6:GLU:HB3	2:E:116:THR:CG2	2.42	0.50
2:E:177:ALA:HB2	2:E:186:LEU:HD23	1.94	0.50
3:C:31:THR:C	3:C:33:SER:N	2.70	0.49
1:D:345:CYS:HB2	1:D:348:ASN:HD22	1.77	0.49
3:C:40:TYR:HE2	3:C:93:GLN:HG2	1.77	0.49
1:A:457:LYS:HA	1:A:460:LEU:HD12	1.95	0.49
2:B:211:SER:HB3	2:B:213:THR:HG23	1.94	0.49
3:F:40:TYR:HE2	3:F:93:GLN:HG2	1.78	0.48
3:F:167:TRP:CD1	3:F:167:TRP:N	2.81	0.48
1:D:190:TYR:HD1	1:D:194:TYR:CE2	2.30	0.48
2:B:152:LYS:HD3	2:B:185:THR:HG21	1.95	0.48
1:A:165:GLN:C	1:A:482:THR:HG22	2.39	0.48
2:B:178:VAL:CG2	3:C:164:LEU:HD13	2.44	0.48
2:E:175:PHE:CD2	3:F:168:THR:HG23	2.50	0.47
1:D:193:ILE:HD11	1:D:202:LYS:HD3	1.95	0.47
1:D:457:LYS:HA	1:D:460:LEU:HD12	1.96	0.47
3:C:148:ILE:HG13	3:C:202:HIS:HB2	1.96	0.47
3:C:167:TRP:CD1	3:C:167:TRP:N	2.82	0.47
2:B:6:GLU:HB3	2:B:116:THR:CG2	2.44	0.47
1:D:351:CYS:O	1:D:449:THR:HA	2.15	0.47
1:A:404:TYR:C	1:A:406:TYR:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:TYR:O	2:E:106:GLY:HA2	2.15	0.46
3:F:38:HIS:ND1	3:F:53:ARG:O	2.49	0.46
1:A:438:ILE:O	1:A:442:ILE:HG13	2.15	0.46
1:A:166:GLU:N	1:A:482:THR:HG22	2.31	0.46
1:A:420:ILE:HG21	1:A:483:PHE:HB2	1.98	0.46
1:D:229:ASN:HA	1:D:232:ILE:HD12	1.98	0.46
1:D:380:LEU:O	1:D:384:THR:OG1	2.34	0.46
3:C:154:ILE:HD11	3:C:183:LEU:HD21	1.98	0.46
2:B:69:THR:HB	2:B:82:GLN:HB3	1.97	0.46
1:D:405:ILE:HG13	1:D:406:TYR:CE2	2.51	0.46
3:F:8:PRO:HG3	3:F:11:LEU:HD13	1.98	0.46
2:E:197:TRP:HZ3	2:E:202:ILE:H	1.64	0.45
1:A:506:ASN:HD21	1:D:399:LYS:HD2	1.80	0.45
1:D:420:ILE:HG21	1:D:483:PHE:HB2	1.99	0.45
2:E:152:LYS:HE2	2:E:185:THR:HG21	1.99	0.45
3:C:50:LEU:HD21	3:C:53:ARG:HD2	1.98	0.45
1:A:351:CYS:O	1:A:449:THR:HA	2.16	0.45
3:F:59:GLU:HB2	3:F:62:VAL:CG2	2.46	0.45
1:D:438:ILE:O	1:D:442:ILE:HG13	2.16	0.45
1:D:180:THR:CA	1:D:471:THR:HG21	2.47	0.45
1:A:378:LYS:HA	1:A:381:SER:HB2	1.99	0.45
3:C:41:GLN:HB2	3:C:51:LEU:HD12	1.98	0.45
3:C:170:GLN:HE21	3:C:175:SER:HB3	1.80	0.45
1:A:312:LYS:HA	1:A:315:ILE:HD12	1.99	0.44
1:A:347:ASN:HB3	1:A:350:PHE:H	1.82	0.44
1:D:234:THR:HG21	1:D:310:LYS:HG3	1.98	0.44
3:F:193:HIS:O	3:F:215:ARG:NH1	2.48	0.44
1:A:180:THR:CA	1:A:471:THR:HG21	2.47	0.44
1:A:383:MET:HG2	1:A:483:PHE:CE2	2.52	0.44
2:B:42:GLU:CD	2:B:42:GLU:N	2.74	0.44
1:A:479:LEU:HA	1:A:482:THR:OG1	2.18	0.44
3:C:146:LYS:O	3:C:167:TRP:HZ3	2.00	0.44
1:D:401:MET:HE1	1:D:501:LEU:HD21	1.99	0.44
2:B:75:ALA:HB1	2:E:75:ALA:CB	2.35	0.44
3:F:185:LEU:HD22	3:F:189:GLU:HB3	2.00	0.43
2:B:178:VAL:HG21	3:C:164:LEU:HD13	1.99	0.43
3:F:41:GLN:HB2	3:F:51:LEU:HD12	1.99	0.43
1:A:188:LEU:HD21	1:A:460:LEU:HD23	2.00	0.43
1:A:347:ASN:OD1	1:A:350:PHE:HB2	2.19	0.43
2:E:42:GLU:CD	2:E:42:GLU:N	2.76	0.43
1:D:505:PHE:O	1:D:505:PHE:CG	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:208:HIS:NE2	2:E:210:ALA:HB3	2.33	0.43
3:F:201:THR:HG22	3:F:208:PRO:HB3	2.01	0.43
1:A:502:GLN:O	1:D:399:LYS:NZ	2.51	0.43
1:D:410:ILE:HD11	1:D:493:ILE:HG22	2.00	0.43
2:B:22:CYS:HB3	2:B:79:LEU:HB3	2.01	0.42
3:F:94:HIS:CE1	3:F:101:THR:H	2.37	0.42
3:F:111:LYS:HA	3:F:144:TYR:OH	2.19	0.42
1:A:484:TYR:CD1	1:A:487:GLU:HG2	2.51	0.42
1:A:485:SER:HA	1:A:488:LYS:HE3	2.01	0.42
1:A:505:PHE:HE2	1:D:501:LEU:HD23	1.83	0.42
2:B:203:THR:HB	2:B:218:LYS:HA	2.01	0.42
1:D:378:LYS:HA	1:D:381:SER:HB2	2.00	0.42
2:B:76:LYS:HD3	2:E:76:LYS:HA	2.01	0.42
3:F:37:PHE:CZ	3:F:92:CYS:HB2	2.55	0.42
3:F:54:TYR:O	3:F:56:SER:N	2.52	0.42
1:A:437:ILE:HG21	1:A:465:GLU:HG2	2.02	0.42
1:D:188:LEU:HD21	1:D:460:LEU:HD23	2.00	0.42
2:E:3:GLN:N	2:E:25:SER:O	2.53	0.42
3:C:94:HIS:CE1	3:C:101:THR:H	2.37	0.42
1:A:367:LEU:HB3	1:A:469:PHE:CE2	2.55	0.41
2:B:11:LEU:CG	2:B:156:PRO:HG3	2.50	0.41
2:B:180:GLN:HB3	2:B:180:GLN:HE21	1.73	0.41
3:C:185:LEU:HD22	3:C:189:GLU:HB3	2.01	0.41
1:D:351:CYS:HB3	1:D:455:LEU:HG	2.02	0.41
3:C:201:THR:HG22	3:C:208:PRO:HB3	2.01	0.41
2:E:29:PHE:CD2	2:E:74:ASN:HA	2.55	0.41
1:A:397:LEU:O	1:A:401:MET:HB3	2.20	0.41
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.89	0.41
1:D:405:ILE:HG13	1:D:406:TYR:CD2	2.56	0.41
3:C:53:ARG:HD3	3:C:59:GLU:OE1	2.21	0.41
3:C:8:PRO:HG3	3:C:11:LEU:HD13	2.03	0.41
3:C:140:LEU:HD21	3:C:200:ALA:CB	2.51	0.41
1:A:227:ILE:H	1:A:227:ILE:HD12	1.87	0.40
1:A:367:LEU:HB3	1:A:469:PHE:HE2	1.86	0.40
1:D:367:LEU:HB3	1:D:469:PHE:CE2	2.56	0.40
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.56	0.40
2:B:147:LEU:HD12	2:B:219:ILE:HD12	2.03	0.40
1:D:353:THR:HG22	1:D:356:ILE:HD12	2.01	0.40
3:F:153:LYS:HA	3:F:158:GLU:HA	2.03	0.40
1:A:351:CYS:HB2	1:A:450:PHE:O	2.21	0.40
3:C:153:LYS:HA	3:C:158:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:203:THR:HB	2:E:218:LYS:HA	2.03	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	284/526 (54%)	261 (92%)	19 (7%)	4 (1%)	9	34
1	D	285/526 (54%)	261 (92%)	22 (8%)	2 (1%)	18	49
2	B	209/258 (81%)	186 (89%)	20 (10%)	3 (1%)	9	34
2	E	209/258 (81%)	182 (87%)	23 (11%)	4 (2%)	6	27
3	C	213/238 (90%)	190 (89%)	15 (7%)	8 (4%)	2	15
3	F	213/238 (90%)	187 (88%)	21 (10%)	5 (2%)	5	23
All	All	1413/2044 (69%)	1267 (90%)	120 (8%)	26 (2%)	6	28

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	TYR
3	C	172	SER
2	E	55	ASP
2	E	197	TRP
3	F	55	ALA
1	A	399	LYS
1	A	402	GLY
1	A	405	ILE
2	B	55	ASP
2	B	153	GLY
3	C	32	SER

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Mol	Chain	Res	Type
3	C	162	GLY
2	E	181	SER
3	F	58	LEU
2	B	197	TRP
3	C	170	GLN
3	F	170	GLN
3	C	60	SER
3	C	161	ASN
1	D	348	ASN
2	E	201	SER
3	F	172	SER
3	C	173	LYS
3	F	161	ASN
3	C	36	TYR
1	D	404	TYR

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	279/511 (55%)	227 (81%)	52 (19%)	1	8
1	D	280/511 (55%)	232 (83%)	48 (17%)	2	10
2	B	182/219 (83%)	150 (82%)	32 (18%)	2	9
2	E	182/219 (83%)	150 (82%)	32 (18%)	2	9
3	C	190/211 (90%)	155 (82%)	35 (18%)	1	8
3	F	190/211 (90%)	156 (82%)	34 (18%)	2	9
All	All	1303/1882 (69%)	1070 (82%)	233 (18%)	2	9

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	165	GLN
1	A	168	GLU

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Mol	Chain	Res	Type
1	A	171	LEU
1	A	178	HIS
1	A	180	THR
1	A	189	SER
1	A	193	ILE
1	A	198	SER
1	A	203	TYR
1	A	213	ILE
1	A	226	ASP
1	A	238	LEU
1	A	309	THR
1	A	313	LYS
1	A	314	LEU
1	A	316	LYS
1	A	317	CYS
1	A	318	ILE
1	A	327	LYS
1	A	347	ASN
1	A	362	GLU
1	A	366	LYS
1	A	367	LEU
1	A	368	ILE
1	A	381	SER
1	A	389	GLN
1	A	392	LEU
1	A	393	LEU
1	A	398	ASN
1	A	401	MET
1	A	407	ILE
1	A	410	ILE
1	A	413	ILE
1	A	433	ASP
1	A	442	ILE
1	A	445	ASN
1	A	451	GLN
1	A	455	LEU
1	A	458	ARG
1	A	459	ILE
1	A	470	ILE
1	A	472	SER
1	A	473	ASP
1	A	477	GLN

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Mol	Chain	Res	Type
1	A	487	GLU
1	A	490	LEU
1	A	493	ILE
1	A	495	HIS
1	A	496	HIS
1	A	497	LEU
1	A	501	LEU
2	B	3	GLN
2	B	5	VAL
2	B	12	VAL
2	B	38	ARG
2	B	42	GLU
2	B	53	ASP
2	B	67	ARG
2	B	83	MET
2	B	84	SER
2	B	86	LEU
2	B	88	SER
2	B	96	CYS
2	B	101	ASN
2	B	107	ASP
2	B	119	THR
2	B	120	VAL
2	B	122	SER
2	B	124	LYS
2	B	136	VAL
2	B	146	THR
2	B	147	LEU
2	B	157	GLU
2	B	160	THR
2	B	162	THR
2	B	164	ASN
2	B	170	SER
2	B	179	LEU
2	B	180	GLN
2	B	196	THR
2	B	203	THR
2	B	211	SER
2	B	220	GLU
3	C	1	ASP
3	C	3	VAL
3	C	10	SER

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Mol	Chain	Res	Type
3	C	15	LEU
3	C	22	SER
3	C	26	SER
3	C	31	THR
3	C	46	GLN
3	C	51	LEU
3	C	60	SER
3	C	71	SER
3	C	76	THR
3	C	79	ILE
3	C	84	GLU
3	C	87	THR
3	C	89	THR
3	C	93	GLN
3	C	98	ILE
3	C	108	LEU
3	C	118	THR
3	C	120	SER
3	C	127	GLU
3	C	146	LYS
3	C	149	ASN
3	C	150	VAL
3	C	158	GLU
3	C	173	LYS
3	C	178	SER
3	C	179	MET
3	C	184	THR
3	C	195	SER
3	C	197	THR
3	C	201	THR
3	C	206	THR
3	C	210	VAL
1	D	162	ASP
1	D	165	GLN
1	D	168	GLU
1	D	171	LEU
1	D	172	ASP
1	D	180	THR
1	D	189	SER
1	D	193	ILE
1	D	198	SER
1	D	213	ILE

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Mol	Chain	Res	Type
1	D	226	ASP
1	D	228	LYS
1	D	238	LEU
1	D	313	LYS
1	D	314	LEU
1	D	316	LYS
1	D	317	CYS
1	D	327	LYS
1	D	345	CYS
1	D	350	PHE
1	D	362	GLU
1	D	366	LYS
1	D	367	LEU
1	D	368	ILE
1	D	381	SER
1	D	384	THR
1	D	392	LEU
1	D	394	LEU
1	D	400	LYS
1	D	404	TYR
1	D	405	ILE
1	D	407	ILE
1	D	433	ASP
1	D	442	ILE
1	D	445	ASN
1	D	451	GLN
1	D	455	LEU
1	D	458	ARG
1	D	459	ILE
1	D	470	ILE
1	D	472	SER
1	D	473	ASP
1	D	477	GLN
1	D	487	GLU
1	D	490	LEU
1	D	495	HIS
1	D	497	LEU
1	D	500	VAL
2	E	3	GLN
2	E	5	VAL
2	E	12	VAL
2	E	38	ARG

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Mol	Chain	Res	Type
2	E	42	GLU
2	E	53	ASP
2	E	67	ARG
2	E	85	SER
2	E	96	CYS
2	E	101	ASN
2	E	107	ASP
2	E	120	VAL
2	E	122	SER
2	E	124	LYS
2	E	136	VAL
2	E	146	THR
2	E	147	LEU
2	E	157	GLU
2	E	160	THR
2	E	162	THR
2	E	164	ASN
2	E	170	SER
2	E	179	LEU
2	E	180	GLN
2	E	183	LEU
2	E	185	THR
2	E	196	THR
2	E	200	GLN
2	E	201	SER
2	E	203	THR
2	E	211	SER
2	E	220	GLU
3	F	1	ASP
3	F	3	VAL
3	F	10	SER
3	F	15	LEU
3	F	22	SER
3	F	26	SER
3	F	33	SER
3	F	38	HIS
3	F	46	GLN
3	F	60	SER
3	F	71	SER
3	F	76	THR
3	F	79	ILE
3	F	87	THR

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Mol	Chain	Res	Type
3	F	89	THR
3	F	93	GLN
3	F	98	ILE
3	F	108	LEU
3	F	118	THR
3	F	120	SER
3	F	127	GLU
3	F	141	ASN
3	F	148	ILE
3	F	149	ASN
3	F	158	GLU
3	F	169	ASP
3	F	174	ASP
3	F	179	MET
3	F	184	THR
3	F	194	ASN
3	F	197	THR
3	F	201	THR
3	F	206	THR
3	F	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	225	ASN
1	A	320	ASN
1	A	326	ASN
1	A	396	ASN
1	A	445	ASN
1	A	477	GLN
1	A	506	ASN
2	B	173	HIS
2	B	180	GLN
3	C	94	HIS
3	C	128	GLN
3	C	142	ASN
1	D	229	ASN
1	D	320	ASN
1	D	321	HIS
1	D	326	ASN
1	D	338	ASN

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Mol	Chain	Res	Type
1	D	348	ASN
1	D	349	ASN
1	D	385	ASN
1	D	388	GLN
1	D	389	GLN
1	D	445	ASN
1	D	477	GLN
2	E	74	ASN
2	E	101	ASN
2	E	173	HIS
3	F	94	HIS
3	F	128	GLN
3	F	141	ASN
3	F	142	ASN
3	F	165	ASN
3	F	193	HIS
3	F	214	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](#)

There are no ligands in this entry.

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	288/526 (54%)	0.29	10 (3%)	47 27	67, 108, 171, 199	0
1	D	289/526 (54%)	0.22	7 (2%)	59 38	77, 113, 174, 203	0
2	B	213/258 (82%)	-0.00	2 (0%)	81 63	51, 84, 123, 136	0
2	E	213/258 (82%)	0.03	3 (1%)	73 53	51, 84, 119, 142	0
3	C	215/238 (90%)	0.19	5 (2%)	61 39	57, 90, 122, 141	1 (0%)
3	F	215/238 (90%)	0.22	4 (1%)	66 45	55, 99, 129, 143	1 (0%)
All	All	1433/2044 (70%)	0.17	31 (2%)	62 41	51, 97, 153, 203	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	66	PHE	3.7
1	A	405	ILE	3.3
1	A	226	ASP	3.3
1	D	160	SER	3.2
3	C	1	ASP	2.9
1	D	422	ASN	2.9
1	D	165	GLN	2.8
2	B	11	LEU	2.7
2	E	145	VAL	2.5
2	E	212	SER	2.5
1	D	162	ASP	2.5
3	C	98	ILE	2.4
3	F	98	ILE	2.4
1	A	309	THR	2.4
3	F	51	LEU	2.4
1	A	192	SER	2.3
1	A	234	THR	2.2
1	A	313	LYS	2.2
1	D	373	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	55	ALA	2.2
3	C	32	SER	2.2
3	C	101	THR	2.1
1	A	493	ILE	2.1
1	A	413	ILE	2.1
2	E	168	LEU	2.1
3	F	58	LEU	2.1
1	A	169	GLY	2.1
2	B	168	LEU	2.1
1	A	350	PHE	2.1
1	D	419	HIS	2.0
1	D	404	TYR	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.