



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:42 AM UTC

PDB ID : 4XMN / pdb_00004xmnn
Title : Structure of the yeast coat nucleoporin complex, space group P212121
Authors : Stuwe, T.; Correia, A.R.; Lin, D.H.; Paduch, M.; Lu, V.T.; Kossiakoff, A.A.;
Hoelz, A.
Deposited on : 2015-01-14
Resolution : 7.60 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:

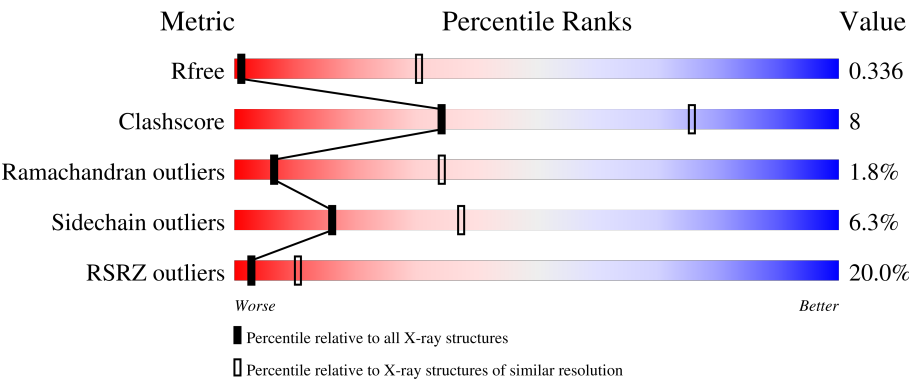
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 7.60 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	297	13% 65% 24% • 8%
2	B	652	16% 56% 17% • 23%
3	F	454	13% 68% 21% • 8%
4	E	1045	20% 72% 13% • 14%
5	D	685	5% 21% 79%

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Mol	Chain	Length	Quality of chain
6	L	217	18% 78% 16%
7	H	267	17% 65% 13% 19%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19816 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q04491

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	503	Total	C	N	O	S	Se	0	0	0
			3765	2393	640	722	6	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MSE	-	initiating methionine	UNP P49687
B	62	GLY	-	expression tag	UNP P49687
B	63	SER	-	expression tag	UNP P49687
B	64	SER	-	expression tag	UNP P49687
B	65	HIS	-	expression tag	UNP P49687
B	66	HIS	-	expression tag	UNP P49687
B	67	HIS	-	expression tag	UNP P49687
B	68	HIS	-	expression tag	UNP P49687
B	69	HIS	-	expression tag	UNP P49687
B	70	HIS	-	expression tag	UNP P49687
B	71	SER	-	expression tag	UNP P49687
B	72	ASP	-	expression tag	UNP P49687
B	73	GLN	-	expression tag	UNP P49687
B	74	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	419	Total	C	N	O	S	Se	0	0	0
			3404	2178	557	657	5	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P52891
F	-1	PRO	-	expression tag	UNP P52891
F	0	HIS	-	expression tag	UNP P52891
F	1	MSE	-	expression tag	UNP P52891

- Molecule 4 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	896	Total	C	N	O	S	0	0	0
			6622	4232	1099	1275	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	MET	-	initiating methionine	UNP P35729
E	-6	HIS	-	expression tag	UNP P35729
E	-5	HIS	-	expression tag	UNP P35729
E	-4	HIS	-	expression tag	UNP P35729
E	-3	HIS	-	expression tag	UNP P35729
E	-2	HIS	-	expression tag	UNP P35729
E	-1	HIS	-	expression tag	UNP P35729
E	0	SER	-	expression tag	UNP P35729

- Molecule 5 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	143	Total	C	N	O	0	0	0
			713	427	143	143			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	60	MSE	-	initiating methionine	UNP P46673
D	61	GLY	-	expression tag	UNP P46673
D	62	SER	-	expression tag	UNP P46673

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Chain	Residue	Modelled	Actual	Comment	Reference
D	63	SER	-	expression tag	UNP P46673
D	64	HIS	-	expression tag	UNP P46673
D	65	HIS	-	expression tag	UNP P46673
D	66	HIS	-	expression tag	UNP P46673
D	67	HIS	-	expression tag	UNP P46673
D	68	HIS	-	expression tag	UNP P46673
D	69	HIS	-	expression tag	UNP P46673
D	70	SER	-	expression tag	UNP P46673
D	71	ASP	-	expression tag	UNP P46673
D	72	GLN	-	expression tag	UNP P46673
D	744	MSE	-	expression tag	UNP P46673

- Molecule 6 is a protein called Antibody 87 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	209	Total	C	N	O	S	0	0	0
			1592	991	269	326	6			

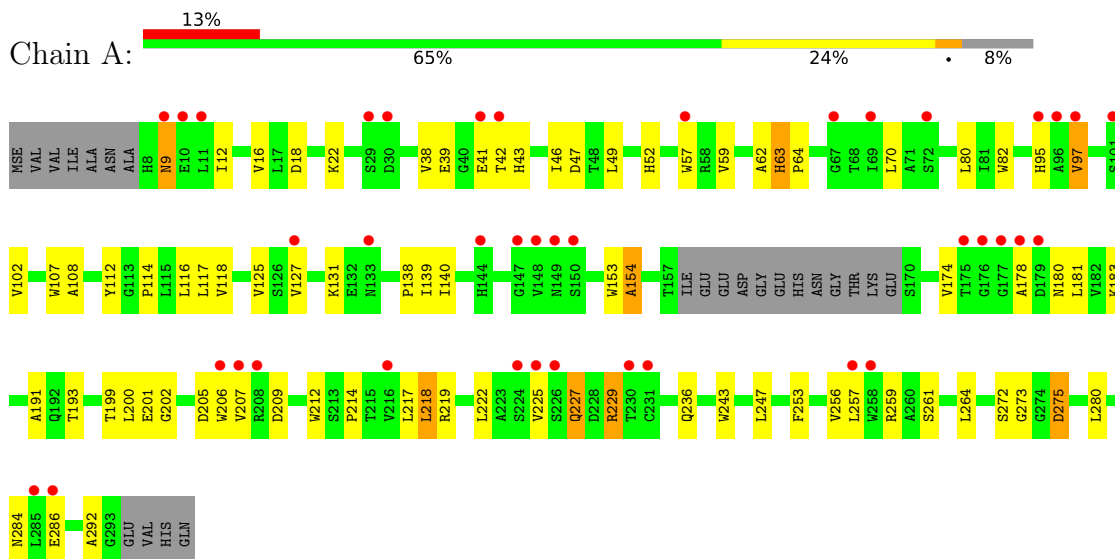
- Molecule 7 is a protein called Antibody 87 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	215	Total	C	N	O	S	0	0	0
			1560	977	265	312	6			

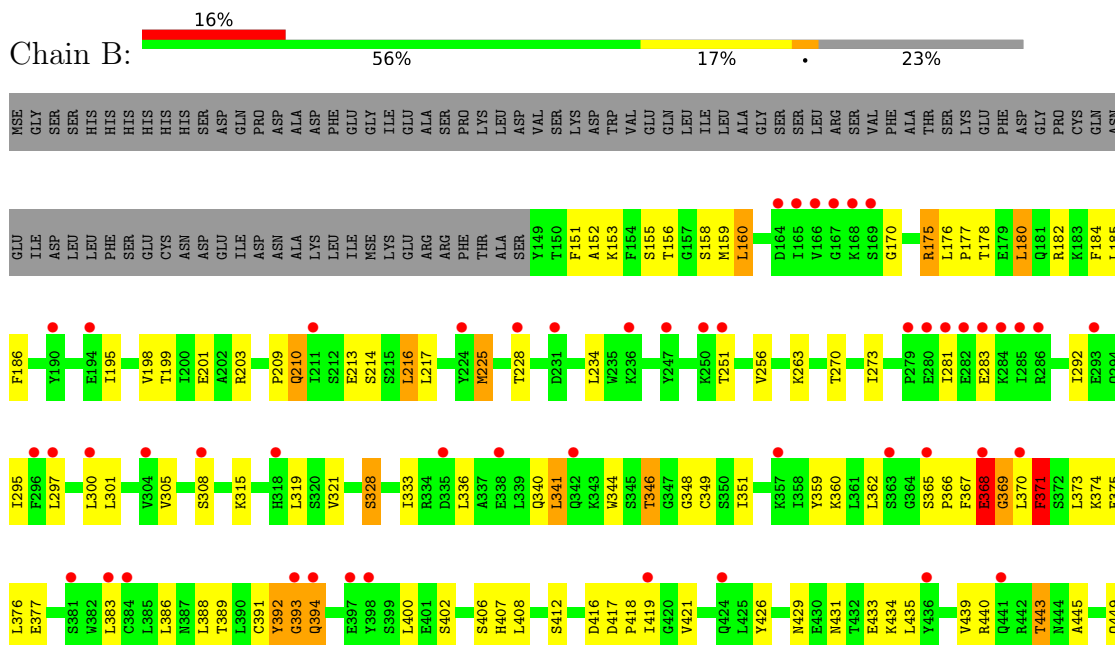
3 Residue-property plots

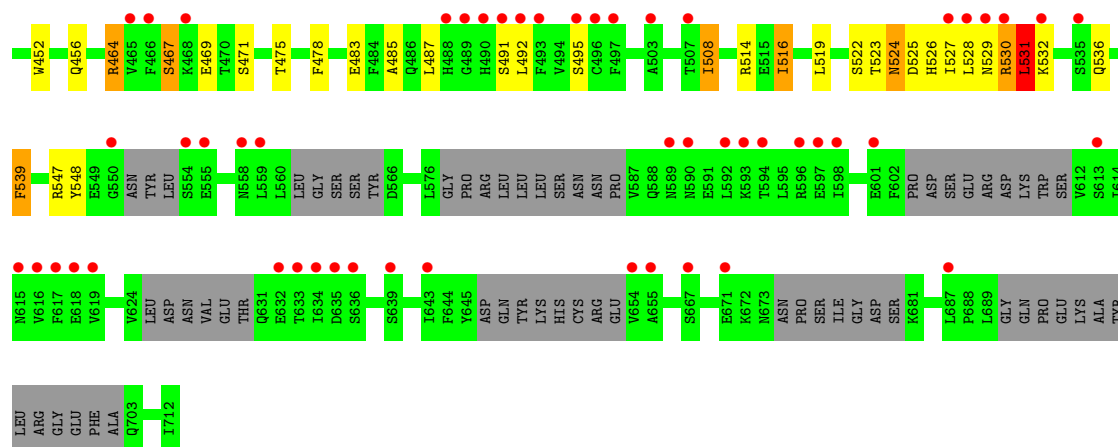
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein transport protein SEC13

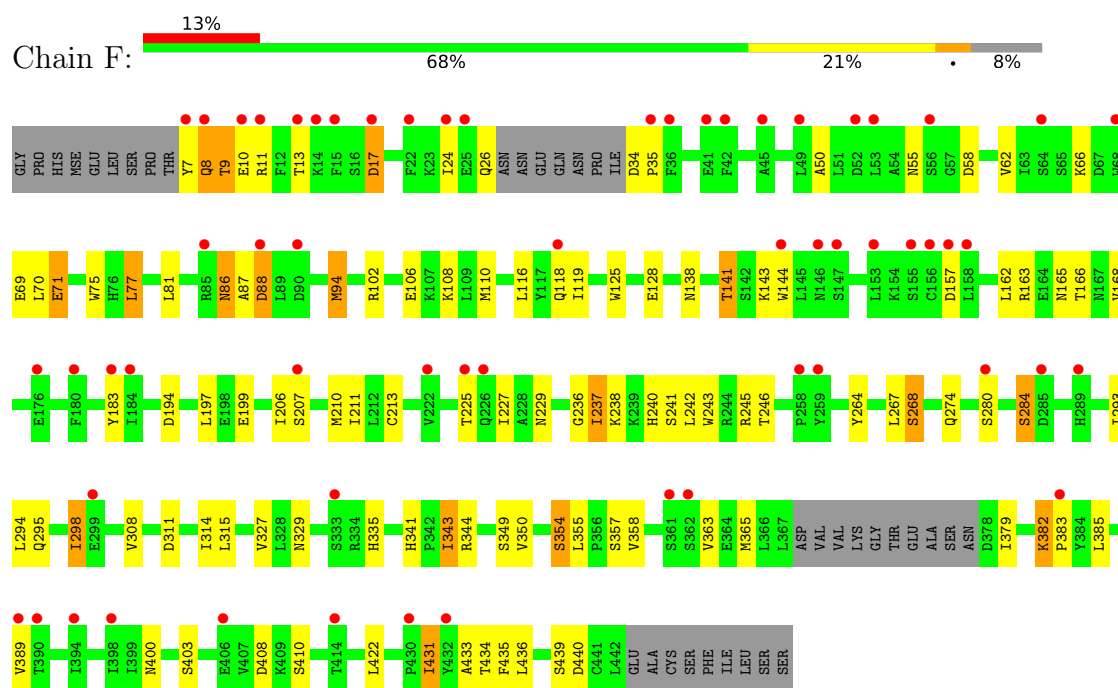


• Molecule 2: Nucleoporin NUP145

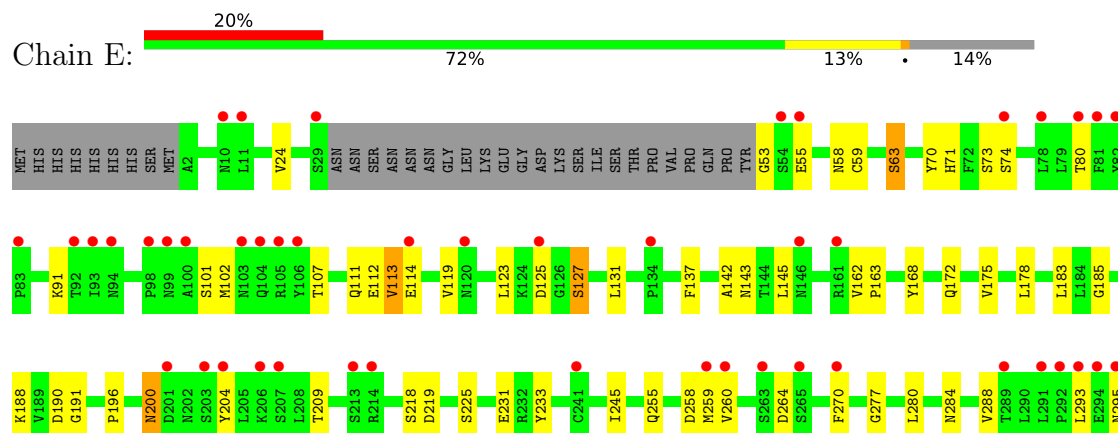




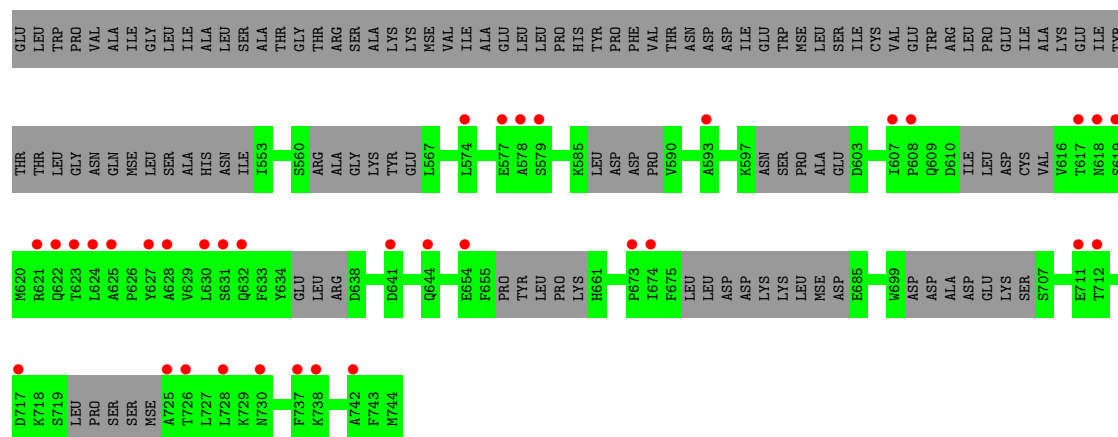
• Molecule 3: Nucleoporin NUP84



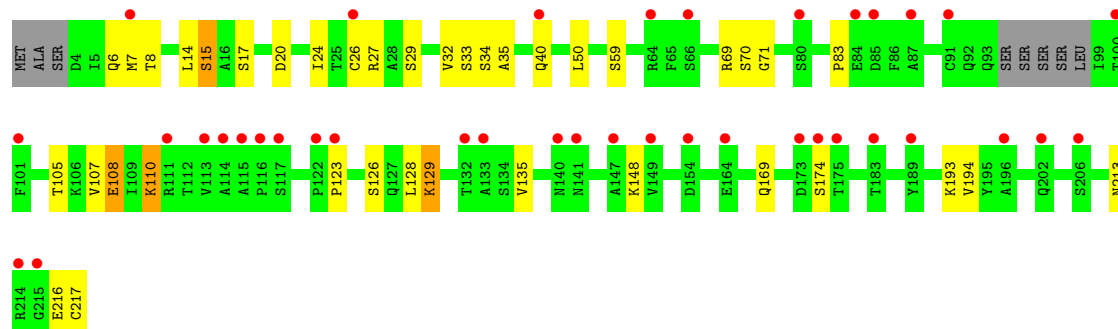
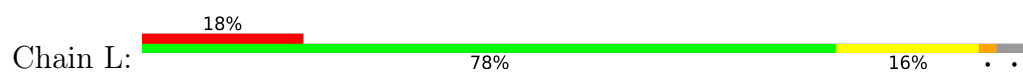
• Molecule 4: Nucleoporin NUP120



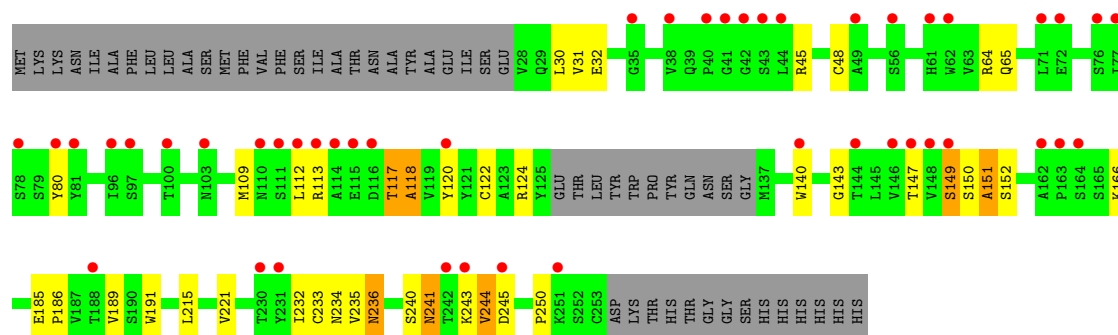




● Molecule 6: Antibody 87 light chain



● Molecule 7: Antibody 87 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	117.13Å 179.95Å 441.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 7.60 49.61 – 7.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.61-7.60) 99.2 (49.61-7.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 7.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1809)	Depositor
R, R_{free}	0.318 , 0.347 0.311 , 0.336	Depositor DCC
R_{free} test set	1355 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	597.7	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 823.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	19816	wwPDB-VP
Average B, all atoms (Å ²)	536.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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	0.39	1/2220 (0.0%)	0.86	5/3028 (0.2%)
2	B	0.39	0/3813	0.94	3/5147 (0.1%)
3	F	0.41	0/3465	0.94	5/4693 (0.1%)
4	E	0.33	0/6730	0.80	2/9158 (0.0%)
5	D	0.28	0/700	0.91	0/958
6	L	0.39	0/1623	0.95	2/2199 (0.1%)
7	H	0.39	0/1594	1.12	14/2172 (0.6%)
All	All	0.37	1/20145 (0.0%)	0.90	31/27355 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	THR	CA-C	5.19	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	244	VAL	N-CA-C	8.56	120.09	108.11
1	A	154	ALA	CA-C-N	-8.39	112.08	120.31
1	A	154	ALA	C-N-CA	-8.39	112.08	120.31
7	H	140	TRP	N-CA-C	7.65	121.39	109.07
3	F	335	HIS	CA-C-N	7.16	126.68	119.24
3	F	335	HIS	C-N-CA	7.16	126.68	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	818	PRO	N-CA-CB	6.63	110.29	103.00
6	L	32	VAL	N-CA-C	-6.52	100.55	109.55
2	B	369	GLY	N-CA-C	6.50	120.80	111.12
7	H	117	THR	N-CA-C	-6.34	101.73	110.35
7	H	245	ASP	N-CA-C	-6.19	97.00	108.02
1	A	42	THR	N-CA-C	6.18	118.53	108.63
7	H	189	VAL	N-CA-C	6.10	116.66	108.11
7	H	30	LEU	N-CA-C	-6.07	100.39	110.17
7	H	232	ILE	N-CA-C	6.05	116.73	107.77
3	F	168	VAL	N-CA-C	6.00	116.66	110.36
6	L	128	LEU	N-CA-C	-5.69	105.08	111.28
2	B	516	ILE	N-CA-C	5.66	117.07	110.62
7	H	140	TRP	CA-C-N	5.64	125.46	120.10
7	H	140	TRP	C-N-CA	5.64	125.46	120.10
1	A	63	HIS	CA-C-N	5.58	125.25	119.56
1	A	63	HIS	C-N-CA	5.58	125.25	119.56
7	H	221	VAL	CA-C-N	-5.54	114.22	119.76
7	H	221	VAL	C-N-CA	-5.54	114.22	119.76
2	B	256	VAL	N-CA-C	-5.50	105.14	110.42
7	H	122	CYS	N-CA-C	-5.49	98.60	108.48
3	F	24	ILE	N-CA-C	5.42	120.50	113.07
7	H	185	GLU	C-N-CD	-5.39	108.75	120.60
3	F	236	GLY	N-CA-C	-5.22	103.95	112.83
7	H	152	SER	N-CA-C	5.20	116.64	110.19
4	E	763	THR	N-CA-C	-5.08	105.93	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	GLU	Mainchain
2	B	368	GLU	Peptide
2	B	371	PHE	Peptide
2	B	392	TYR	Peptide

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	2160	0	2096	51	0
2	B	3765	0	3484	85	0
3	F	3404	0	3378	63	1
4	E	6622	0	5907	73	1
5	D	713	0	308	0	0
6	L	1592	0	1546	25	0
7	H	1560	0	1512	17	0
All	All	19816	0	18231	288	1

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 (288) 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)
4:E:451:ARG:HH12	6:L:69:ARG:HD3	1.27	0.97
4:E:325:ALA:HA	6:L:59:SER:HB2	1.50	0.94
3:F:314:ILE:HG22	3:F:315:LEU:HG	1.61	0.82
1:A:18:ASP:OD2	2:B:548:TYR:OH	1.97	0.80
4:E:293:LEU:HD13	4:E:297:LEU:HD12	1.63	0.79
4:E:113:VAL:HG23	4:E:114:GLU:H	1.51	0.76
4:E:404:VAL:HG11	4:E:438:GLU:HA	1.70	0.74
7:H:235:VAL:HB	7:H:244:VAL:HB	1.69	0.73
3:F:70:LEU:HD22	3:F:343:ILE:HD11	1.72	0.72
3:F:8:GLN:C	3:F:10:GLU:H	2.00	0.69
4:E:451:ARG:NH1	6:L:69:ARG:HD3	2.06	0.69
6:L:126:SER:O	6:L:129:LYS:HB3	1.92	0.69
3:F:62:VAL:HG12	3:F:66:LYS:HE3	1.75	0.69
6:L:193:LYS:HE3	6:L:213:ASN:HB3	1.74	0.68
2:B:297:LEU:HD23	2:B:300:LEU:HD12	1.75	0.68
6:L:15:SER:HB3	6:L:110:LYS:HE3	1.75	0.68
2:B:178:THR:HG21	2:B:485:ALA:HB2	1.75	0.67
2:B:426:TYR:O	2:B:464:ARG:NH2	2.28	0.67
2:B:416:ASP:HA	2:B:443:THR:HG21	1.75	0.67
4:E:55:GLU:HB2	4:E:74:SER:HA	1.77	0.66
2:B:152:ALA:HB1	2:B:160:LEU:HD11	1.78	0.65
4:E:678:VAL:HG11	4:E:720:PHE:HA	1.79	0.65
1:A:12:ILE:HD12	2:B:170:GLY:HA3	1.79	0.65
2:B:483:GLU:CD	2:B:514:ARG:HH22	2.04	0.65
2:B:300:LEU:HD23	2:B:388:LEU:HD21	1.78	0.65
2:B:292:ILE:HD12	2:B:292:ILE:H	1.61	0.65
4:E:335:VAL:HG13	4:E:352:ILE:HB	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:448:THR:OG1	6:L:71:GLY:N	2.26	0.64
3:F:71:GLU:OE1	3:F:75:TRP:NE1	2.29	0.64
7:H:149:SER:OG	7:H:150:SER:N	2.31	0.64
4:E:829:SER:HA	4:E:841:ALA:HB1	1.80	0.63
6:L:6:GLN:HB2	6:L:29:SER:HB3	1.81	0.62
2:B:367:PHE:O	2:B:369:GLY:N	2.30	0.62
2:B:209:PRO:HB3	2:B:532:LYS:HB2	1.82	0.62
4:E:609:GLY:O	4:E:613:ILE:HG22	1.99	0.61
6:L:14:LEU:HG	6:L:107:VAL:HG22	1.83	0.61
4:E:511:ARG:HD2	7:H:80:TYR:CE2	2.35	0.61
4:E:295:ASN:ND2	4:E:329:TRP:O	2.33	0.61
1:A:64:PRO:HB3	2:B:548:TYR:HB2	1.82	0.61
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.83	0.61
2:B:184:PHE:HE2	2:B:225:MSE:HE3	1.64	0.61
3:F:410:SER:HA	3:F:436:LEU:HD11	1.82	0.60
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.83	0.60
6:L:24:ILE:HG12	6:L:105:THR:HG21	1.82	0.60
2:B:525:ASP:O	2:B:528:LEU:HB2	2.03	0.59
3:F:433:ALA:HB1	3:F:439:SER:OG	2.03	0.59
3:F:343:ILE:HD13	3:F:344:ARG:N	2.17	0.59
4:E:329:TRP:HB3	4:E:355:TRP:HB3	1.85	0.59
2:B:152:ALA:HB1	2:B:160:LEU:CD1	2.33	0.58
2:B:199:THR:HB	2:B:213:GLU:HB2	1.86	0.58
6:L:40:GLN:HB2	6:L:50:LEU:HD11	1.86	0.58
2:B:483:GLU:OE2	2:B:514:ARG:NH2	2.29	0.58
2:B:180:LEU:HD21	2:B:185:LEU:HD13	1.86	0.58
6:L:216:GLU:O	6:L:217:CYS:HB2	2.04	0.57
2:B:360:LYS:HG3	2:B:366:PRO:HA	1.85	0.57
4:E:101:SER:HA	4:E:123:LEU:HA	1.86	0.57
4:E:245:ILE:HB	4:E:255:GLN:HB2	1.87	0.57
2:B:389:THR:O	2:B:393:GLY:HA3	2.05	0.57
6:L:15:SER:OG	6:L:108:GLU:OE1	2.22	0.57
4:E:448:THR:HG21	6:L:70:SER:HA	1.85	0.56
2:B:433:GLU:OE1	2:B:467:SER:OG	2.20	0.56
4:E:342:LEU:HD13	4:E:379:ILE:HD12	1.85	0.56
2:B:359:TYR:CE2	3:F:210:MSE:HE1	2.40	0.56
4:E:63:SER:OG	4:E:112:GLU:OE1	2.23	0.56
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.40	0.56
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.41	0.56
2:B:525:ASP:HA	2:B:528:LEU:HD12	1.88	0.55
3:F:34:ASP:HB3	3:F:35:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:200:ASN:O	4:E:200:ASN:ND2	2.39	0.55
1:A:217:LEU:HD22	1:A:218:LEU:H	1.71	0.55
3:F:237:ILE:HD11	3:F:240:HIS:HA	1.87	0.55
4:E:325:ALA:HA	6:L:59:SER:CB	2.32	0.55
7:H:64:ARG:HB3	7:H:120:TYR:CD2	2.42	0.55
2:B:519:LEU:O	2:B:529:ASN:ND2	2.40	0.54
4:E:58:ASN:HB3	4:E:70:TYR:CZ	2.42	0.54
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.88	0.54
2:B:305:VAL:HG13	3:F:314:ILE:HD11	1.89	0.54
2:B:492:LEU:HD12	2:B:508:ILE:HD13	1.89	0.54
3:F:341:HIS:CE1	3:F:343:ILE:HD12	2.42	0.54
4:E:511:ARG:HD2	7:H:80:TYR:HE2	1.73	0.54
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.22	0.54
2:B:180:LEU:HD11	2:B:478:PHE:HE1	1.71	0.54
4:E:125:ASP:OD1	4:E:127:SER:OG	2.19	0.54
2:B:359:TYR:HA	2:B:362:LEU:HD12	1.90	0.54
2:B:156:THR:HG22	2:B:514:ARG:HD2	1.90	0.54
3:F:13:THR:O	3:F:17:ASP:N	2.31	0.53
7:H:65:GLN:O	7:H:118:ALA:HB1	2.08	0.53
2:B:365:SER:HB3	2:B:368:GLU:HB2	1.90	0.53
4:E:119:VAL:HB	4:E:131:LEU:HB2	1.89	0.53
1:A:178:ALA:HB1	1:A:206:TRP:CE2	2.43	0.53
2:B:524:ASN:O	2:B:528:LEU:HG	2.09	0.53
4:E:659:TYR:OH	4:E:743:ASN:O	2.21	0.53
7:H:31:VAL:O	7:H:48:CYS:HA	2.09	0.52
1:A:116:LEU:O	1:A:127:VAL:HA	2.10	0.52
2:B:182:ARG:HD2	2:B:449:GLN:OE1	2.10	0.52
4:E:508:LYS:O	4:E:512:THR:HG23	2.09	0.52
2:B:435:LEU:O	2:B:439:VAL:HG23	2.09	0.52
1:A:275:ASP:OD1	1:A:275:ASP:N	2.42	0.52
2:B:305:VAL:HG21	3:F:311:ASP:HB3	1.92	0.52
3:F:379:ILE:HG13	3:F:385:LEU:HD23	1.90	0.52
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.92	0.52
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.45	0.51
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.75	0.51
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.45	0.51
2:B:159:MSE:SE	2:B:175:ARG:HH21	2.43	0.51
3:F:431:ILE:HD12	3:F:431:ILE:H	1.74	0.51
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.45	0.51
3:F:294:LEU:O	3:F:298:ILE:HD12	2.10	0.51
2:B:178:THR:HG22	2:B:180:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:102:MET:HE3	4:E:163:PRO:HD2	1.93	0.51
1:A:261:SER:CB	2:B:153:LYS:HA	2.40	0.51
3:F:280:SER:HB2	3:F:284:SER:HB3	1.92	0.51
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.93	0.51
2:B:492:LEU:HD11	2:B:508:ILE:HG23	1.92	0.50
4:E:400:LYS:HE3	4:E:736:ASN:HA	1.93	0.50
7:H:109:MET:HB3	7:H:112:LEU:HD21	1.92	0.50
2:B:491:SER:O	2:B:495:SER:OG	2.28	0.50
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.46	0.50
2:B:281:ILE:HB	2:B:301:LEU:HD21	1.92	0.50
7:H:117:THR:O	7:H:118:ALA:HB2	2.11	0.50
4:E:245:ILE:HG21	4:E:311:LEU:HD23	1.94	0.50
3:F:86:ASN:C	3:F:88:ASP:H	2.20	0.50
3:F:245:ARG:HG2	3:F:315:LEU:HB2	1.94	0.49
4:E:537:THR:HA	4:E:746:CYS:CB	2.42	0.49
3:F:227:ILE:C	3:F:229:ASN:H	2.20	0.49
4:E:102:MET:HB3	4:E:107:THR:HG21	1.94	0.49
2:B:359:TYR:HE2	3:F:210:MSE:HE1	1.78	0.49
4:E:448:THR:HG21	6:L:69:ARG:O	2.13	0.49
2:B:186:PHE:CD2	2:B:487:LEU:HD11	2.48	0.49
2:B:392:TYR:O	2:B:394:GLN:N	2.39	0.49
2:B:523:THR:HA	2:B:526:HIS:HB2	1.94	0.49
4:E:541:PRO:HD2	4:E:544:MET:HE2	1.95	0.49
2:B:374:LYS:O	2:B:377:GLU:HB2	2.13	0.49
7:H:32:GLU:OE1	7:H:143:GLY:N	2.36	0.49
3:F:350:VAL:HG22	3:F:355:LEU:HD22	1.95	0.49
4:E:386:LEU:HD23	4:E:621:GLN:HA	1.95	0.49
2:B:270:THR:OG1	2:B:391:CYS:SG	2.71	0.49
3:F:106:GLU:O	3:F:110:MSE:HG2	2.13	0.49
4:E:522:ASN:O	4:E:526:ARG:HG3	2.12	0.49
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.95	0.48
2:B:526:HIS:C	2:B:528:LEU:N	2.69	0.48
2:B:526:HIS:C	2:B:530:ARG:HD2	2.38	0.48
4:E:70:TYR:HA	4:E:80:THR:O	2.12	0.48
3:F:293:ILE:HD11	3:F:327:VAL:HG21	1.95	0.48
3:F:8:GLN:O	3:F:10:GLU:N	2.45	0.48
4:E:591:MET:HE1	4:E:630:THR:OG1	2.13	0.48
1:A:191:ALA:C	1:A:193:THR:H	2.22	0.48
4:E:570:LEU:O	4:E:574:LEU:HB2	2.14	0.48
1:A:259:ARG:NH1	2:B:151:PHE:HB2	2.29	0.48
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:33:SER:C	6:L:35:ALA:H	2.22	0.48
4:E:500:GLU:HB2	4:E:507:PHE:CZ	2.49	0.47
1:A:272:SER:OG	2:B:152:ALA:HB3	2.14	0.47
2:B:186:PHE:HD2	2:B:487:LEU:HD11	1.79	0.47
4:E:508:LYS:HG2	4:E:511:ARG:NH2	2.29	0.47
2:B:156:THR:HG22	2:B:514:ARG:CD	2.44	0.47
4:E:91:LYS:NZ	4:E:142:ALA:O	2.34	0.47
3:F:116:LEU:O	3:F:119:ILE:HB	2.15	0.47
1:A:16:VAL:HG21	1:A:59:VAL:O	2.14	0.47
4:E:531:LYS:HB3	4:E:553:ILE:HG12	1.96	0.47
7:H:240:SER:O	7:H:241:ASN:C	2.58	0.47
2:B:393:GLY:O	2:B:394:GLN:HB2	2.13	0.47
1:A:9:ASN:HD22	1:A:9:ASN:HA	1.50	0.47
4:E:288:VAL:HG13	4:E:336:LEU:HD22	1.95	0.47
1:A:217:LEU:HD13	1:A:218:LEU:N	2.30	0.47
3:F:431:ILE:H	3:F:431:ILE:CD1	2.28	0.47
4:E:596:PHE:CZ	4:E:704:SER:HA	2.50	0.47
1:A:174:VAL:HA	1:A:183:LYS:O	2.15	0.46
4:E:288:VAL:HG12	4:E:300:MET:HB3	1.97	0.46
7:H:236:ASN:ND2	7:H:243:LYS:HD3	2.30	0.46
1:A:108:ALA:HB1	1:A:112:TYR:HD1	1.81	0.46
1:A:18:ASP:OD1	1:A:18:ASP:N	2.47	0.46
2:B:292:ILE:HA	2:B:295:ILE:HD12	1.98	0.46
3:F:194:ASP:HA	3:F:197:LEU:HD12	1.97	0.46
3:F:431:ILE:HD12	3:F:431:ILE:N	2.30	0.46
7:H:65:GLN:C	7:H:118:ALA:HB1	2.40	0.46
7:H:236:ASN:HD21	7:H:243:LYS:HD3	1.80	0.46
4:E:137:PHE:CD1	4:E:145:LEU:HD13	2.51	0.46
2:B:315:LYS:HG3	3:F:162:LEU:HB3	1.97	0.46
3:F:8:GLN:C	3:F:10:GLU:N	2.68	0.46
1:A:229:ARG:HH11	1:A:229:ARG:HB2	1.81	0.46
2:B:531:LEU:O	2:B:532:LYS:HG2	2.16	0.46
4:E:59:CYS:HB2	4:E:464:THR:OG1	2.15	0.46
3:F:382:LYS:HA	3:F:383:PRO:HD3	1.78	0.46
2:B:333:ILE:HD11	3:F:213:CYS:HB2	1.97	0.45
1:A:214:PRO:HG2	1:A:264:LEU:HA	1.98	0.45
4:E:111:GLN:HG3	4:E:168:TYR:CG	2.52	0.45
4:E:436:HIS:CD2	4:E:438:GLU:H	2.34	0.45
1:A:38:VAL:O	1:A:39:GLU:HG3	2.17	0.45
4:E:634:LEU:O	4:E:638:VAL:HG13	2.16	0.45
6:L:7:MET:HE3	6:L:26:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:C	1:A:275:ASP:H	2.25	0.44
3:F:7:TYR:O	3:F:9:THR:N	2.50	0.44
3:F:241:SER:O	3:F:245:ARG:HD2	2.17	0.44
6:L:33:SER:O	6:L:35:ALA:N	2.49	0.44
1:A:227:GLN:OE1	1:A:256:VAL:HG11	2.18	0.44
3:F:385:LEU:O	3:F:389:VAL:HG23	2.16	0.44
4:E:53:GLY:HA2	4:E:73:SER:HA	1.98	0.44
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.18	0.44
4:E:354:LEU:HD21	4:E:460:ALA:HB1	1.99	0.44
4:E:382:VAL:HG21	4:E:495:TYR:CD1	2.52	0.44
3:F:86:ASN:OD1	3:F:400:ASN:ND2	2.50	0.44
6:L:169:GLN:HG2	6:L:174:SER:HA	1.99	0.44
2:B:328:SER:HA	3:F:238:LYS:HE3	2.00	0.44
3:F:183:TYR:CE2	3:F:199:GLU:HG3	2.52	0.44
4:E:24:VAL:HG11	4:E:143:ASN:HA	2.00	0.44
1:A:219:ARG:HB2	1:A:236:GLN:O	2.18	0.44
2:B:373:LEU:HB3	2:B:376:LEU:HD12	1.99	0.44
3:F:157:ASP:OD1	3:F:163:ARG:NH2	2.47	0.44
4:E:185:GLY:O	4:E:196:PRO:HA	2.18	0.44
4:E:451:ARG:NH1	6:L:69:ARG:HH11	2.15	0.44
6:L:194:VAL:HG22	6:L:213:ASN:ND2	2.32	0.44
2:B:393:GLY:O	2:B:394:GLN:CB	2.66	0.44
4:E:466:TYR:HB3	4:E:470:ILE:HB	2.00	0.44
4:E:736:ASN:C	4:E:738:ARG:H	2.25	0.44
6:L:17:SER:HB2	6:L:20:ASP:CG	2.42	0.44
2:B:297:LEU:O	2:B:300:LEU:HB2	2.18	0.43
2:B:375:GLU:C	2:B:377:GLU:H	2.26	0.43
3:F:143:LYS:HG3	3:F:144:TRP:N	2.33	0.43
3:F:349:SER:OG	3:F:358:VAL:HG21	2.18	0.43
2:B:315:LYS:HE3	3:F:162:LEU:HB3	2.00	0.43
2:B:452:TRP:CD1	2:B:475:THR:HA	2.53	0.43
1:A:95:HIS:NE2	1:A:138:PRO:HB3	2.33	0.43
1:A:118:VAL:O	1:A:125:VAL:HA	2.18	0.43
4:E:427:LEU:HD13	4:E:442:TYR:CE1	2.53	0.43
6:L:108:GLU:OE2	6:L:169:GLN:NE2	2.51	0.43
2:B:321:VAL:HA	3:F:246:THR:HG21	2.00	0.43
4:E:678:VAL:HG11	4:E:720:PHE:CA	2.46	0.43
4:E:53:GLY:HA3	4:E:71:HIS:HB3	2.01	0.43
4:E:225:SER:OG	4:E:277:GLY:O	2.36	0.42
3:F:264:TYR:O	3:F:268:SER:OG	2.31	0.42
3:F:267:LEU:O	3:F:295:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:433:ALA:O	3:F:435:PHE:N	2.44	0.42
7:H:150:SER:HB2	7:H:151:ALA:H	1.59	0.42
1:A:280:LEU:HB2	1:A:292:ALA:O	2.19	0.42
2:B:341:LEU:HD12	2:B:341:LEU:HA	1.89	0.42
3:F:237:ILE:C	3:F:237:ILE:HD12	2.45	0.42
2:B:273:ILE:HG23	2:B:383:LEU:HG	2.01	0.42
3:F:77:LEU:HG	3:F:125:TRP:CD2	2.55	0.42
7:H:191:TRP:CZ3	7:H:233:CYS:HB3	2.55	0.42
1:A:259:ARG:HB2	1:A:272:SER:HB2	2.02	0.42
3:F:343:ILE:HD13	3:F:344:ARG:H	1.84	0.42
4:E:190:ASP:OD2	4:E:191:GLY:N	2.52	0.42
1:A:181:LEU:HD22	1:A:199:THR:CG2	2.50	0.42
2:B:386:LEU:HA	2:B:407:HIS:CE1	2.55	0.42
2:B:418:PRO:HB3	2:B:445:ALA:HB1	2.01	0.42
2:B:471:SER:O	2:B:475:THR:OG1	2.30	0.42
3:F:293:ILE:HD11	3:F:327:VAL:CG2	2.49	0.42
4:E:218:SER:OG	4:E:219:ASP:N	2.53	0.42
2:B:526:HIS:C	2:B:528:LEU:H	2.27	0.42
2:B:536:GLN:HA	2:B:539:PHE:CE2	2.54	0.42
4:E:345:GLU:O	4:E:347:SER:N	2.53	0.42
1:A:209:ASP:OD1	1:A:259:ARG:HD3	2.20	0.41
2:B:176:LEU:HA	2:B:177:PRO:HD2	1.86	0.41
2:B:431:ASN:HB2	2:B:434:LYS:HB3	2.01	0.41
2:B:539:PHE:CD1	2:B:539:PHE:C	2.98	0.41
3:F:94:MSE:HE2	3:F:108:LYS:HB2	2.02	0.41
3:F:363:VAL:HG11	3:F:408:ASP:OD1	2.20	0.41
4:E:233:TYR:CG	4:E:311:LEU:HD22	2.55	0.41
4:E:297:LEU:HD23	4:E:297:LEU:HA	1.92	0.41
1:A:57:TRP:HD1	1:A:102:VAL:O	2.02	0.41
2:B:417:ASP:O	2:B:421:VAL:HG23	2.21	0.41
6:L:123:PRO:HD3	6:L:135:VAL:HG22	2.02	0.41
1:A:284:ASN:OD1	1:A:286:GLU:HB2	2.21	0.41
3:F:354:SER:O	3:F:358:VAL:HG23	2.21	0.41
1:A:16:VAL:HG23	1:A:59:VAL:HG23	2.01	0.41
2:B:492:LEU:CD1	2:B:508:ILE:HD13	2.50	0.41
4:E:601:PHE:O	4:E:602:ILE:C	2.63	0.41
1:A:59:VAL:HB	1:A:70:LEU:HD11	2.03	0.41
2:B:216:LEU:O	2:B:217:LEU:HD23	2.21	0.41
3:F:81:LEU:HD12	3:F:350:VAL:HG12	2.03	0.41
3:F:242:LEU:O	3:F:243:TRP:C	2.64	0.41
2:B:203:ARG:NE	2:B:210:GLN:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:TRP:C	2:B:346:THR:H	2.29	0.41
3:F:102:ARG:NH2	3:F:308:VAL:HG22	2.36	0.40
3:F:207:SER:HA	3:F:210:MSE:HE3	2.03	0.40
4:E:258:ASP:OD1	4:E:260:VAL:HG22	2.20	0.40
4:E:346:ALA:CB	4:E:369:ASN:HD22	2.35	0.40
2:B:526:HIS:O	2:B:528:LEU:N	2.54	0.40
3:F:50:ALA:HB1	3:F:69:GLU:HG3	2.03	0.40
2:B:263:LYS:HD3	2:B:263:LYS:HA	1.78	0.40
2:B:340:GLN:HB2	3:F:206:ILE:HG21	2.03	0.40
4:E:163:PRO:HA	4:E:178:LEU:HA	2.03	0.40
1:A:63:HIS:CD2	1:A:64:PRO:HD2	2.56	0.40
1:A:253:PHE:CD1	1:A:257:LEU:HD11	2.56	0.40
2:B:155:SER:HB3	2:B:159:MSE:H	1.87	0.40
3:F:183:TYR:HE2	3:F:199:GLU:HG3	1.85	0.40
7:H:117:THR:HG23	7:H:147:THR:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:329:ASN:OD1	4:E:204:TYR:OH[2_454]	1.97	0.23

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	270/297 (91%)	227 (84%)	37 (14%)	6 (2%)	5	29
2	B	485/652 (74%)	447 (92%)	28 (6%)	10 (2%)	5	30
3	F	413/454 (91%)	369 (89%)	33 (8%)	11 (3%)	4	25
4	E	858/1045 (82%)	797 (93%)	51 (6%)	10 (1%)	10	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	123/685 (18%)	123 (100%)	0	0	100	100
6	L	205/217 (94%)	195 (95%)	7 (3%)	3 (2%)	8	40
7	H	211/267 (79%)	198 (94%)	8 (4%)	5 (2%)	4	27
All	All	2565/3617 (71%)	2356 (92%)	164 (6%)	45 (2%)	6	34

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	SER
2	B	368	GLU
2	B	371	PHE
2	B	394	GLN
3	F	9	THR
3	F	11	ARG
3	F	138	ASN
3	F	165	ASN
7	H	118	ALA
1	A	218	LEU
2	B	180	LEU
2	B	348	GLY
2	B	429	ASN
2	B	527	ILE
3	F	8	GLN
3	F	55	ASN
3	F	141	THR
3	F	354	SER
3	F	434	THR
4	E	113	VAL
4	E	598	LYS
4	E	602	ILE
6	L	129	LYS
7	H	149	SER
3	F	440	ASP
4	E	346	ALA
6	L	34	SER
1	A	131	LYS
2	B	531	LEU
3	F	87	ALA
4	E	264	ASP
4	E	284	ASN
4	E	600	ASP

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Mol	Chain	Res	Type
6	L	110	LYS
1	A	114	PRO
1	A	247	LEU
4	E	780	HIS
7	H	151	ALA
4	E	231	GLU
7	H	241	ASN
4	E	737	ILE
1	A	202	GLY
2	B	393	GLY
1	A	97	VAL
7	H	186	PRO

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	233/251 (93%)	223 (96%)	10 (4%)	26	47
2	B	367/584 (63%)	323 (88%)	44 (12%)	5	17
3	F	387/410 (94%)	361 (93%)	26 (7%)	15	36
4	E	639/980 (65%)	609 (95%)	30 (5%)	23	45
6	L	183/191 (96%)	177 (97%)	6 (3%)	33	55
7	H	173/223 (78%)	165 (95%)	8 (5%)	24	45
All	All	1982/2639 (75%)	1858 (94%)	124 (6%)	16	37

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	22	LYS
1	A	43	HIS
1	A	46	ILE
1	A	47	ASP
1	A	139	ILE

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Mol	Chain	Res	Type
1	A	225	VAL
1	A	227	GLN
1	A	229	ARG
1	A	275	ASP
2	B	160	LEU
2	B	175	ARG
2	B	195	ILE
2	B	198	VAL
2	B	201	GLU
2	B	210	GLN
2	B	214	SER
2	B	216	LEU
2	B	225	MSE
2	B	228	THR
2	B	234	LEU
2	B	251	THR
2	B	283	GLU
2	B	308	SER
2	B	319	LEU
2	B	328	SER
2	B	336	LEU
2	B	341	LEU
2	B	346	THR
2	B	349	CYS
2	B	351	ILE
2	B	368	GLU
2	B	370	LEU
2	B	371	PHE
2	B	400	LEU
2	B	402	SER
2	B	406	SER
2	B	408	LEU
2	B	412	SER
2	B	419	ILE
2	B	440	ARG
2	B	443	THR
2	B	456	GLN
2	B	464	ARG
2	B	467	SER
2	B	469	GLU
2	B	508	ILE
2	B	516	ILE

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Mol	Chain	Res	Type
2	B	522	SER
2	B	524	ASN
2	B	530	ARG
2	B	531	LEU
2	B	539	PHE
2	B	547	ARG
3	F	17	ASP
3	F	26	GLN
3	F	58	ASP
3	F	71	GLU
3	F	77	LEU
3	F	86	ASN
3	F	88	ASP
3	F	94	MSE
3	F	118	GLN
3	F	128	GLU
3	F	141	THR
3	F	166	THR
3	F	211	ILE
3	F	225	THR
3	F	237	ILE
3	F	268	SER
3	F	274	GLN
3	F	284	SER
3	F	298	ILE
3	F	343	ILE
3	F	357	SER
3	F	365	MSE
3	F	382	LYS
3	F	403	SER
3	F	422	LEU
3	F	431	ILE
4	E	63	SER
4	E	127	SER
4	E	162	VAL
4	E	172	GLN
4	E	175	VAL
4	E	183	LEU
4	E	188	LYS
4	E	200	ASN
4	E	209	THR
4	E	259	MET

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Mol	Chain	Res	Type
4	E	270	PHE
4	E	280	LEU
4	E	305	VAL
4	E	314	THR
4	E	328	ILE
4	E	335	VAL
4	E	338	ARG
4	E	341	GLU
4	E	370	ASP
4	E	404	VAL
4	E	408	PHE
4	E	428	SER
4	E	590	GLN
4	E	600	ASP
4	E	605	ILE
4	E	638	VAL
4	E	644	THR
4	E	663	LEU
4	E	690	VAL
4	E	703	ASP
6	L	8	THR
6	L	15	SER
6	L	27	ARG
6	L	83	PRO
6	L	108	GLU
6	L	148	LYS
7	H	45	ARG
7	H	113	ARG
7	H	124	ARG
7	H	166	LYS
7	H	215	LEU
7	H	234	ASN
7	H	236	ASN
7	H	250	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	63	HIS
1	A	91	GLN
1	A	103	ASN

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Mol	Chain	Res	Type
1	A	188	ASN
2	B	210	GLN
2	B	329	ASN
2	B	405	GLN
2	B	461	ASN
2	B	488	HIS
2	B	490	HIS
3	F	26	GLN
3	F	335	HIS
3	F	360	HIS
4	E	116	GLN
4	E	154	ASN
4	E	200	ASN
4	E	239	GLN
4	E	255	GLN
4	E	350	ASN
4	E	369	ASN
4	E	393	HIS
4	E	566	ASN
4	E	575	ASN
4	E	584	ASN
4	E	588	ASN
4	E	620	HIS
6	L	127	GLN
6	L	213	ASN
7	H	108	GLN
7	H	110	ASN
7	H	201	HIS

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	274/297 (92%)	1.08	40 (14%) 6 14	579, 633, 655, 668	0
2	B	495/652 (75%)	1.08	102 (20%) 2 10	466, 557, 629, 666	0
3	F	412/454 (90%)	0.92	60 (14%) 6 14	455, 526, 597, 626	0
4	E	896/1045 (85%)	1.21	206 (22%) 2 9	424, 509, 574, 666	0
5	D	140/685 (20%)	1.41	35 (25%) 2 8	555, 634, 690, 699	0
6	L	209/217 (96%)	1.19	38 (18%) 3 11	422, 477, 527, 558	0
7	H	215/267 (80%)	1.15	46 (21%) 2 9	451, 495, 558, 613	0
All	All	2641/3617 (73%)	1.13	527 (19%) 3 10	422, 522, 644, 699	0

All (527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	600	ASP	17.5
6	L	173	ASP	11.7
4	E	601	PHE	11.6
2	B	166	VAL	11.2
7	H	111	SER	10.8
4	E	842	LEU	9.8
2	B	282	GLU	9.7
1	A	208	ARG	9.2
4	E	684	SER	8.9
5	D	711	GLU	8.7
1	A	149	ASN	8.6
2	B	165	ILE	8.5
4	E	295	ASN	8.5
3	F	52	ASP	8.3
1	A	225	VAL	8.2
2	B	598	ILE	8.0
1	A	207	VAL	7.9

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Mol	Chain	Res	Type	RSRZ
2	B	601	GLU	7.9
5	D	627	TYR	7.9
4	E	646	ILE	7.8
4	E	841	ALA	7.6
6	L	174	SER	7.6
4	E	460	ALA	7.4
6	L	141	ASN	7.2
4	E	690	VAL	7.1
1	A	224	SER	7.0
4	E	599	LYS	6.9
1	A	226	SER	6.8
4	E	415	TYR	6.8
1	A	177	GLY	6.8
2	B	335	ASP	6.4
7	H	243	LYS	6.4
4	E	839	GLU	6.3
7	H	148	VAL	6.3
4	E	682	ASP	6.3
1	A	286	GLU	6.3
4	E	292	PRO	6.3
4	E	822	SER	6.2
2	B	616	VAL	6.2
3	F	156	CYS	6.2
4	E	540	LEU	6.2
3	F	8	GLN	6.2
1	A	176	GLY	6.2
4	E	450	LEU	6.1
4	E	454	LYS	6.0
5	D	641	ASP	6.0
7	H	116	ASP	6.0
4	E	54	SER	6.0
4	E	541	PRO	6.0
1	A	231	CYS	5.9
4	E	74	SER	5.9
4	E	821	HIS	5.9
4	E	55	GLU	5.8
3	F	14	LYS	5.7
2	B	559	LEU	5.7
4	E	552	ASP	5.7
2	B	597	GLU	5.7
3	F	15	PHE	5.7
1	A	41	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
4	E	691	LYS	5.6
4	E	840	PHE	5.6
4	E	431	LYS	5.5
5	D	617	THR	5.5
4	E	325	ALA	5.5
4	E	636	THR	5.5
4	E	602	ILE	5.5
4	E	829	SER	5.4
2	B	615	ASN	5.4
2	B	441	GLN	5.3
2	B	489	GLY	5.2
4	E	845	ILE	5.2
3	F	49	LEU	5.2
5	D	628	ALA	5.2
3	F	53	LEU	5.1
5	D	631	SER	5.0
4	E	643	ASP	5.0
3	F	56	SER	5.0
4	E	476	PHE	5.0
4	E	29	SER	4.9
7	H	78	SER	4.9
4	E	744	VAL	4.9
7	H	38	VAL	4.8
3	F	25	GLU	4.8
4	E	844	CYS	4.8
5	D	619	SER	4.7
2	B	285	ILE	4.7
2	B	618	GLU	4.7
6	L	164	GLU	4.7
7	H	242	THR	4.7
4	E	419	ILE	4.6
3	F	144	TRP	4.6
2	B	281	ILE	4.6
7	H	41	GLY	4.6
2	B	167	GLY	4.5
4	E	512	THR	4.5
6	L	91	CYS	4.5
2	B	466	PHE	4.5
6	L	115	ALA	4.5
4	E	80	THR	4.5
4	E	98	PRO	4.4
4	E	762	MET	4.4

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Mol	Chain	Res	Type	RSRZ
3	F	158	LEU	4.4
1	A	148	VAL	4.4
6	L	122	PRO	4.4
3	F	7	TYR	4.4
4	E	681	LYS	4.3
4	E	509	TYR	4.3
4	E	683	SER	4.3
4	E	458	ASN	4.3
2	B	308	SER	4.3
4	E	241	CYS	4.3
1	A	230	THR	4.3
3	F	42	PHE	4.3
4	E	544	MET	4.3
2	B	465	VAL	4.2
4	E	685	GLU	4.2
7	H	112	LEU	4.2
4	E	596	PHE	4.2
4	E	579	ILE	4.2
4	E	689	GLY	4.2
7	H	72	GLU	4.2
4	E	495	TYR	4.1
2	B	555	GLU	4.1
2	B	632	GLU	4.1
6	L	202	GLN	4.1
4	E	531	LYS	4.1
2	B	495	SER	4.1
1	A	285	LEU	4.1
4	E	294	GLU	4.1
4	E	494	PHE	4.1
3	F	361	SER	4.1
4	E	203	SER	4.1
4	E	214	ARG	4.1
6	L	7	MET	4.1
3	F	45	ALA	4.0
2	B	318	HIS	4.0
4	E	104	GLN	4.0
1	A	147	GLY	4.0
2	B	211	ILE	4.0
4	E	446	LEU	3.9
2	B	636	SER	3.9
4	E	207	SER	3.9
2	B	528	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
7	H	43	SER	3.9
2	B	284	LYS	3.9
2	B	496	CYS	3.9
4	E	447	GLU	3.9
4	E	534	ASP	3.9
1	A	133	ASN	3.9
5	D	607	ILE	3.9
4	E	259	MET	3.9
2	B	283	GLU	3.9
4	E	846	SER	3.9
4	E	414	ARG	3.9
4	E	843	LYS	3.8
4	E	99	ASN	3.8
7	H	110	ASN	3.8
1	A	175	THR	3.8
7	H	245	ASP	3.8
4	E	901	ARG	3.8
1	A	57	TRP	3.7
5	D	623	THR	3.7
5	D	725	ALA	3.7
2	B	613	SER	3.7
4	E	324	SER	3.7
4	E	260	VAL	3.7
7	H	163	PRO	3.7
4	E	461	SER	3.7
2	B	532	LYS	3.7
4	E	442	TYR	3.7
5	D	630	LEU	3.6
7	H	96	ILE	3.6
7	H	44	LEU	3.6
2	B	554	SER	3.6
4	E	388	ASP	3.6
5	D	621	ARG	3.6
2	B	424	GLN	3.6
7	H	49	ALA	3.5
5	D	730	ASN	3.5
6	L	66	SER	3.5
4	E	146	ASN	3.5
4	E	329	TRP	3.5
6	L	40	GLN	3.5
2	B	635	ASP	3.5
4	E	594	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	593	LYS	3.5
4	E	106	TYR	3.5
3	F	153	LEU	3.5
5	D	632	GLN	3.5
4	E	511	ARG	3.4
2	B	492	LEU	3.4
2	B	589	ASN	3.4
3	F	259	TYR	3.4
4	E	1005	ASN	3.4
2	B	357	LYS	3.4
3	F	10	GLU	3.4
5	D	712	THR	3.4
2	B	398	TYR	3.4
3	F	285	ASP	3.4
5	D	717	ASP	3.4
4	E	628	ARG	3.4
7	H	56	SER	3.4
4	E	853	LEU	3.4
3	F	17	ASP	3.4
7	H	103	ASN	3.4
1	A	10	GLU	3.3
1	A	206	TRP	3.3
4	E	423	ALA	3.3
4	E	746	CYS	3.3
4	E	717	ASN	3.3
4	E	386	LEU	3.3
7	H	97	SER	3.3
4	E	513	LEU	3.3
4	E	635	LEU	3.3
6	L	113	VAL	3.3
4	E	289	THR	3.3
2	B	194	GLU	3.3
2	B	490	HIS	3.2
2	B	687	LEU	3.2
4	E	823	ALA	3.2
3	F	157	ASP	3.2
2	B	617	PHE	3.2
1	A	97	VAL	3.2
3	F	147	SER	3.2
6	L	132	THR	3.2
3	F	430	PRO	3.2
3	F	36	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
6	L	111	ARG	3.2
5	D	578	ALA	3.2
1	A	178	ALA	3.2
2	B	394	GLN	3.2
4	E	687	SER	3.2
2	B	436	TYR	3.2
4	E	204	TYR	3.2
1	A	216	VAL	3.2
2	B	286	ARG	3.2
2	B	643	ILE	3.2
4	E	632	GLN	3.1
4	E	893	HIS	3.1
1	A	72	SER	3.1
4	E	607	PHE	3.1
6	L	214	ARG	3.1
4	E	389	LEU	3.1
3	F	41	GLU	3.1
4	E	459	GLU	3.1
2	B	342	GLN	3.1
2	B	535	SER	3.1
6	L	175	THR	3.1
1	A	144	HIS	3.1
2	B	596	ARG	3.1
4	E	296	GLY	3.1
5	D	726	THR	3.1
7	H	149	SER	3.1
4	E	453	VAL	3.1
7	H	80	TYR	3.0
2	B	639	SER	3.0
4	E	999	CYS	3.0
2	B	558	ASN	3.0
2	B	468	LYS	3.0
4	E	645	GLU	3.0
4	E	263	SER	3.0
5	D	577	GLU	3.0
1	A	96	ALA	3.0
2	B	164	ASP	3.0
4	E	94	ASN	3.0
2	B	169	SER	3.0
2	B	251	THR	3.0
2	B	419	ILE	3.0
4	E	330	SER	3.0

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Mol	Chain	Res	Type	RSRZ
7	H	147	THR	3.0
4	E	515	GLY	3.0
4	E	885	VAL	3.0
5	D	624	LEU	3.0
4	E	902	THR	3.0
4	E	745	GLU	3.0
4	E	639	LEU	2.9
7	H	231	TYR	2.9
4	E	638	VAL	2.9
3	F	207	SER	2.9
4	E	270	PHE	2.9
5	D	673	PRO	2.9
4	E	398	VAL	2.9
4	E	443	LEU	2.9
4	E	574	LEU	2.9
3	F	24	ILE	2.9
5	D	608	PRO	2.9
4	E	759	MET	2.9
4	E	848	SER	2.9
7	H	144	THR	2.9
3	F	289	HIS	2.8
1	A	95	HIS	2.8
1	A	69	ILE	2.8
1	A	258	TRP	2.8
4	E	399	THR	2.8
2	B	280	GLU	2.8
7	H	113	ARG	2.8
2	B	338	GLU	2.8
2	B	381	SER	2.8
2	B	493	PHE	2.8
4	E	201	ASP	2.8
3	F	176	GLU	2.8
3	F	406	GLU	2.8
5	D	622	GLN	2.8
6	L	123	PRO	2.8
4	E	93	ILE	2.7
2	B	190	TYR	2.7
4	E	649	GLN	2.7
4	E	826	TYR	2.7
5	D	674	ILE	2.7
4	E	743	ASN	2.7
4	E	981	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	E	420	PHE	2.7
4	E	213	SER	2.7
3	F	22	PHE	2.7
2	B	293	GLU	2.7
2	B	368	GLU	2.7
7	H	77	ILE	2.7
2	B	247	TYR	2.7
4	E	608	ASP	2.7
7	H	162	ALA	2.7
3	F	35	PRO	2.7
2	B	384	CYS	2.7
6	L	117	SER	2.7
3	F	88	ASP	2.6
2	B	654	VAL	2.6
5	D	738	LYS	2.6
6	L	116	PRO	2.6
2	B	529	ASN	2.6
6	L	85	ASP	2.6
4	E	811	LEU	2.6
5	D	644	GLN	2.6
4	E	92	THR	2.6
3	F	155	SER	2.6
4	E	504	SER	2.6
4	E	810	ASP	2.6
4	E	595	ILE	2.6
1	A	150	SER	2.6
4	E	125	ASP	2.6
6	L	215	GLY	2.6
4	E	1003	VAL	2.6
4	E	813	CYS	2.6
7	H	115	GLU	2.6
7	H	146	VAL	2.6
4	E	134	PRO	2.6
6	L	206	SER	2.6
2	B	497	PHE	2.6
3	F	398	ILE	2.6
2	B	370	LEU	2.6
3	F	13	THR	2.6
3	F	68	TRP	2.5
1	A	30	ASP	2.5
2	B	634	ILE	2.5
5	D	654	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
4	E	967	PHE	2.5
3	F	280	SER	2.5
3	F	333	SER	2.5
4	E	428	SER	2.5
7	H	164	SER	2.5
4	E	983	GLN	2.5
5	D	625	ALA	2.5
4	E	825	TYR	2.5
4	E	384	LYS	2.5
4	E	543	SER	2.5
6	L	147	ALA	2.5
4	E	206	LYS	2.5
4	E	318	ASN	2.5
6	L	64	ARG	2.5
2	B	365	SER	2.5
2	B	397	GLU	2.5
2	B	671	GLU	2.5
3	F	118	GLN	2.5
4	E	293	LEU	2.5
4	E	353	VAL	2.5
7	H	61	HIS	2.5
6	L	84	GLU	2.5
4	E	864	PHE	2.5
3	F	222	VAL	2.5
5	D	593	ALA	2.5
2	B	488	HIS	2.4
4	E	562	PHE	2.4
3	F	362	SER	2.4
5	D	742	ALA	2.4
4	E	375	ASN	2.4
4	E	971	ASN	2.4
1	A	42	THR	2.4
3	F	64	SER	2.4
4	E	120	ASN	2.4
4	E	105	ARG	2.4
6	L	149	VAL	2.4
4	E	697	GLN	2.4
4	E	827	GLN	2.4
1	A	101	SER	2.4
2	B	300	LEU	2.4
2	B	550	GLY	2.4
5	D	574	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
7	H	35	GLY	2.4
2	B	527	ILE	2.4
4	E	397	ILE	2.4
4	E	508	LYS	2.4
6	L	101	PHE	2.4
2	B	383	LEU	2.4
2	B	363	SER	2.4
2	B	491	SER	2.4
4	E	400	LYS	2.4
4	E	982	TYR	2.4
4	E	539	GLU	2.3
4	E	911	GLU	2.3
2	B	655	ALA	2.3
2	B	530	ARG	2.3
1	A	179	ASP	2.3
3	F	90	ASP	2.3
2	B	507	THR	2.3
6	L	183	THR	2.3
3	F	11	ARG	2.3
4	E	11	LEU	2.3
7	H	120	TYR	2.3
6	L	189	TYR	2.3
2	B	590	ASN	2.3
7	H	251	LYS	2.3
3	F	225	THR	2.3
4	E	879	PHE	2.3
3	F	394	ILE	2.3
7	H	114	ALA	2.3
1	A	257	LEU	2.3
4	E	866	GLU	2.3
4	E	10	ASN	2.3
2	B	633	THR	2.3
2	B	393	GLY	2.3
4	E	725	ARG	2.3
4	E	1008	SER	2.3
7	H	76	SER	2.3
7	H	42	GLY	2.3
1	A	11	LEU	2.3
1	A	127	VAL	2.3
6	L	133	ALA	2.3
6	L	154	ASP	2.3
7	H	62	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	184	ILE	2.2
4	E	564	ILE	2.2
2	B	236	LYS	2.2
4	E	1006	VAL	2.2
6	L	114	ALA	2.2
4	E	81	PHE	2.2
4	E	516	PHE	2.2
4	E	291	LEU	2.2
4	E	501	THR	2.2
6	L	26	CYS	2.2
1	A	29	SER	2.2
3	F	389	VAL	2.2
4	E	978	ALA	2.2
4	E	78	LEU	2.2
2	B	231	ASP	2.2
4	E	808	TRP	2.2
4	E	100	ALA	2.2
4	E	721	MET	2.2
6	L	87	ALA	2.2
3	F	180	PHE	2.2
3	F	432	TYR	2.2
4	E	781	ASP	2.2
2	B	228	THR	2.2
7	H	188	THR	2.2
4	E	328	ILE	2.2
3	F	383	PRO	2.2
4	E	556	ASN	2.2
6	L	140	ASN	2.2
4	E	565	THR	2.2
7	H	230	THR	2.2
3	F	299	GLU	2.2
2	B	503	ALA	2.1
7	H	100	THR	2.1
4	E	393	HIS	2.1
4	E	265	SER	2.1
4	E	82	TYR	2.1
6	L	196	ALA	2.1
3	F	258	PRO	2.1
5	D	737	PHE	2.1
1	A	9	ASN	2.1
4	E	103	ASN	2.1
5	D	618	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	619	VAL	2.1
3	F	85	ARG	2.1
3	F	226	GLN	2.1
2	B	279	PRO	2.1
4	E	83	PRO	2.1
7	H	40	PRO	2.1
3	F	414	THR	2.1
6	L	100	THR	2.1
7	H	140	TRP	2.1
3	F	183	TYR	2.1
2	B	592	LEU	2.1
2	B	594	THR	2.1
3	F	146	ASN	2.1
4	E	838	GLN	2.1
4	E	979	GLU	2.1
2	B	168	LYS	2.1
2	B	296	PHE	2.1
4	E	625	ILE	2.1
4	E	686	PHE	2.1
4	E	824	PHE	2.1
4	E	985	ILE	2.1
4	E	299	GLN	2.1
4	E	438	GLU	2.1
2	B	297	LEU	2.0
4	E	970	LEU	2.0
1	A	67	GLY	2.0
4	E	849	ALA	2.0
2	B	667	SER	2.0
6	L	80	SER	2.0
4	E	356	LYS	2.0
4	E	570	LEU	2.0
4	E	875	LEU	2.0
4	E	889	LEU	2.0
5	D	728	LEU	2.0
7	H	71	LEU	2.0
4	E	390	GLN	2.0
4	E	114	GLU	2.0
4	E	763	THR	2.0
4	E	888	VAL	2.0
4	E	161	ARG	2.0
2	B	224	TYR	2.0
7	H	81	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
4	E	780	HIS	2.0
2	B	304	VAL	2.0
4	E	355	TRP	2.0
2	B	250	LYS	2.0
3	F	390	THR	2.0
5	D	579	SER	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.