



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:15 PM UTC

PDB ID : 5GS1 / pdb_00005gs1
Title : Crystal structure of homo-specific diabody
Authors : Kim, J.H.; Song, D.H.; Youn, S.J.; Kim, J.W.; Cho, G.; Lee, H.; Lee, J.O.
Deposited on : 2016-08-13
Resolution : 2.00 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:

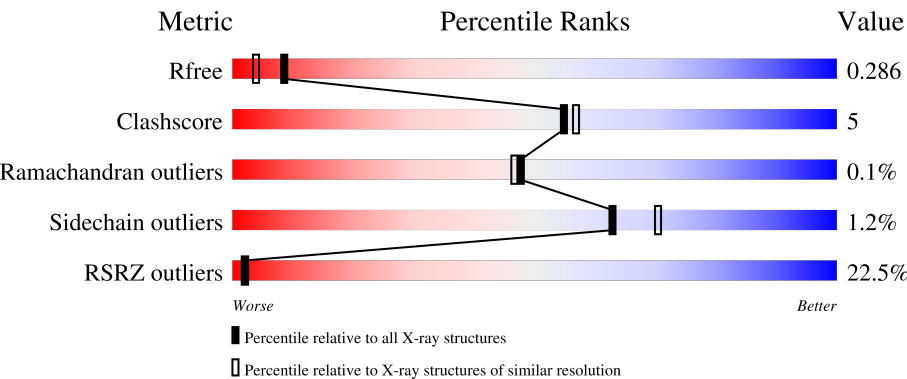
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	108	2% 90% 8%
1	M	108	25% 86% 12%
1	O	108	30% 86% 12%
1	Q	108	8% 91% 7%
2	B	124	8% 88% 7% 5%

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Mol	Chain	Length	Quality of chain
2	N	124	
2	P	124	
2	R	124	
3	C	232	
3	D	232	
3	E	232	
3	F	232	
3	G	232	
3	H	232	
3	I	232	
3	J	232	
3	K	232	
3	L	232	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25820 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			803	502	134	165	2			
1	M	106	Total	C	N	O	S	0	0	0
			803	502	134	165	2			
1	O	106	Total	C	N	O	S	0	0	0
			803	502	134	165	2			
1	Q	106	Total	C	N	O	S	0	0	0
			803	502	134	165	2			

- Molecule 2 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	S	0	0	0
			901	569	156	172	4			
2	N	118	Total	C	N	O	S	0	0	0
			901	569	156	172	4			
2	P	118	Total	C	N	O	S	0	0	0
			901	569	156	172	4			
2	R	118	Total	C	N	O	S	0	0	0
			901	569	156	172	4			

- Molecule 3 is a protein called diabody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			
3	D	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			
3	E	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			
3	F	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	223	Total	C	N	O	S	0	0	0
			1698	1068	289	335	6			
3	H	224	Total	C	N	O	S	0	0	0
			1704	1071	290	337	6			
3	I	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			
3	J	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			
3	K	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			
3	L	229	Total	C	N	O	S	0	0	0
			1726	1082	295	343	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	84	Total	O	0	0
			84	84		
4	C	183	Total	O	0	0
			183	183		
4	D	145	Total	O	0	0
			145	145		
4	E	110	Total	O	0	0
			110	110		
4	F	101	Total	O	0	0
			101	101		
4	G	50	Total	O	0	0
			50	50		
4	H	58	Total	O	0	0
			58	58		
4	I	157	Total	O	0	0
			157	157		
4	J	168	Total	O	0	0
			168	168		
4	K	191	Total	O	0	0
			191	191		
4	L	142	Total	O	0	0
			142	142		
4	M	44	Total	O	0	0
			44	44		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	38	Total 38	O 38	0	0
4	O	37	Total 37	O 37	0	0
4	P	67	Total 67	O 67	0	0
4	Q	51	Total 51	O 51	0	0
4	R	107	Total 107	O 107	0	0

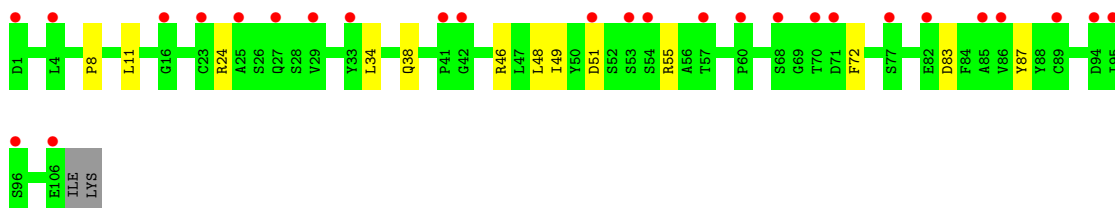
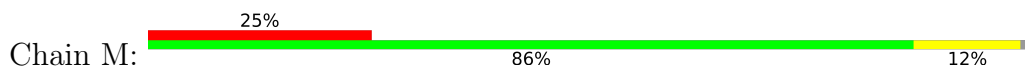
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

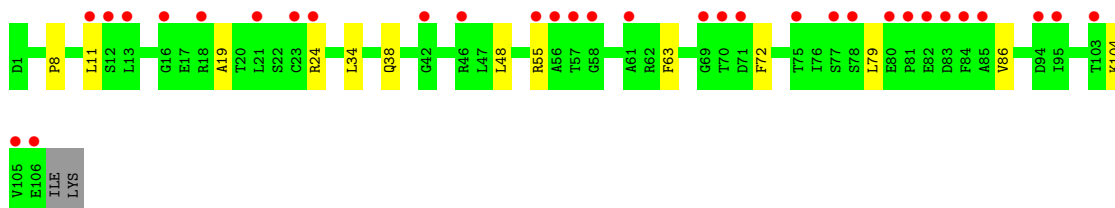
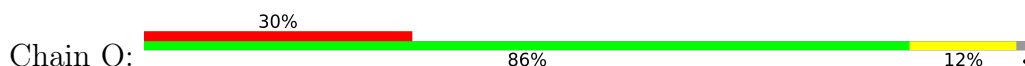
- Molecule 1: light chain



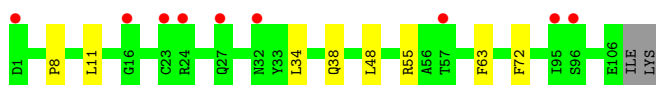
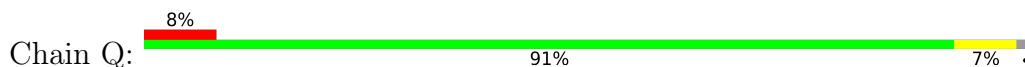
- Molecule 1: light chain



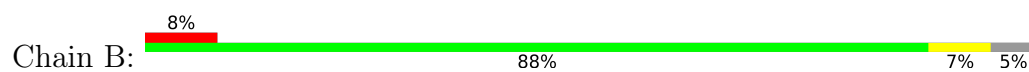
- Molecule 1: light chain



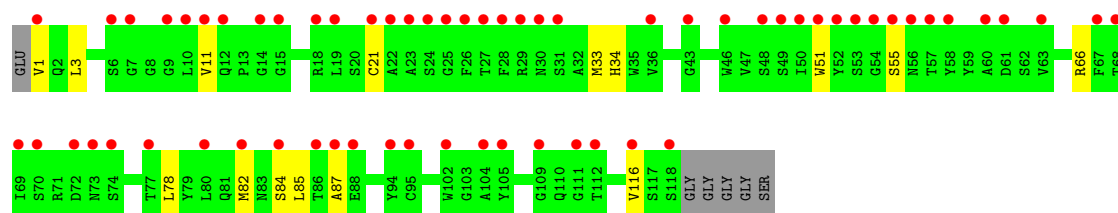
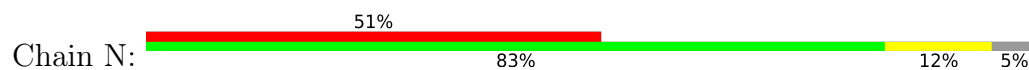
- Molecule 1: light chain



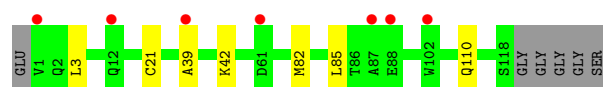
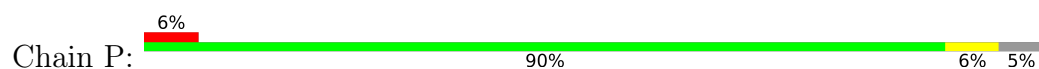
- Molecule 2: heavy chain



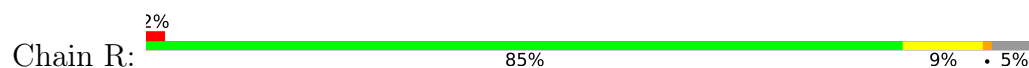
- Molecule 2: heavy chain



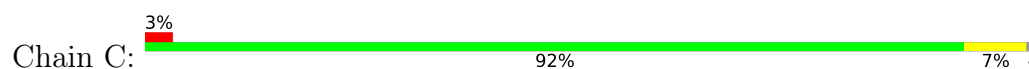
- Molecule 2: heavy chain



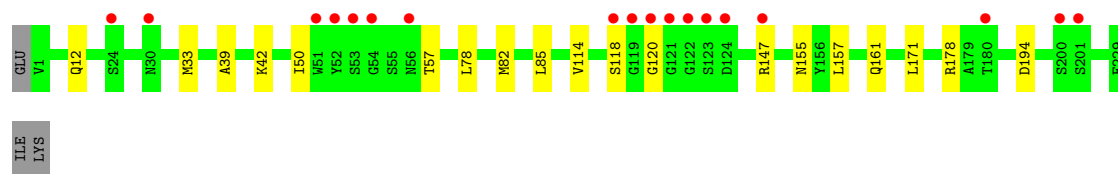
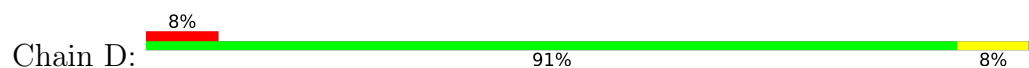
- Molecule 2: heavy chain



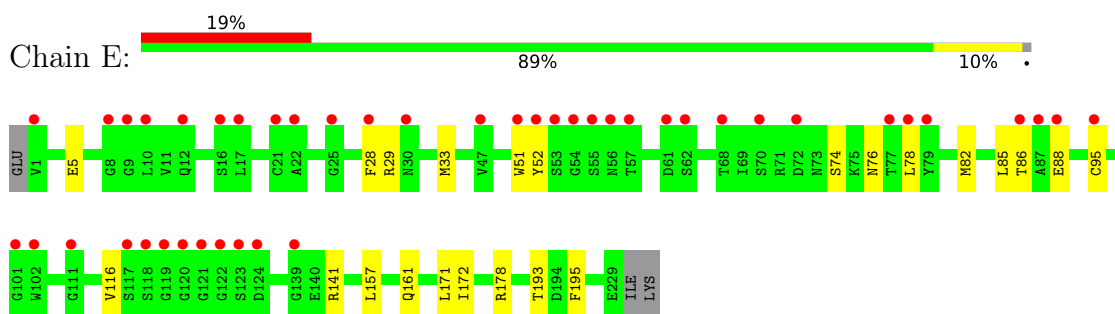
- Molecule 3: diabody



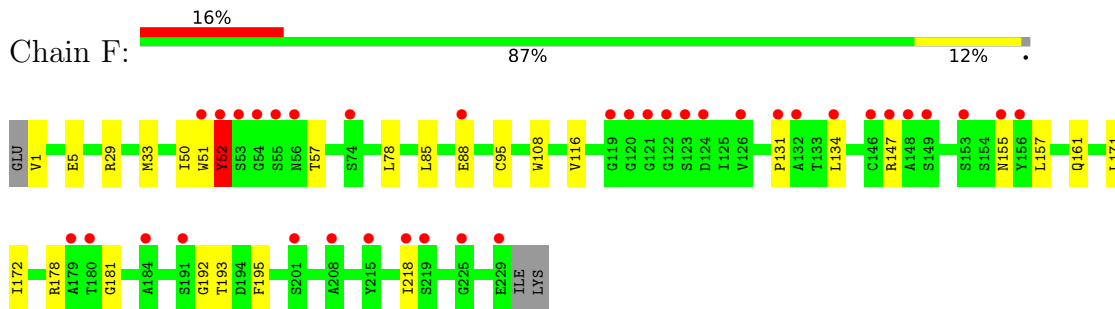
- Molecule 3: diabody



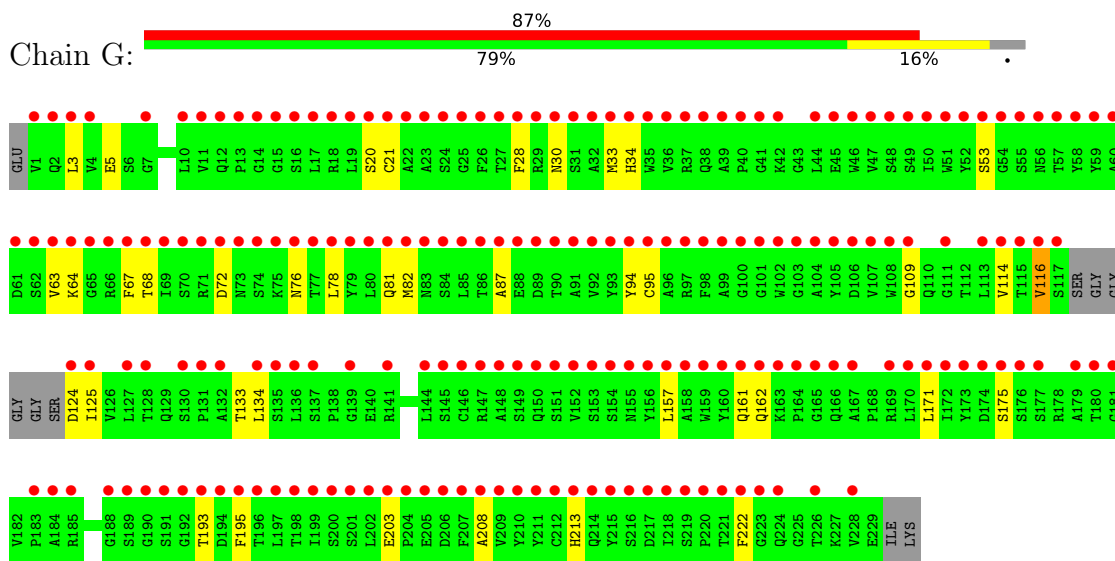
- Molecule 3: diabody



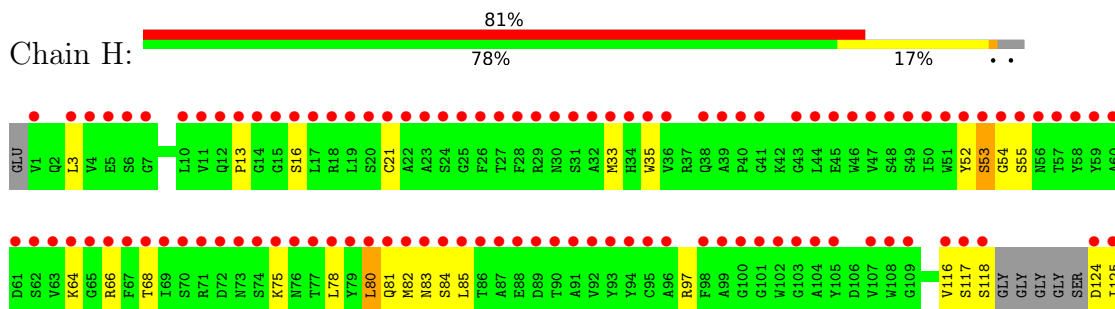
- Molecule 3: diabody

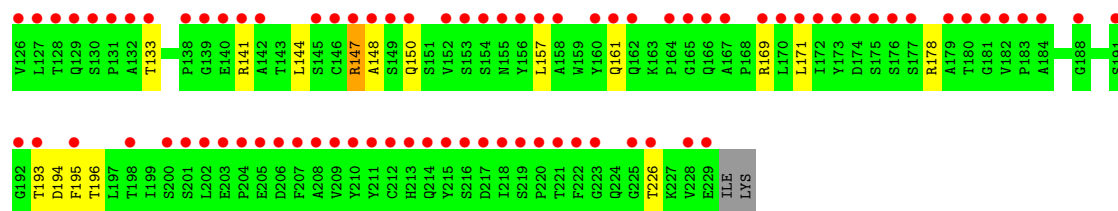


- Molecule 3: diabody

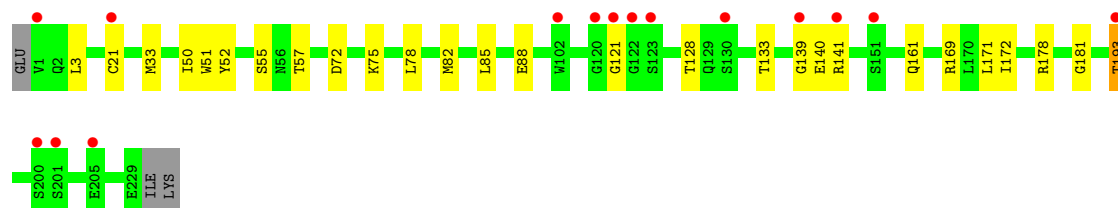
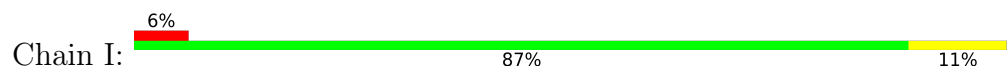


- Molecule 3: diabody

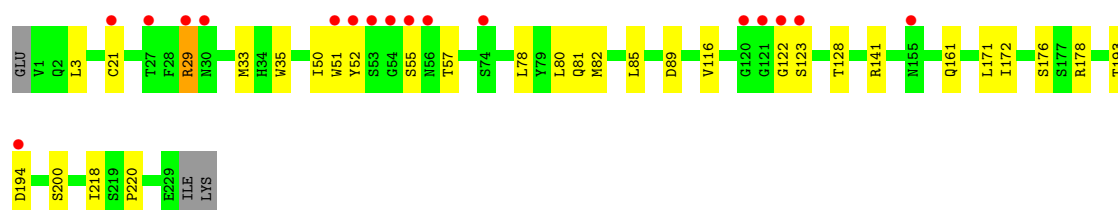
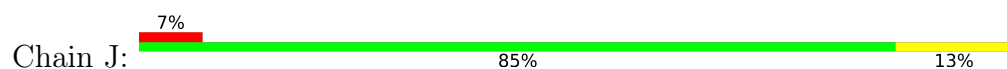




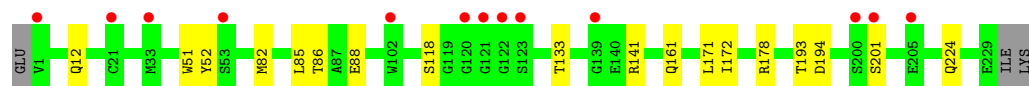
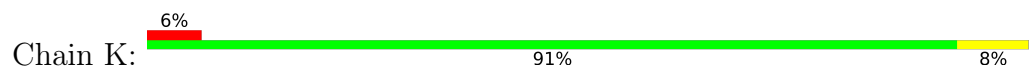
• Molecule 3: diabody



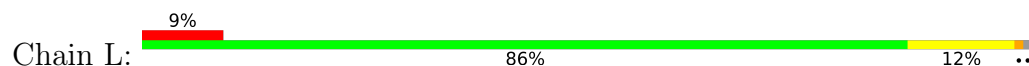
• Molecule 3: diabody



• Molecule 3: diabody



• Molecule 3: diabody



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.12Å 128.81Å 259.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.05 – 2.00 20.05 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.05-2.00) 96.2 (20.05-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.25 (at 1.99Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.267 , 0.286 0.267 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (0.78%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25820	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.78 % 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 1.1822e-06. 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 [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/822	0.35	0/1120
1	M	0.12	0/822	0.35	0/1120
1	O	0.12	0/822	0.40	0/1120
1	Q	0.10	0/822	0.37	0/1120
2	B	0.12	0/924	0.35	0/1255
2	N	0.14	0/924	0.37	0/1255
2	P	0.12	0/924	0.35	0/1255
2	R	0.11	0/924	0.36	0/1255
3	C	0.10	0/1769	0.33	0/2406
3	D	0.10	0/1769	0.34	0/2406
3	E	0.12	0/1769	0.36	0/2406
3	F	0.14	0/1769	0.42	1/2406 (0.0%)
3	G	0.18	0/1740	0.40	0/2367
3	H	0.14	0/1746	0.46	1/2375 (0.0%)
3	I	0.13	0/1769	0.38	0/2406
3	J	0.13	0/1769	0.38	0/2406
3	K	0.12	0/1769	0.36	0/2406
3	L	0.12	0/1769	0.36	0/2406
All	All	0.13	0/24622	0.38	2/33490 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	52	TYR	N-CA-C	6.10	118.93	109.60
3	H	53	SER	N-CA-C	5.48	118.13	107.71

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	803	0	768	10	0
1	M	803	0	768	10	0
1	O	803	0	768	8	0
1	Q	803	0	768	4	0
2	B	901	0	856	6	0
2	N	901	0	856	11	0
2	P	901	0	856	5	0
2	R	901	0	856	10	0
3	C	1726	0	1639	9	0
3	D	1726	0	1639	15	0
3	E	1726	0	1639	14	0
3	F	1726	0	1639	17	0
3	G	1698	0	1616	24	1
3	H	1704	0	1621	35	0
3	I	1726	0	1639	17	0
3	J	1726	0	1639	19	0
3	K	1726	0	1639	12	0
3	L	1726	0	1639	18	0
4	A	61	0	0	2	0
4	B	84	0	0	2	0
4	C	183	0	0	0	0
4	D	145	0	0	3	0
4	E	110	0	0	2	0
4	F	101	0	0	4	0
4	G	50	0	0	8	1
4	H	58	0	0	10	0
4	I	157	0	0	5	0
4	J	168	0	0	4	0
4	K	191	0	0	4	0
4	L	142	0	0	2	0
4	M	44	0	0	2	0
4	N	38	0	0	3	0
4	O	37	0	0	1	0
4	P	67	0	0	1	0
4	Q	51	0	0	0	0
4	R	107	0	0	4	0
All	All	25820	0	22845	223	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 5.

All (223) 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)
3:I:139:GLY:O	1:O:24:ARG:NH1	2.04	0.89
1:A:24:ARG:NH1	4:A:201:HOH:O	2.12	0.81
3:G:72:ASP:O	4:G:301:HOH:O	2.04	0.75
3:J:81:GLN:NE2	4:J:302:HOH:O	2.18	0.74
3:D:120:GLY:HA2	2:P:110:GLN:HB3	1.70	0.73
1:A:18:ARG:NH2	3:H:194:ASP:OD2	2.23	0.72
1:M:24:ARG:NH2	4:M:201:HOH:O	2.21	0.71
3:I:72:ASP:OD2	3:I:75:LYS:NZ	2.23	0.71
3:L:178:ARG:NH1	4:L:303:HOH:O	2.24	0.70
2:R:12:GLN:NE2	4:R:202:HOH:O	2.20	0.70
3:G:34:HIS:O	4:G:302:HOH:O	2.09	0.69
3:K:141:ARG:NH2	4:K:304:HOH:O	2.25	0.69
3:D:12:GLN:NE2	4:D:301:HOH:O	2.25	0.69
3:H:144:LEU:HD21	3:H:226:THR:HG21	1.76	0.68
3:I:88:GLU:OE2	4:I:301:HOH:O	2.12	0.68
3:G:95:CYS:O	4:G:303:HOH:O	2.11	0.67
2:R:86:THR:HG22	2:R:88:GLU:H	1.59	0.67
2:B:12:GLN:NE2	4:K:303:HOH:O	2.26	0.67
3:K:224:GLN:NE2	4:K:305:HOH:O	2.27	0.66
3:G:33:MET:HB3	3:G:78:LEU:HD22	1.79	0.65
3:G:175:SER:OG	4:G:304:HOH:O	2.13	0.65
3:D:178:ARG:NH1	4:D:303:HOH:O	2.29	0.65
1:A:24:ARG:NH2	3:H:141:ARG:H	1.96	0.64
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.79	0.64
1:A:24:ARG:NH2	4:H:302:HOH:O	2.31	0.64
1:M:46:ARG:NH2	4:M:204:HOH:O	2.31	0.64
3:G:30:ASN:ND2	4:G:308:HOH:O	2.32	0.62
3:C:82:MET:HB3	3:C:85:LEU:HD21	1.81	0.62
1:A:71:ASP:OD2	3:H:141:ARG:NH2	2.31	0.62
3:C:141:ARG:NH2	3:J:194:ASP:OD2	2.28	0.62
1:M:38:GLN:HB2	1:M:48:LEU:HD11	1.81	0.62
2:N:51:TRP:HB3	2:N:55:SER:OG	1.99	0.61
1:A:24:ARG:HH21	3:H:141:ARG:H	1.49	0.61
4:I:301:HOH:O	3:J:89:ASP:OD1	2.17	0.60
3:H:52:TYR:CD1	3:H:54:GLY:HA3	2.37	0.59
3:D:161:GLN:HB2	3:D:171:LEU:HD11	1.83	0.59
3:H:83:ASN:OD1	4:H:301:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:GLN:HB2	3:C:171:LEU:HD11	1.85	0.59
2:P:39:ALA:HB3	2:P:42:LYS:HD3	1.84	0.59
1:Q:38:GLN:HB2	1:Q:48:LEU:HD11	1.84	0.59
2:N:34:HIS:HB3	4:N:201:HOH:O	2.02	0.58
2:P:110:GLN:NE2	4:P:203:HOH:O	2.37	0.58
3:H:53:SER:HA	3:H:55:SER:N	2.18	0.58
1:Q:8:PRO:HG2	1:Q:11:LEU:HG	1.85	0.58
3:L:12:GLN:NE2	4:L:301:HOH:O	2.18	0.58
3:J:176:SER:OG	4:J:301:HOH:O	2.16	0.57
3:D:194:ASP:OD2	3:E:141:ARG:NH2	2.39	0.56
3:H:147:ARG:NH2	4:H:311:HOH:O	2.37	0.56
3:K:161:GLN:HB2	3:K:171:LEU:HD11	1.87	0.56
3:H:148:ALA:O	3:H:193:THR:OG1	2.23	0.56
3:E:33:MET:HB3	3:E:78:LEU:HD22	1.87	0.56
3:H:97:ARG:NH1	4:H:303:HOH:O	2.39	0.56
3:F:161:GLN:HB2	3:F:171:LEU:HD11	1.87	0.56
3:L:11:VAL:HG11	3:L:17:LEU:HD13	1.87	0.55
3:F:50:ILE:HG13	3:F:57:THR:HG22	1.87	0.55
3:H:81:GLN:NE2	4:H:301:HOH:O	2.12	0.55
3:J:172:ILE:HD13	3:J:178:ARG:HA	1.89	0.55
3:L:52:TYR:HD1	3:L:54:GLY:H	1.54	0.55
3:H:85:LEU:HB3	3:H:116:VAL:HG21	1.87	0.55
3:L:172:ILE:HD13	3:L:178:ARG:HA	1.87	0.55
3:E:172:ILE:HD13	3:E:178:ARG:HA	1.88	0.55
3:E:29:ARG:NH1	1:M:55:ARG:O	2.30	0.54
2:R:66:ARG:NH2	4:R:207:HOH:O	2.39	0.54
3:L:51:TRP:HB3	3:L:55:SER:OG	2.07	0.54
3:K:194:ASP:OD1	4:K:301:HOH:O	2.19	0.54
3:I:141:ARG:NH1	4:O:201:HOH:O	2.40	0.54
2:R:88:GLU:OE2	4:R:201:HOH:O	2.18	0.54
3:F:1:VAL:N	4:F:304:HOH:O	2.41	0.54
3:G:82:MET:HE1	3:G:114:VAL:HG21	1.90	0.54
3:H:161:GLN:HB2	3:H:171:LEU:HD11	1.90	0.54
3:F:33:MET:HB3	3:F:78:LEU:HD22	1.90	0.54
3:I:172:ILE:HD13	3:I:178:ARG:HA	1.90	0.54
3:E:161:GLN:HB2	3:E:171:LEU:HD11	1.89	0.53
3:G:161:GLN:HB2	3:G:171:LEU:HD11	1.90	0.53
3:I:161:GLN:HB2	3:I:171:LEU:HD11	1.90	0.53
2:R:82:MET:HB3	2:R:85:LEU:HD21	1.91	0.52
3:H:33:MET:HB3	3:H:78:LEU:HD22	1.92	0.52
3:G:109:GLY:N	4:G:303:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:124:ASP:N	3:H:124:ASP:OD1	2.42	0.52
1:O:8:PRO:HG2	1:O:11:LEU:HG	1.92	0.52
2:N:66:ARG:NH1	2:N:84:SER:O	2.43	0.52
3:J:218:ILE:O	3:J:220:PRO:HD3	2.10	0.51
2:P:82:MET:HB3	2:P:85:LEU:HD21	1.92	0.51
3:H:178:ARG:NH1	4:H:307:HOH:O	2.42	0.51
3:H:68:THR:HB	3:H:81:GLN:HB3	1.91	0.51
3:H:83:ASN:ND2	4:H:305:HOH:O	2.42	0.51
1:O:55:ARG:HD3	1:O:63:PHE:O	2.11	0.51
3:J:161:GLN:HB2	3:J:171:LEU:HD11	1.91	0.51
3:K:82:MET:HB3	3:K:85:LEU:HD21	1.93	0.50
3:G:64:LYS:O	3:H:13:PRO:HB2	2.12	0.50
2:N:11:VAL:HG13	4:N:202:HOH:O	2.10	0.50
2:N:116:VAL:HG13	4:N:202:HOH:O	2.11	0.50
3:D:33:MET:HB3	3:D:78:LEU:HD22	1.94	0.50
3:L:161:GLN:HB2	3:L:171:LEU:HD11	1.94	0.50
4:G:313:HOH:O	3:L:141:ARG:NH2	2.45	0.50
3:G:124:ASP:OD1	3:G:124:ASP:N	2.44	0.50
2:B:1:VAL:N	4:B:202:HOH:O	2.32	0.50
3:H:66:ARG:NH1	3:H:84:SER:O	2.43	0.50
3:G:5:GLU:HG3	3:G:95:CYS:SG	2.52	0.49
3:I:181:GLY:O	4:I:302:HOH:O	2.19	0.49
1:M:49:ILE:HD13	1:M:55:ARG:HA	1.93	0.49
2:N:82:MET:HB3	2:N:85:LEU:HD21	1.92	0.49
3:D:82:MET:HB3	3:D:85:LEU:HD21	1.94	0.49
3:I:82:MET:HB3	3:I:85:LEU:HD21	1.94	0.49
1:Q:55:ARG:HD3	1:Q:63:PHE:O	2.13	0.49
3:H:82:MET:HB3	3:H:85:LEU:HD21	1.94	0.49
1:O:38:GLN:HB2	1:O:48:LEU:HD11	1.94	0.49
1:A:17:GLU:HG2	3:H:147:ARG:NH2	2.27	0.48
3:D:147:ARG:NH2	4:E:302:HOH:O	2.41	0.48
3:I:169:ARG:NH2	4:I:305:HOH:O	2.35	0.48
2:N:1:VAL:HG13	2:N:1:VAL:O	2.13	0.48
2:B:33:MET:HB3	2:B:78:LEU:HD22	1.95	0.48
3:L:33:MET:HB3	3:L:78:LEU:HD22	1.94	0.48
3:K:172:ILE:HD13	3:K:178:ARG:HA	1.95	0.48
2:R:21:CYS:HB3	2:R:78:LEU:HB3	1.95	0.47
3:F:85:LEU:HB3	3:F:116:VAL:HG21	1.96	0.47
3:G:162:GLN:O	3:G:208:ALA:HB1	2.14	0.47
3:F:108:TRP:O	3:I:121:GLY:HA2	2.15	0.47
3:G:94:TYR:HB3	4:G:303:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:LEU:HB3	2:P:21:CYS:SG	2.55	0.47
3:C:33:MET:HB3	3:C:78:LEU:HD22	1.95	0.47
3:D:155:ASN:ND2	4:D:304:HOH:O	2.41	0.47
3:D:82:MET:HE1	3:D:114:VAL:HG21	1.97	0.47
3:I:193:THR:HG23	4:I:432:HOH:O	2.14	0.47
3:J:33:MET:HB3	3:J:78:LEU:HD22	1.96	0.47
3:J:3:LEU:HB3	3:J:21:CYS:SG	2.55	0.46
3:E:51:TRP:CG	3:E:52:TYR:H	2.33	0.46
2:R:86:THR:HG22	2:R:88:GLU:HG2	1.97	0.46
3:L:3:LEU:HB3	3:L:21:CYS:SG	2.55	0.46
3:H:82:MET:HE2	3:H:85:LEU:HD21	1.98	0.46
2:N:66:ARG:HD2	2:N:84:SER:HB2	1.97	0.46
2:B:51:TRP:CG	2:B:52:TYR:H	2.34	0.45
2:B:55:SER:O	4:B:201:HOH:O	2.21	0.45
2:B:82:MET:HB3	2:B:85:LEU:HD21	1.97	0.45
3:E:86:THR:OG1	3:E:88:GLU:OE1	2.34	0.45
3:F:157:LEU:HD22	3:F:195:PHE:CG	2.50	0.45
3:H:35:TRP:CE2	3:H:80:LEU:HB2	2.52	0.45
3:H:169:ARG:HE	3:H:169:ARG:HB3	1.58	0.45
3:L:86:THR:OG1	3:L:88:GLU:OE1	2.35	0.45
1:A:49:ILE:HD13	1:A:55:ARG:HA	1.98	0.45
3:E:157:LEU:HD22	3:E:195:PHE:CG	2.52	0.45
3:H:141:ARG:O	4:H:302:HOH:O	2.20	0.45
3:J:51:TRP:CG	3:J:52:TYR:H	2.35	0.45
3:C:121:GLY:HA2	3:C:122:GLY:HA3	1.77	0.44
3:I:3:LEU:HB3	3:I:21:CYS:SG	2.57	0.44
1:M:8:PRO:HG2	1:M:11:LEU:HG	1.99	0.44
3:F:155:ASN:HD21	3:F:192:GLY:H	1.65	0.44
1:O:86:VAL:HG22	1:O:104:LYS:HB2	2.00	0.44
3:C:194:ASP:OD2	3:J:141:ARG:NH2	2.51	0.43
3:L:50:ILE:HG13	3:L:57:THR:HG22	1.99	0.43
3:J:50:ILE:HG13	3:J:57:THR:HG22	2.00	0.43
3:J:85:LEU:HB3	3:J:116:VAL:HG21	1.99	0.43
3:E:29:ARG:NH1	1:M:55:ARG:HB3	2.33	0.43
3:I:50:ILE:HG13	3:I:57:THR:HG22	2.00	0.43
4:F:302:HOH:O	3:K:201:SER:HA	2.18	0.43
3:D:12:GLN:HG3	3:D:118:SER:HA	2.01	0.43
3:F:181:GLY:O	3:H:150:GLN:NE2	2.49	0.43
2:N:33:MET:HB3	2:N:78:LEU:HD22	2.00	0.43
3:G:68:THR:HB	3:G:81:GLN:HB3	2.01	0.43
3:F:51:TRP:CG	3:F:52:TYR:H	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:200:SER:O	4:J:303:HOH:O	2.22	0.43
3:F:29:ARG:NH2	4:F:303:HOH:O	2.39	0.43
3:H:117:SER:OG	3:H:118:SER:N	2.52	0.43
3:H:144:LEU:O	3:H:196:THR:HA	2.19	0.43
3:C:51:TRP:CG	3:C:52:TYR:H	2.36	0.42
1:O:19:ALA:HB2	1:O:79:LEU:HD11	2.01	0.42
3:E:82:MET:HB3	3:E:85:LEU:HD21	2.01	0.42
3:F:5:GLU:HG3	3:F:95:CYS:SG	2.59	0.42
2:R:33:MET:HB3	2:R:78:LEU:HD22	2.00	0.42
3:G:213:HIS:HB2	3:G:222:PHE:CD1	2.53	0.42
3:K:51:TRP:CG	3:K:52:TYR:H	2.36	0.42
3:H:52:TYR:CE1	3:H:54:GLY:HA3	2.54	0.42
3:L:162:GLN:O	3:L:208:ALA:HB1	2.19	0.42
3:D:39:ALA:HB3	3:D:42:LYS:HE2	2.00	0.42
1:M:83:ASP:O	1:M:87:TYR:OH	2.31	0.42
3:D:147:ARG:NH1	4:E:302:HOH:O	2.48	0.42
3:G:3:LEU:HB3	3:G:21:CYS:SG	2.59	0.42
3:H:3:LEU:HB3	3:H:21:CYS:SG	2.59	0.42
1:O:34:LEU:HD13	1:O:72:PHE:CD1	2.54	0.42
3:G:87:ALA:HA	3:G:116:VAL:HG13	2.02	0.42
3:I:33:MET:HB3	3:I:78:LEU:HD22	2.00	0.42
3:J:123:SER:HB2	4:J:422:HOH:O	2.19	0.42
1:Q:34:LEU:HD13	1:Q:72:PHE:CD1	2.54	0.42
3:G:28:PHE:CD2	3:G:76:ASN:HA	2.55	0.42
1:M:34:LEU:HD13	1:M:72:PHE:CD1	2.55	0.42
2:N:3:LEU:HB3	2:N:21:CYS:SG	2.60	0.42
2:N:87:ALA:HA	2:N:116:VAL:HB	2.02	0.42
2:R:109:GLY:HA2	4:R:206:HOH:O	2.19	0.42
3:I:51:TRP:CG	3:I:52:TYR:H	2.38	0.42
3:K:86:THR:OG1	3:L:62:SER:O	2.24	0.42
3:E:88:GLU:HG2	3:F:88:GLU:OE2	2.19	0.41
3:F:1:VAL:N	4:F:306:HOH:O	2.44	0.41
3:H:16:SER:HB2	4:H:301:HOH:O	2.20	0.41
3:J:51:TRP:HB3	3:J:55:SER:OG	2.20	0.41
3:K:12:GLN:NE2	3:K:118:SER:HA	2.34	0.41
3:D:147:ARG:NE	3:D:194:ASP:OD1	2.52	0.41
3:F:131:PRO:HG2	3:F:134:LEU:HD21	2.02	0.41
3:G:134:LEU:HD23	3:G:134:LEU:HA	1.95	0.41
3:F:147:ARG:NH2	3:K:141:ARG:HB2	2.34	0.41
3:J:35:TRP:CE2	3:J:80:LEU:HB2	2.56	0.41
3:I:140:GLU:HA	1:O:24:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:50:ILE:HG13	3:D:57:THR:HG22	2.03	0.41
3:G:63:VAL:HB	3:G:67:PHE:CG	2.56	0.41
3:L:178:ARG:HG2	3:L:182:VAL:HB	2.02	0.41
3:C:11:VAL:HG11	3:C:17:LEU:HD13	2.03	0.41
3:E:5:GLU:HG3	3:E:95:CYS:SG	2.61	0.41
3:J:82:MET:HB3	3:J:85:LEU:HD21	2.03	0.41
3:E:28:PHE:CD2	3:E:76:ASN:HA	2.55	0.41
3:G:28:PHE:HB3	3:G:76:ASN:OD1	2.21	0.41
3:I:52:TYR:CZ	3:I:55:SER:HB3	2.56	0.41
3:L:218:ILE:O	3:L:220:PRO:HD3	2.20	0.41
1:A:27:GLN:OE1	4:A:202:HOH:O	2.22	0.41
3:G:203:GLU:OE1	3:G:203:GLU:N	2.54	0.41
3:E:52:TYR:CD1	1:M:51:ASP:HB3	2.56	0.40
3:H:157:LEU:HD13	3:H:195:PHE:CD2	2.56	0.40
3:C:5:GLU:HG3	3:C:95:CYS:SG	2.61	0.40
3:F:172:ILE:HD13	3:F:178:ARG:HA	2.03	0.40
3:G:157:LEU:HD13	3:G:195:PHE:CD2	2.56	0.40
3:J:29:ARG:CZ	3:J:29:ARG:HB3	2.50	0.40
3:L:141:ARG:HG3	3:L:200:SER:O	2.21	0.40
3:K:88:GLU:HB3	3:L:88:GLU:HG2	2.02	0.40
2:R:51:TRP:CG	2:R:52:TYR:H	2.38	0.40
3:H:169:ARG:NH1	4:H:309:HOH:O	2.36	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:G:53:SER:O	4:G:304:HOH:O[3_454]	2.19	0.01

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	104/108 (96%)	101 (97%)	3 (3%)	0	100	100
1	M	104/108 (96%)	101 (97%)	3 (3%)	0	100	100
1	O	104/108 (96%)	102 (98%)	2 (2%)	0	100	100
1	Q	104/108 (96%)	101 (97%)	3 (3%)	0	100	100
2	B	116/124 (94%)	113 (97%)	3 (3%)	0	100	100
2	N	116/124 (94%)	112 (97%)	4 (3%)	0	100	100
2	P	116/124 (94%)	113 (97%)	3 (3%)	0	100	100
2	R	116/124 (94%)	113 (97%)	3 (3%)	0	100	100
3	C	227/232 (98%)	221 (97%)	6 (3%)	0	100	100
3	D	227/232 (98%)	217 (96%)	10 (4%)	0	100	100
3	E	227/232 (98%)	223 (98%)	4 (2%)	0	100	100
3	F	227/232 (98%)	217 (96%)	9 (4%)	1 (0%)	30	27
3	G	219/232 (94%)	213 (97%)	6 (3%)	0	100	100
3	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
3	I	227/232 (98%)	221 (97%)	6 (3%)	0	100	100
3	J	227/232 (98%)	221 (97%)	5 (2%)	1 (0%)	30	27
3	K	227/232 (98%)	223 (98%)	4 (2%)	0	100	100
3	L	227/232 (98%)	223 (98%)	4 (2%)	0	100	100
All	All	3135/3248 (96%)	3048 (97%)	85 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	122	GLY
3	F	52	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	90/92 (98%)	90 (100%)	0	100	100
1	M	90/92 (98%)	90 (100%)	0	100	100
1	O	90/92 (98%)	90 (100%)	0	100	100
1	Q	90/92 (98%)	90 (100%)	0	100	100
2	B	93/95 (98%)	93 (100%)	0	100	100
2	N	93/95 (98%)	93 (100%)	0	100	100
2	P	93/95 (98%)	93 (100%)	0	100	100
2	R	93/95 (98%)	92 (99%)	1 (1%)	65	73
3	C	184/187 (98%)	184 (100%)	0	100	100
3	D	184/187 (98%)	183 (100%)	1 (0%)	81	87
3	E	184/187 (98%)	181 (98%)	3 (2%)	55	62
3	F	184/187 (98%)	182 (99%)	2 (1%)	65	73
3	G	182/187 (97%)	177 (97%)	5 (3%)	39	42
3	H	183/187 (98%)	177 (97%)	6 (3%)	33	34
3	I	184/187 (98%)	181 (98%)	3 (2%)	55	62
3	J	184/187 (98%)	181 (98%)	3 (2%)	55	62
3	K	184/187 (98%)	182 (99%)	2 (1%)	65	73
3	L	184/187 (98%)	179 (97%)	5 (3%)	39	42
All	All	2569/2618 (98%)	2538 (99%)	31 (1%)	63	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	157	LEU
3	E	74	SER
3	E	116	VAL
3	E	193	THR
3	F	193	THR
3	F	218	ILE
3	G	20	SER
3	G	116	VAL
3	G	125	ILE
3	G	133	THR
3	G	193	THR
3	H	64	LYS
3	H	75	LYS
3	H	80	LEU

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Mol	Chain	Res	Type
3	H	125	ILE
3	H	133	THR
3	H	147	ARG
3	I	128	THR
3	I	133	THR
3	I	193	THR
3	J	29	ARG
3	J	128	THR
3	J	193	THR
3	K	133	THR
3	K	193	THR
3	L	2	GLN
3	L	12	GLN
3	L	133	THR
3	L	141	ARG
3	L	193	THR
2	R	86	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	81	GLN
3	C	81	GLN
3	C	83	ASN
3	D	81	GLN
3	D	83	ASN
3	E	224	GLN
3	F	155	ASN
3	F	224	GLN
3	G	213	HIS
3	H	81	GLN
3	H	161	GLN
3	H	166	GLN
3	I	81	GLN
3	I	83	ASN
3	J	81	GLN
3	J	83	ASN
3	K	2	GLN
3	K	81	GLN
3	K	83	ASN
3	L	56	ASN
3	L	81	GLN

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Mol	Chain	Res	Type
3	L	83	ASN
1	M	39	GLN
2	N	38	GLN
2	N	81	GLN
2	N	83	ASN
2	P	81	GLN
2	P	83	ASN
1	Q	101	GLN
2	R	81	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [i](#)

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	106/108 (98%)	0.01	2 (1%) 66 66	8, 20, 36, 58	0
1	M	106/108 (98%)	1.59	27 (25%) 1 1	30, 37, 51, 70	0
1	O	106/108 (98%)	1.53	32 (30%) 1 1	21, 37, 54, 68	0
1	Q	106/108 (98%)	0.54	9 (8%) 16 15	14, 30, 41, 64	0
2	B	118/124 (95%)	0.26	10 (8%) 16 15	8, 16, 45, 68	0
2	N	118/124 (95%)	2.27	63 (53%) 0 0	29, 40, 58, 73	0
2	P	118/124 (95%)	0.39	7 (5%) 28 27	12, 22, 37, 54	0
2	R	118/124 (95%)	-0.11	3 (2%) 58 58	7, 15, 34, 48	0
3	C	229/232 (98%)	0.17	8 (3%) 47 46	8, 19, 39, 113	0
3	D	229/232 (98%)	0.37	18 (7%) 18 17	10, 23, 44, 112	0
3	E	229/232 (98%)	1.14	44 (19%) 3 3	13, 32, 52, 110	0
3	F	229/232 (98%)	0.97	36 (15%) 5 4	12, 33, 58, 118	0
3	G	223/232 (96%)	3.38	201 (90%) 0 0	37, 51, 66, 93	0
3	H	224/232 (96%)	3.24	189 (84%) 0 0	37, 51, 71, 100	0
3	I	229/232 (98%)	0.27	15 (6%) 24 23	8, 19, 46, 70	0
3	J	229/232 (98%)	0.30	17 (7%) 20 19	7, 19, 46, 69	0
3	K	229/232 (98%)	0.15	13 (5%) 29 28	7, 16, 39, 66	0
3	L	229/232 (98%)	0.49	21 (9%) 14 13	7, 21, 51, 69	0
All	All	3175/3248 (97%)	0.97	715 (22%) 2 2	7, 28, 59, 118	0

All (715) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	51	TRP	10.6
3	G	53	SER	8.4
3	C	121	GLY	8.3

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Mol	Chain	Res	Type	RSRZ
3	E	120	GLY	7.6
2	N	53	SER	7.5
3	G	87	ALA	7.2
3	E	121	GLY	6.9
3	H	52	TYR	6.8
3	H	49	SER	6.8
3	E	53	SER	6.8
3	G	57	THR	6.7
3	H	208	ALA	6.6
3	H	67	PHE	6.6
2	N	51	TRP	6.6
3	H	46	TRP	6.5
3	G	60	ALA	6.5
3	G	117	SER	6.5
3	G	203	GLU	6.3
3	L	52	TYR	6.3
3	G	55	SER	6.2
3	F	120	GLY	6.2
3	F	121	GLY	6.2
3	I	121	GLY	6.1
3	H	117	SER	6.1
3	G	61	ASP	6.0
3	H	63	VAL	6.0
3	H	68	THR	6.0
3	G	90	THR	5.9
3	G	52	TYR	5.9
3	H	31	SER	5.8
3	I	122	GLY	5.8
2	N	24	SER	5.8
3	G	49	SER	5.8
3	G	54	GLY	5.8
3	H	56	ASN	5.7
3	G	63	VAL	5.6
3	G	59	TYR	5.6
3	G	102	TRP	5.5
3	G	84	SER	5.5
2	N	52	TYR	5.5
3	H	15	GLY	5.5
3	G	14	GLY	5.4
3	G	68	THR	5.4
3	C	119	GLY	5.4
3	H	58	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
3	G	30	ASN	5.3
3	H	50	ILE	5.3
3	E	123	SER	5.3
3	J	53	SER	5.3
3	H	14	GLY	5.3
2	B	52	TYR	5.2
3	G	150	GLN	5.2
3	G	193	THR	5.2
3	G	69	ILE	5.2
3	H	200	SER	5.2
3	L	51	TRP	5.2
3	G	215	TYR	5.2
3	F	53	SER	5.2
3	G	48	SER	5.2
3	F	56	ASN	5.2
3	D	53	SER	5.1
3	J	55	SER	5.1
3	G	12	GLN	5.1
3	G	31	SER	5.1
3	H	102	TRP	5.0
2	N	1	VAL	5.0
3	G	158	ALA	5.0
3	H	57	THR	5.0
3	G	95	CYS	4.9
2	B	56	ASN	4.9
3	H	161	GLN	4.9
3	G	56	ASN	4.9
3	D	121	GLY	4.9
3	H	69	ILE	4.8
3	L	54	GLY	4.8
2	N	21	CYS	4.8
3	H	146	CYS	4.8
3	H	179	ALA	4.8
3	G	21	CYS	4.8
3	G	201	SER	4.8
3	H	177	SER	4.8
3	H	21	CYS	4.8
1	O	78	SER	4.8
3	G	91	ALA	4.8
3	J	52	TYR	4.7
3	G	67	PHE	4.7
3	F	123	SER	4.7

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Mol	Chain	Res	Type	RSRZ
3	H	87	ALA	4.7
3	G	50	ILE	4.7
3	H	95	CYS	4.6
3	H	193	THR	4.6
3	H	23	ALA	4.6
3	E	119	GLY	4.6
3	K	122	GLY	4.6
3	H	98	PHE	4.6
3	I	200	SER	4.6
3	H	152	VAL	4.6
3	H	25	GLY	4.6
3	G	220	PRO	4.6
3	H	24	SER	4.6
3	G	47	VAL	4.6
3	H	82	MET	4.6
3	G	184	ALA	4.6
3	G	58	TYR	4.6
3	F	218	ILE	4.6
3	G	66	ARG	4.6
3	J	56	ASN	4.6
3	H	118	SER	4.6
2	B	54	GLY	4.5
3	C	120	GLY	4.5
3	E	122	GLY	4.5
3	G	1	VAL	4.5
3	H	72	ASP	4.5
3	G	200	SER	4.5
3	G	208	ALA	4.5
3	H	59	TYR	4.5
3	H	48	SER	4.5
3	G	219	SER	4.4
3	G	46	TRP	4.4
1	O	55	ARG	4.4
2	N	55	SER	4.4
3	G	205	GLU	4.3
3	G	179	ALA	4.3
2	N	63	VAL	4.3
3	G	41	GLY	4.3
3	E	88	GLU	4.3
3	G	139	GLY	4.2
3	G	156	TYR	4.2
3	G	192	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
3	G	212	CYS	4.2
3	H	219	SER	4.2
3	G	96	ALA	4.2
3	H	209	VAL	4.2
3	G	83	ASN	4.2
3	G	51	TRP	4.2
3	G	223	GLY	4.2
3	G	89	ASP	4.2
3	H	74	SER	4.2
2	N	30	ASN	4.2
3	G	134	LEU	4.2
3	J	121	GLY	4.1
3	G	28	PHE	4.1
3	H	54	GLY	4.1
1	O	23	CYS	4.1
3	G	82	MET	4.1
3	L	53	SER	4.1
3	L	55	SER	4.1
3	H	22	ALA	4.1
3	G	15	GLY	4.1
3	K	121	GLY	4.1
3	H	85	LEU	4.1
3	J	54	GLY	4.1
3	I	139	GLY	4.0
3	J	122	GLY	4.0
3	H	78	LEU	4.0
3	G	148	ALA	4.0
3	D	123	SER	4.0
3	H	172	ILE	4.0
3	H	60	ALA	4.0
3	G	17	LEU	4.0
3	H	53	SER	4.0
3	H	86	THR	4.0
3	D	52	TYR	4.0
3	H	12	GLN	4.0
3	H	32	ALA	3.9
3	G	189	SER	3.9
3	H	176	SER	3.9
3	G	86	THR	3.9
2	N	95	CYS	3.9
3	H	147	ARG	3.9
3	H	116	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	N	56	ASN	3.9
3	G	85	LEU	3.9
3	H	30	ASN	3.9
3	G	226	THR	3.9
3	G	11	VAL	3.8
3	G	111	GLY	3.8
3	H	99	ALA	3.8
3	E	56	ASN	3.8
3	G	45	GLU	3.8
3	G	77	THR	3.8
3	G	92	VAL	3.8
3	H	192	GLY	3.8
2	P	102	TRP	3.8
3	D	118	SER	3.8
3	H	104	ALA	3.8
3	H	11	VAL	3.8
3	H	165	GLY	3.8
3	H	225	GLY	3.8
3	H	70	SER	3.7
3	H	154	SER	3.7
3	H	128	THR	3.7
3	C	61	ASP	3.7
3	G	217	ASP	3.7
3	H	47	VAL	3.7
3	G	104	ALA	3.7
3	G	62	SER	3.7
3	G	145	SER	3.7
3	H	84	SER	3.7
3	H	28	PHE	3.7
1	M	85	ALA	3.7
3	G	163	LYS	3.7
3	J	51	TRP	3.7
3	H	73	ASN	3.7
2	B	55	SER	3.7
3	L	200	SER	3.7
3	H	169	ARG	3.7
1	M	70	THR	3.7
3	G	180	THR	3.7
2	N	58	TYR	3.7
3	H	80	LEU	3.6
3	C	122	GLY	3.6
3	G	36	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
3	G	228	VAL	3.6
3	G	173	TYR	3.6
3	G	207	PHE	3.6
3	G	146	CYS	3.6
3	G	161	GLN	3.6
3	G	107	VAL	3.6
3	H	217	ASP	3.6
1	O	84	PHE	3.6
3	G	125	ILE	3.6
3	H	226	THR	3.6
1	O	61	ALA	3.6
3	F	52	TYR	3.6
3	G	211	TYR	3.6
3	H	156	TYR	3.6
3	G	35	TRP	3.5
3	G	27	THR	3.5
3	H	77	THR	3.5
3	H	88	GLU	3.5
3	H	83	ASN	3.5
3	G	78	LEU	3.5
3	G	16	SER	3.5
2	N	46	TRP	3.5
3	H	64	LYS	3.5
2	N	23	ALA	3.5
3	H	127	LEU	3.5
3	K	200	SER	3.5
3	E	61	ASP	3.5
3	G	160	TYR	3.5
3	H	36	VAL	3.5
3	G	214	GLN	3.5
3	G	98	PHE	3.5
3	H	109	GLY	3.5
3	H	181	GLY	3.5
3	H	202	LEU	3.5
3	G	124	ASP	3.5
3	H	124	ASP	3.5
3	H	125	ILE	3.4
1	O	77	SER	3.4
3	F	119	GLY	3.4
3	G	154	SER	3.4
3	H	19	LEU	3.4
3	H	20	SER	3.4

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Mol	Chain	Res	Type	RSRZ
3	G	29	ARG	3.4
3	F	146	CYS	3.4
2	N	86	THR	3.4
2	R	1	VAL	3.4
3	H	13	PRO	3.4
3	H	39	ALA	3.4
3	H	157	LEU	3.4
3	G	105	TYR	3.4
3	G	204	PRO	3.4
3	H	62	SER	3.4
3	K	123	SER	3.4
3	F	51	TRP	3.4
1	M	89	CYS	3.4
2	B	53	SER	3.4
2	N	118	SER	3.4
3	F	122	GLY	3.4
3	H	100	GLY	3.4
3	H	167	ALA	3.4
3	L	30	ASN	3.3
3	H	27	THR	3.3
2	N	31	SER	3.3
3	D	122	GLY	3.3
3	G	165	GLY	3.3
3	H	145	SER	3.3
3	H	191	SER	3.3
3	G	81	GLN	3.3
3	H	17	LEU	3.3
3	G	73	ASN	3.3
3	G	101	GLY	3.3
3	E	87	ALA	3.3
3	G	32	ALA	3.3
3	H	222	PHE	3.3
2	B	51	TRP	3.3
3	G	13	PRO	3.3
3	G	213	HIS	3.3
3	G	22	ALA	3.3
3	H	66	ARG	3.3
1	O	80	GLU	3.3
2	R	62	SER	3.2
3	G	190	GLY	3.2
3	H	203	GLU	3.2
1	O	95	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	76	ASN	3.2
3	H	221	THR	3.2
3	H	43	GLY	3.2
3	H	101	GLY	3.2
3	G	183	PRO	3.2
1	M	25	ALA	3.2
3	H	158	ALA	3.2
3	H	184	ALA	3.2
3	G	94	TYR	3.2
3	H	105	TYR	3.2
1	O	83	ASP	3.2
3	H	89	ASP	3.2
3	H	130	SER	3.2
1	O	57	THR	3.2
3	G	115	THR	3.2
3	H	220	PRO	3.2
2	P	1	VAL	3.2
2	N	22	ALA	3.2
3	G	79	TYR	3.2
3	H	204	PRO	3.2
3	G	127	LEU	3.1
3	G	194	ASP	3.1
3	G	202	LEU	3.1
3	H	170	LEU	3.1
3	H	94	TYR	3.1
3	H	153	SER	3.1
3	H	207	PHE	3.1
2	N	68	THR	3.1
3	E	9	GLY	3.1
3	J	120	GLY	3.1
3	H	81	GLN	3.1
2	N	11	VAL	3.1
3	G	147	ARG	3.1
3	G	88	GLU	3.1
3	G	218	ILE	3.1
3	H	205	GLU	3.1
3	D	200	SER	3.1
3	G	70	SER	3.1
3	H	223	GLY	3.1
1	A	24	ARG	3.1
3	H	206	ASP	3.1
3	H	45	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
3	H	132	ALA	3.1
3	H	44	LEU	3.1
2	N	69	ILE	3.1
3	L	218	ILE	3.1
3	H	35	TRP	3.1
3	G	177	SER	3.1
3	H	6	SER	3.1
3	H	201	SER	3.1
3	J	123	SER	3.1
3	D	120	GLY	3.1
3	L	56	ASN	3.1
3	G	132	ALA	3.1
3	E	1	VAL	3.1
2	N	67	PHE	3.0
3	H	55	SER	3.0
3	H	216	SER	3.0
1	O	24	ARG	3.0
3	H	103	GLY	3.0
3	G	196	THR	3.0
3	L	207	PHE	3.0
3	G	162	GLN	3.0
3	H	148	ALA	3.0
3	G	153	SER	3.0
3	H	175	SER	3.0
3	K	53	SER	3.0
3	D	51	TRP	3.0
3	G	206	ASP	3.0
3	H	215	TYR	3.0
3	H	129	GLN	3.0
3	H	150	GLN	3.0
2	N	48	SER	3.0
3	J	21	CYS	3.0
2	N	116	VAL	3.0
3	G	152	VAL	3.0
1	O	82	GLU	3.0
3	E	54	GLY	3.0
2	N	57	THR	3.0
3	G	198	THR	3.0
3	H	173	TYR	3.0
3	G	114	VAL	2.9
3	F	225	GLY	2.9
3	G	172	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	77	THR	2.9
3	G	149	SER	2.9
3	G	39	ALA	2.9
3	E	25	GLY	2.9
3	G	170	LEU	2.9
2	N	12	GLN	2.9
3	G	195	PHE	2.9
1	O	18	ARG	2.8
3	H	33	MET	2.8
3	H	180	THR	2.8
3	H	198	THR	2.8
3	C	200	SER	2.8
3	G	26	PHE	2.8
3	H	210	TYR	2.8
1	M	42	GLY	2.8
3	D	54	GLY	2.8
3	F	179	ALA	2.8
3	G	100	GLY	2.8
3	H	1	VAL	2.8
3	K	1	VAL	2.8
3	C	123	SER	2.8
3	H	155	ASN	2.8
3	H	61	ASP	2.8
3	G	167	ALA	2.8
3	G	10	LEU	2.8
3	H	171	LEU	2.8
3	D	180	THR	2.8
3	G	116	VAL	2.8
3	H	182	VAL	2.8
3	F	155	ASN	2.8
3	H	71	ARG	2.8
3	G	33	MET	2.8
2	N	109	GLY	2.8
3	G	109	GLY	2.8
3	E	79	TYR	2.8
3	G	113	LEU	2.8
3	G	157	LEU	2.8
2	N	27	THR	2.8
3	F	131	PRO	2.8
3	C	53	SER	2.7
3	H	213	HIS	2.7
2	B	88	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	203	GLU	2.7
2	N	54	GLY	2.7
3	E	52	TYR	2.7
3	G	3	LEU	2.7
3	H	79	TYR	2.7
3	H	183	PRO	2.7
3	I	1	VAL	2.7
2	P	61	ASP	2.7
2	N	87	ALA	2.7
3	H	195	PHE	2.7
1	M	57	THR	2.7
3	G	93	TYR	2.7
3	H	126	VAL	2.7
2	N	49	SER	2.7
3	H	212	CYS	2.7
3	F	54	GLY	2.7
3	G	188	GLY	2.7
3	H	65	GLY	2.7
3	L	122	GLY	2.7
3	G	99	ALA	2.7
3	G	44	LEU	2.7
3	G	40	PRO	2.7
3	G	130	SER	2.7
3	I	201	SER	2.7
3	J	74	SER	2.7
3	G	174	ASP	2.7
3	E	111	GLY	2.7
3	E	102	TRP	2.7
3	I	102	TRP	2.7
1	O	85	ALA	2.6
2	N	26	PHE	2.6
3	H	34	HIS	2.6
1	Q	1	ASP	2.6
3	F	74	SER	2.6
3	G	24	SER	2.6
1	Q	23	CYS	2.6
2	N	14	GLY	2.6
2	N	15	GLY	2.6
3	H	108	TRP	2.6
3	G	171	LEU	2.6
3	G	222	PHE	2.6
3	H	149	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	194	ASP	2.6
3	H	160	TYR	2.6
1	M	95	ILE	2.6
3	E	21	CYS	2.6
3	D	119	GLY	2.6
2	N	104	ALA	2.6
3	G	159	TRP	2.6
2	N	80	LEU	2.6
3	G	144	LEU	2.6
3	G	164	PRO	2.6
1	M	53	SER	2.6
3	G	135	SER	2.6
3	H	26	PHE	2.6
3	F	126	VAL	2.6
3	H	214	GLN	2.6
1	O	106	GLU	2.6
2	N	88	GLU	2.6
1	M	41	PRO	2.6
1	Q	24	ARG	2.6
3	G	128	THR	2.6
1	M	96	SER	2.6
3	G	19	LEU	2.6
3	G	80	LEU	2.6
3	H	140	GLU	2.5
1	M	33	TYR	2.5
3	F	215	TYR	2.5
3	G	181	GLY	2.5
3	I	21	CYS	2.5
3	L	21	CYS	2.5
3	G	97	ARG	2.5
2	P	87	ALA	2.5
3	G	23	ALA	2.5
3	H	90	THR	2.5
3	F	191	SER	2.5
3	G	191	SER	2.5
3	L	201	SER	2.5
3	E	10	LEU	2.5
3	G	38	GLN	2.5
3	F	229	GLU	2.5
3	H	218	ILE	2.5
3	H	228	VAL	2.5
1	O	71	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	133	THR	2.5
1	O	56	ALA	2.5
3	G	20	SER	2.5
3	H	96	ALA	2.5
3	E	17	LEU	2.5
2	N	25	GLY	2.5
1	O	105	VAL	2.5
3	H	18	ARG	2.5
3	H	211	TYR	2.5
1	M	77	SER	2.5
2	N	84	SER	2.5
3	E	16	SER	2.5
3	E	55	SER	2.5
3	G	74	SER	2.5
3	G	131	PRO	2.5
2	N	18	ARG	2.5
3	E	28	PHE	2.5
3	G	42	LYS	2.5
3	G	64	LYS	2.5
3	F	147	ARG	2.5
3	G	18	ARG	2.5
3	G	103	GLY	2.5
1	M	82	GLU	2.4
1	Q	27	GLN	2.4
2	N	61	ASP	2.4
3	G	106	ASP	2.4
2	N	6	SER	2.4
2	N	77	THR	2.4
3	E	62	SER	2.4
3	E	86	THR	2.4
3	H	16	SER	2.4
3	F	184	ALA	2.4
2	N	19	LEU	2.4
3	G	197	LEU	2.4
3	G	37	ARG	2.4
3	K	120	GLY	2.4
3	F	88	GLU	2.4
3	G	166	GLN	2.4
3	H	166	GLN	2.4
2	N	36	VAL	2.4
3	F	124	ASP	2.4
3	H	92	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	54	SER	2.4
3	F	219	SER	2.4
3	G	175	SER	2.4
3	H	3	LEU	2.4
3	H	10	LEU	2.4
2	N	111	GLY	2.4
2	N	73	ASN	2.4
3	E	30	ASN	2.4
3	J	30	ASN	2.4
3	G	2	GLN	2.4
1	M	29	VAL	2.4
1	A	77	SER	2.4
3	F	153	SER	2.4
3	G	108	TRP	2.4
3	G	210	TYR	2.4
3	H	164	PRO	2.4
3	G	65	GLY	2.4
3	H	7	GLY	2.4
3	H	76	ASN	2.4
2	B	1	VAL	2.4
2	N	82	MET	2.4
1	O	70	THR	2.4
1	O	81	PRO	2.4
3	G	34	HIS	2.4
2	N	10	LEU	2.3
3	D	147	ARG	2.3
1	O	12	SER	2.3
3	E	47	VAL	2.3
3	F	149	SER	2.3
2	P	12	GLN	2.3
3	F	156	TYR	2.3
3	E	78	LEU	2.3
3	K	139	GLY	2.3
1	M	1	ASP	2.3
3	G	72	ASP	2.3
3	H	174	ASP	2.3
3	G	141	ARG	2.3
1	M	68	SER	2.3
3	L	123	SER	2.3
3	H	4	VAL	2.3
3	F	180	THR	2.3
3	D	56	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	132	ALA	2.3
1	M	4	LEU	2.3
1	M	71	ASP	2.3
2	N	105	TYR	2.3
3	D	124	ASP	2.3
3	H	41	GLY	2.3
3	J	29	ARG	2.3
3	G	137	SER	2.3
3	G	176	SER	2.3
3	G	216	SER	2.3
3	J	27	THR	2.3
2	N	60	ALA	2.3
3	J	194	ASP	2.3
1	O	58	GLY	2.3
3	E	101	GLY	2.3
3	G	7	GLY	2.3
3	H	93	TYR	2.3
3	K	205	GLU	2.2
3	D	201	SER	2.2
3	F	55	SER	2.2
3	E	68	THR	2.2
3	G	4	VAL	2.2
3	J	155	ASN	2.2
1	O	16	GLY	2.2
3	E	8	GLY	2.2
3	E	95	CYS	2.2
3	H	142	ALA	2.2
3	F	134	LEU	2.2
3	E	12	GLN	2.2
3	G	224	GLN	2.2
3	H	38	GLN	2.2
1	Q	96	SER	2.2
2	N	70	SER	2.2
2	N	74	SER	2.2
3	D	24	SER	2.2
3	F	201	SER	2.2
3	G	169	ARG	2.2
1	O	75	THR	2.2
2	N	50	ILE	2.2
3	D	30	ASN	2.2
3	E	57	THR	2.2
3	G	75	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	209	VAL	2.2
3	H	107	VAL	2.2
2	N	7	GLY	2.2
3	I	120	GLY	2.2
1	M	106	GLU	2.2
3	H	5	GLU	2.2
3	H	91	ALA	2.2
3	L	2	GLN	2.2
2	B	62	SER	2.2
3	E	117	SER	2.2
3	I	151	SER	2.2
1	Q	32	ASN	2.2
1	Q	95	ILE	2.2
2	N	112	THR	2.2
3	H	40	PRO	2.2
3	H	138	PRO	2.2
2	N	72	ASP	2.2
3	E	72	ASP	2.2
3	K	33	MET	2.2
3	F	148	ALA	2.2
1	M	23	CYS	2.2
3	K	21	CYS	2.2
3	L	146	CYS	2.2
2	N	29	ARG	2.2
3	E	118	SER	2.2
3	K	201	SER	2.2
3	L	147	ARG	2.2
2	N	94	TYR	2.2
2	B	30	ASN	2.2
3	K	102	TRP	2.2
1	M	51	ASP	2.2
1	M	60	PRO	2.1
3	E	124	ASP	2.2
2	P	88	GLU	2.1
1	O	42	GLY	2.1
1	O	13	LEU	2.1
1	O	21	LEU	2.1
1	O	46	ARG	2.1
3	H	29	ARG	2.1
1	M	94	ASP	2.1
3	H	229	GLU	2.1
3	L	193	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	28	PHE	2.1
2	N	43	GLY	2.1
3	G	25	GLY	2.1
3	H	139	GLY	2.1
3	H	75	LYS	2.1
3	E	70	SER	2.1
3	G	151	SER	2.1
2	R	56	ASN	2.1
3	I	205	GLU	2.1
1	M	27	GLN	2.1
1	O	103	THR	2.1
3	G	185	ARG	2.1
3	G	199	ILE	2.1
1	M	86	VAL	2.1
3	E	22	ALA	2.1
3	F	208	ALA	2.1
3	G	136	LEU	2.1
3	I	123	SER	2.1
3	G	155	ASN	2.1
3	H	162	GLN	2.1
3	H	141	ARG	2.1
3	I	141	ARG	2.1
3	L	141	ARG	2.1
3	H	188	GLY	2.1
2	N	102	TRP	2.1
1	O	11	LEU	2.0
1	O	69	GLY	2.0
3	E	139	GLY	2.0
3	I	130	SER	2.0
2	P	39	ALA	2.0
3	E	51	TRP	2.0
1	O	94	ASP	2.0
3	G	71	ARG	2.0
1	Q	57	THR	2.0
3	G	221	THR	2.0
3	H	131	PRO	2.0
3	I	193	THR	2.0
1	M	16	GLY	2.0
1	Q	16	GLY	2.0
2	N	9	GLY	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.