



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:34 PM UTC

PDB ID : 7JQY / pdb_00007jqy
Title : Crystal structure of Cfl1-D123S from Burkholderia cenocepacia
Authors : Taher, N.M.; Madden, D.R.
Deposited on : 2020-08-11
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

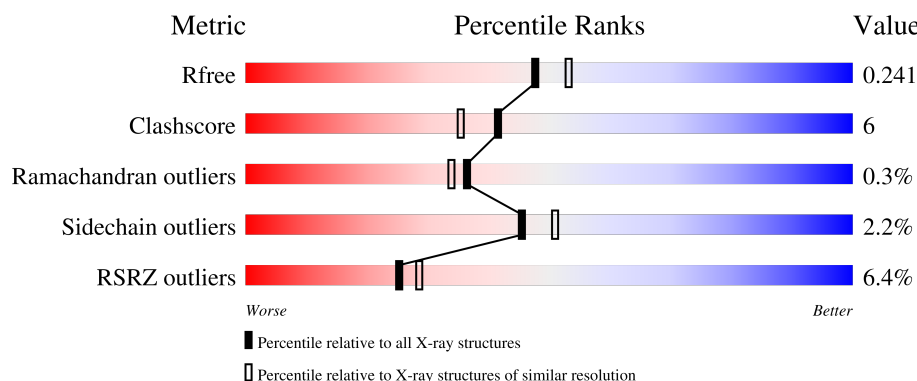
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	309	87% 7% 5%
1	B	309	87% 8% 5%
1	C	309	89% 6% 5%
1	D	309	4% 79% 15% • 5%
1	E	309	3% 80% 14% • 5%

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Mol	Chain	Length	Quality of chain
1	F	309	5% 76% 17% • 5%
1	G	309	28% 71% 19% • 5%
1	H	309	6% 79% 14% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19289 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 Cif-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2308	1479	411	408	10			
1	B	294	Total	C	N	O	S	0	0	0
			2317	1484	412	411	10			
1	C	293	Total	C	N	O	S	0	0	0
			2310	1479	411	410	10			
1	D	294	Total	C	N	O	S	0	0	0
			2317	1484	412	411	10			
1	E	294	Total	C	N	O	S	0	0	0
			2317	1484	412	411	10			
1	F	293	Total	C	N	O	S	0	0	0
			2308	1479	411	408	10			
1	G	293	Total	C	N	O	S	0	0	0
			2308	1479	411	408	10			
1	H	294	Total	C	N	O	S	0	0	0
			2317	1484	412	411	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	SER	ASP	engineered mutation	UNP B4EJL9
B	123	SER	ASP	engineered mutation	UNP B4EJL9
C	123	SER	ASP	engineered mutation	UNP B4EJL9
D	123	SER	ASP	engineered mutation	UNP B4EJL9
E	123	SER	ASP	engineered mutation	UNP B4EJL9
F	123	SER	ASP	engineered mutation	UNP B4EJL9
G	123	SER	ASP	engineered mutation	UNP B4EJL9
H	123	SER	ASP	engineered mutation	UNP B4EJL9

- Molecule 2 is water.

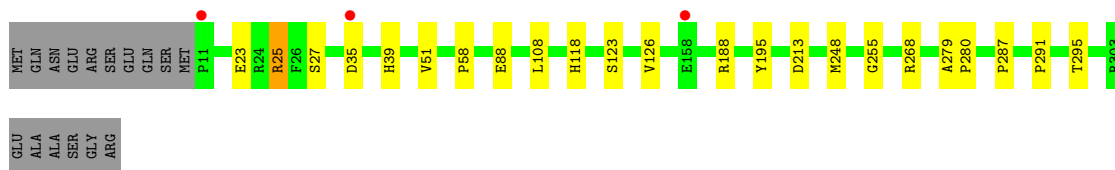
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	183	Total 183	O 183	0	0
2	B	135	Total 135	O 135	0	0
2	C	118	Total 118	O 118	0	0
2	D	94	Total 94	O 94	0	0
2	E	87	Total 87	O 87	0	0
2	F	57	Total 57	O 57	0	0
2	G	64	Total 64	O 64	0	0
2	H	49	Total 49	O 49	0	0

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.

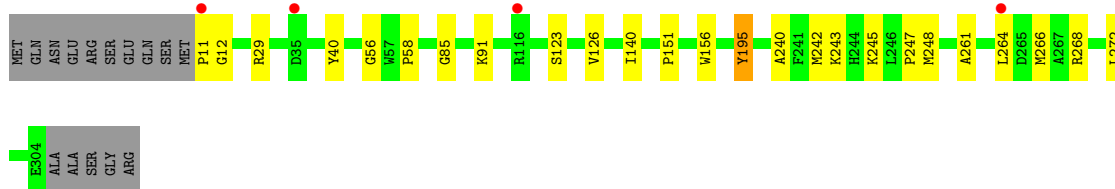
- Molecule 1: Cif-like 1

Chain A: 



- Molecule 1: Cif-like 1

Chain B: 



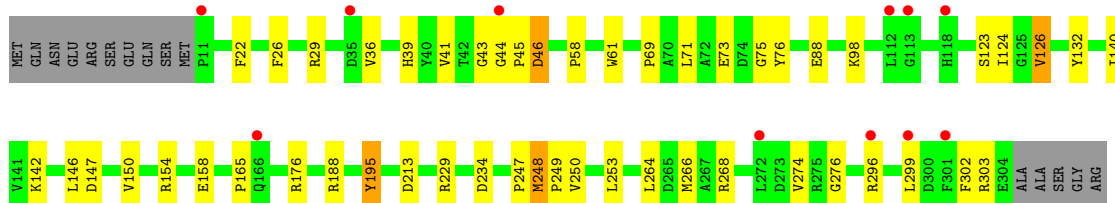
- Molecule 1: Cif-like 1

Chain C: 



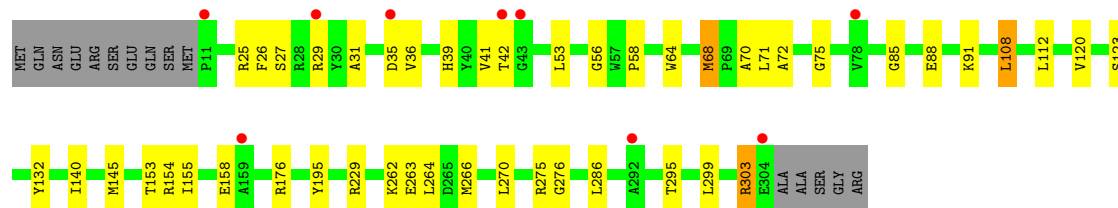
- Molecule 1: Cif-like 1

Chain D: 



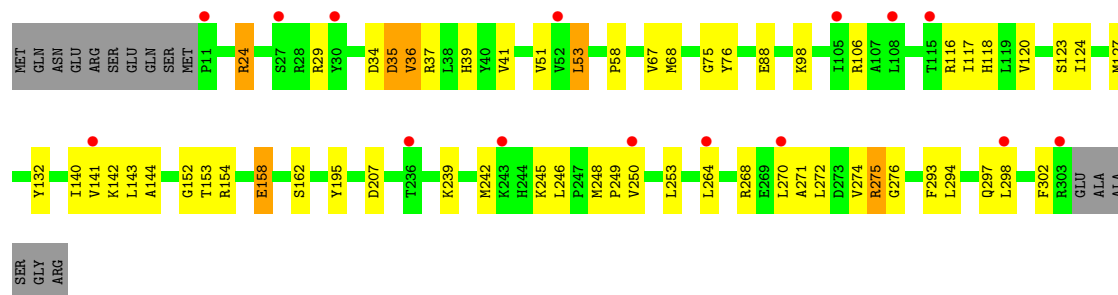
- Molecule 1: Cif-like 1

Chain E: 



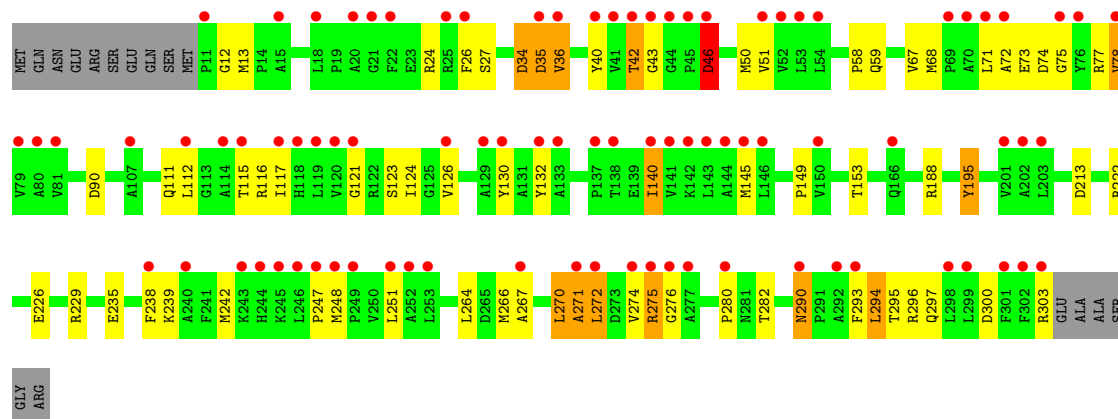
- Molecule 1: Cif-like 1

Chain F: 



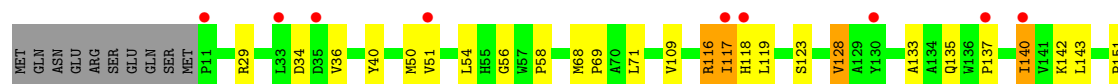
- Molecule 1: Cif-like 1

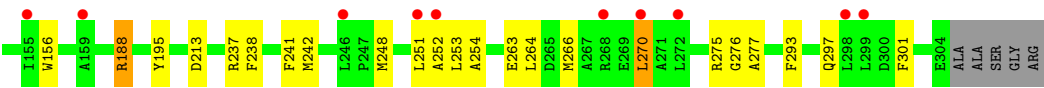
Chain G: 



- Molecule 1: Cif-like 1

Chain H: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.00Å 98.40Å 170.00Å 90.00° 118.60° 90.00°	Depositor
Resolution (Å)	44.71 – 2.15 44.71 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.71-2.15) 99.5 (44.71-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.209 , 0.240 0.211 , 0.241	Depositor DCC
R_{free} test set	7620 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19289	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.33	1/2374 (0.0%)	0.52	0/3225
1	B	0.39	1/2383 (0.0%)	0.56	0/3237
1	C	0.39	0/2375	0.52	1/3226 (0.0%)
1	D	0.64	4/2383 (0.2%)	0.69	6/3237 (0.2%)
1	E	0.63	3/2383 (0.1%)	0.67	3/3237 (0.1%)
1	F	0.81	1/2374 (0.0%)	0.72	4/3225 (0.1%)
1	G	0.82	1/2374 (0.0%)	0.96	19/3225 (0.6%)
1	H	0.78	0/2383	0.72	4/3237 (0.1%)
All	All	0.63	11/19029 (0.1%)	0.68	37/25849 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	286	LEU	C-O	-6.42	1.18	1.24
1	D	36	VAL	C-O	-5.65	1.18	1.23
1	G	296	ARG	C-O	-5.62	1.17	1.24
1	E	31	ALA	C-O	-5.39	1.17	1.24
1	B	195	TYR	C-O	-5.37	1.17	1.24
1	F	37	ARG	C-O	-5.27	1.17	1.24
1	E	68	MET	C-O	-5.20	1.19	1.24
1	D	247	PRO	CA-C	-5.18	1.47	1.52
1	D	195	TYR	C-O	-5.10	1.18	1.24
1	A	25	ARG	C-O	-5.09	1.17	1.23
1	D	22	PHE	C-O	-5.06	1.17	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	36	VAL	N-CA-C	10.07	123.14	108.53
1	G	290	ASN	CA-C-N	7.75	127.30	118.85
1	G	290	ASN	C-N-CA	7.75	127.30	118.85
1	C	23	GLU	N-CA-C	7.20	120.05	111.33
1	G	272	LEU	N-CA-C	6.98	118.53	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	36	VAL	N-CA-C	6.98	117.94	108.17
1	F	34	ASP	N-CA-C	6.35	118.20	111.28
1	E	75	GLY	N-CA-C	6.32	124.04	115.32
1	E	36	VAL	N-CA-C	6.31	118.11	108.71
1	G	78	VAL	N-CA-C	6.27	117.83	108.54
1	D	248	MET	CA-C-N	6.25	126.46	119.90
1	D	248	MET	C-N-CA	6.25	126.46	119.90
1	G	294	LEU	N-CA-C	6.17	118.01	111.28
1	G	73	GLU	CA-C-N	6.13	132.47	122.65
1	G	73	GLU	C-N-CA	6.13	132.47	122.65
1	H	34	ASP	N-CA-C	6.00	117.82	111.28
1	D	44	GLY	CA-C-N	5.99	126.19	119.90
1	D	44	GLY	C-N-CA	5.99	126.19	119.90
1	H	119	LEU	N-CA-C	5.86	118.45	108.90
1	G	12	GLY	N-CA-C	5.79	122.67	112.83
1	G	13	MET	N-CA-C	5.76	118.04	110.08
1	G	46	ASP	N-CA-C	5.75	118.49	111.82
1	H	297	GLN	N-CA-C	5.74	117.53	111.28
1	E	26	PHE	N-CA-C	5.72	118.27	110.55
1	G	24	ARG	N-CA-C	5.68	118.24	111.71
1	G	121	GLY	N-CA-C	5.59	119.46	110.90
1	F	36	VAL	N-CA-C	5.55	116.58	108.53
1	G	75	GLY	N-CA-C	5.53	123.66	114.48
1	G	271	ALA	N-CA-C	5.48	118.39	109.24
1	G	42	THR	N-CA-C	5.28	117.21	109.24
1	G	36	VAL	N-CA-CB	-5.19	101.62	111.21
1	F	75	GLY	N-CA-C	5.18	122.58	115.27
1	F	117	ILE	CB-CA-C	-5.17	103.17	110.82
1	D	165	PRO	CA-C-N	-5.15	113.07	122.38
1	D	165	PRO	C-N-CA	-5.15	113.07	122.38
1	G	271	ALA	CA-C-N	5.10	127.06	120.44
1	G	271	ALA	C-N-CA	5.10	127.06	120.44

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	2308	0	2265	15	0
1	B	2317	0	2271	15	0
1	C	2310	0	2263	14	0
1	D	2317	0	2271	33	0
1	E	2317	0	2271	24	0
1	F	2308	0	2265	39	0
1	G	2308	0	2265	61	0
1	H	2317	0	2271	39	0
2	A	183	0	0	3	0
2	B	135	0	0	2	0
2	C	118	0	0	1	0
2	D	94	0	0	2	0
2	E	87	0	0	0	0
2	F	57	0	0	2	0
2	G	64	0	0	0	0
2	H	49	0	0	0	0
All	All	19289	0	18142	235	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 6.

All (235) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:MET:HB3	1:G:117:ILE:HG22	1.47	0.96
1:G:50:MET:CE	1:G:117:ILE:HG21	1.98	0.94
1:H:116:ARG:HG2	1:H:116:ARG:HH21	1.35	0.91
1:D:142:LYS:HG2	1:D:249:PRO:HB2	1.59	0.84
1:G:50:MET:HE3	1:G:117:ILE:HG21	1.58	0.84
1:H:140:ILE:HG23	1:H:248:MET:HE2	1.63	0.79
1:H:242:MET:HE3	1:H:270:LEU:HD23	1.68	0.75
1:G:247:PRO:HD2	1:G:248:MET:HE3	1.70	0.74
1:F:275:ARG:HH11	1:F:275:ARG:HB3	1.54	0.73
1:G:50:MET:HB3	1:G:117:ILE:CG2	2.19	0.72
1:G:51:VAL:HG13	1:G:51:VAL:O	1.90	0.71
1:G:50:MET:HE2	1:G:117:ILE:HG21	1.71	0.71
1:G:271:ALA:O	1:G:274:VAL:CG2	2.39	0.70
1:H:264:LEU:HD21	1:H:276:GLY:HA3	1.73	0.70
1:H:116:ARG:HH21	1:H:116:ARG:CG	2.03	0.69
1:C:138:THR:HG21	1:G:300:ASP:HB3	1.72	0.69
1:F:35:ASP:OD2	1:F:35:ASP:N	2.23	0.69
1:F:132:TYR:CD1	1:F:140:ILE:HD11	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:ILE:HD11	1:H:142:LYS:C	2.18	0.68
1:D:69:PRO:O	1:D:73:GLU:HG3	1.93	0.68
1:F:242:MET:HE2	1:F:270:LEU:HD11	1.76	0.68
1:E:53:LEU:HD23	1:E:120:VAL:HB	1.75	0.67
1:H:140:ILE:HD11	1:H:143:LEU:HB2	1.78	0.66
1:D:250:VAL:HB	1:D:274:VAL:HG12	1.78	0.66
1:E:153:THR:HG21	1:E:266:MET:HG2	1.79	0.65
1:E:64:TRP:O	1:E:68:MET:HG3	1.97	0.65
1:G:35:ASP:HB2	1:G:36:VAL:HG23	1.77	0.65
1:H:140:ILE:CD1	1:H:143:LEU:HB2	2.27	0.65
1:H:251:LEU:HD12	1:H:275:ARG:HG2	1.80	0.64
1:G:50:MET:HE2	1:G:117:ILE:CG2	2.27	0.63
1:G:188:ARG:HH21	1:G:213:ASP:CG	2.06	0.63
1:H:264:LEU:CD2	1:H:276:GLY:HA3	2.29	0.63
1:G:271:ALA:O	1:G:274:VAL:HG23	2.00	0.62
1:F:294:LEU:O	1:F:298:LEU:HG	1.99	0.62
1:E:25:ARG:NH1	1:E:72:ALA:HB3	2.14	0.62
1:G:46:ASP:OD2	1:G:46:ASP:N	2.32	0.61
1:F:253:LEU:HD22	1:F:293:PHE:HE1	1.65	0.61
1:G:72:ALA:HB2	1:G:78:VAL:HG23	1.82	0.61
1:D:248:MET:HB2	1:D:249:PRO:CD	2.29	0.61
1:H:50:MET:HB3	1:H:117:ILE:HG22	1.83	0.61
1:G:145:MET:HE1	1:G:270:LEU:HD13	1.83	0.60
1:G:275:ARG:HB3	1:G:275:ARG:CZ	2.31	0.60
1:D:264:LEU:HD13	1:D:276:GLY:HA3	1.85	0.59
1:G:282:THR:HG21	1:G:290:ASN:HB2	1.85	0.59
1:F:53:LEU:HD22	1:F:53:LEU:N	2.18	0.58
1:H:254:ALA:HB2	1:H:263:GLU:HG3	1.84	0.58
1:C:123:SER:O	1:C:126:VAL:HG12	2.04	0.58
1:D:46:ASP:OD1	1:D:46:ASP:N	2.33	0.58
1:C:138:THR:HG21	1:G:300:ASP:CB	2.34	0.58
1:C:138:THR:HG21	1:G:300:ASP:CG	2.30	0.57
1:C:153:THR:HG21	1:C:266:MET:HG2	1.87	0.57
1:F:268:ARG:HG2	1:F:274:VAL:HG21	1.85	0.57
1:D:268:ARG:HG2	1:D:274:VAL:HG21	1.86	0.56
1:G:117:ILE:C	1:G:117:ILE:HD12	2.29	0.56
1:D:248:MET:HB2	1:D:249:PRO:HD2	1.86	0.56
1:G:267:ALA:HA	1:G:270:LEU:HD12	1.88	0.56
1:G:35:ASP:OD1	1:G:35:ASP:N	2.38	0.55
1:G:68:MET:HG2	1:G:78:VAL:HG11	1.88	0.55
1:H:238:PHE:O	1:H:242:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:VAL:CG1	1:F:68:MET:HE1	2.37	0.55
1:F:41:VAL:HG12	1:F:68:MET:HE1	1.88	0.55
1:H:140:ILE:HD13	1:H:248:MET:HG3	1.89	0.55
1:H:56:GLY:HA3	1:H:123:SER:HB3	1.88	0.55
1:A:35:ASP:OD2	1:A:35:ASP:N	2.37	0.55
1:C:56:GLY:HA3	1:C:123:SER:HB3	1.89	0.54
1:F:246:LEU:HB2	1:F:271:ALA:HB2	1.89	0.54
1:G:153:THR:HG21	1:G:266:MET:HG2	1.90	0.54
1:F:293:PHE:CD1	1:F:293:PHE:C	2.85	0.54
1:H:54:LEU:HD13	1:H:128:VAL:CG2	2.37	0.54
1:D:154:ARG:O	1:D:158:GLU:HG3	2.08	0.54
1:D:296:ARG:HE	1:D:296:ARG:HA	1.73	0.53
1:G:27:SER:N	1:G:42:THR:O	2.35	0.53
1:H:253:LEU:HD22	1:H:277:ALA:HB3	1.91	0.53
1:D:296:ARG:HH21	1:D:299:LEU:HB2	1.73	0.53
1:F:132:TYR:CE1	1:F:140:ILE:HD11	2.45	0.52
1:A:27:SER:OG	1:B:11:PRO:HA	2.09	0.52
1:G:293:PHE:CE1	1:G:297:GLN:HG3	2.45	0.52
1:E:27:SER:O	1:E:41:VAL:HA	2.09	0.52
1:E:25:ARG:HH11	1:E:72:ALA:HB3	1.74	0.52
1:A:23:GLU:O	1:B:12:GLY:HA2	2.09	0.52
1:D:264:LEU:O	1:D:268:ARG:HG3	2.09	0.51
1:A:268:ARG:NE	2:A:403:HOH:O	2.29	0.51
1:E:70:ALA:CB	1:E:295:THR:HG21	2.40	0.51
1:H:252:ALA:O	1:H:253:LEU:HD23	2.11	0.51
1:B:245:LYS:HE3	1:B:272:LEU:HD23	1.93	0.51
1:B:56:GLY:HA3	1:B:123:SER:HB3	1.93	0.51
1:E:154:ARG:O	1:E:158:GLU:HG3	2.11	0.51
1:F:120:VAL:HG22	1:F:144:ALA:HB3	1.92	0.51
1:G:149:PRO:HA	1:G:266:MET:HE2	1.93	0.51
1:G:188:ARG:NH2	1:G:213:ASP:OD2	2.44	0.50
1:A:188:ARG:HH21	1:A:213:ASP:CG	2.20	0.50
1:G:115:THR:O	1:G:115:THR:OG1	2.22	0.50
1:G:238:PHE:O	1:G:242:MET:HG2	2.12	0.50
1:H:109:VAL:HG11	1:H:117:ILE:HD13	1.94	0.50
1:F:253:LEU:CD2	1:F:293:PHE:HE1	2.24	0.50
1:H:142:LYS:HB3	1:H:301:PHE:CE2	2.47	0.50
1:B:261:ALA:O	1:B:264:LEU:HB2	2.13	0.49
1:F:275:ARG:HB3	1:F:275:ARG:NH1	2.23	0.49
1:G:51:VAL:O	1:G:51:VAL:CG1	2.60	0.49
1:D:126:VAL:HG13	1:D:150:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:SER:O	1:D:126:VAL:HG12	2.12	0.49
1:F:297:GLN:NE2	2:F:405:HOH:O	2.35	0.49
1:G:123:SER:O	1:G:126:VAL:HG12	2.12	0.49
1:G:251:LEU:HD13	1:G:275:ARG:HD3	1.93	0.49
1:D:41:VAL:HG21	1:D:61:TRP:CE2	2.48	0.49
1:D:188:ARG:HH21	1:D:213:ASP:CG	2.21	0.48
1:D:274:VAL:HG22	2:D:402:HOH:O	2.13	0.48
1:D:140:ILE:HB	1:D:248:MET:HE2	1.95	0.48
1:E:70:ALA:HB3	1:E:295:THR:HG21	1.94	0.48
1:G:280:PRO:O	1:G:282:THR:HG23	2.13	0.48
1:D:248:MET:CB	1:D:249:PRO:CD	2.91	0.48
1:E:29:ARG:HD2	1:E:42:THR:CG2	2.44	0.48
1:G:72:ALA:HB2	1:G:78:VAL:CG2	2.43	0.48
1:F:264:LEU:HD13	1:F:276:GLY:HA3	1.96	0.47
1:D:71:LEU:O	1:D:76:TYR:HB2	2.14	0.47
1:E:29:ARG:HD2	1:E:42:THR:HG21	1.97	0.47
1:E:39:HIS:CG	1:E:88:GLU:HB2	2.49	0.47
1:G:40:TYR:OH	1:G:112:LEU:HD21	2.15	0.47
1:A:291:PRO:O	1:A:295:THR:HG23	2.15	0.47
1:E:85:GLY:HA2	1:E:91:LYS:HG3	1.96	0.47
1:E:155:ILE:HD12	1:E:262:LYS:HG2	1.96	0.47
1:G:117:ILE:C	1:G:117:ILE:CD1	2.87	0.46
1:D:98:LYS:NZ	1:D:234:ASP:OD2	2.44	0.46
1:F:207:ASP:OD2	2:F:401:HOH:O	2.21	0.46
1:G:235:GLU:O	1:G:239:LYS:HG3	2.14	0.46
1:A:287:PRO:HD2	2:A:478:HOH:O	2.15	0.46
1:D:45:PRO:HG2	1:D:75:GLY:HA2	1.97	0.46
1:D:123:SER:OG	1:D:124:ILE:N	2.48	0.46
1:F:106:ARG:HA	1:F:132:TYR:OH	2.16	0.46
1:G:117:ILE:HD12	1:G:117:ILE:O	2.16	0.46
1:D:76:TYR:OH	1:D:302:PHE:HB3	2.14	0.46
1:H:151:PRO:HA	1:H:156:TRP:CG	2.51	0.46
1:H:237:ARG:NH2	1:H:241:PHE:HZ	2.14	0.46
1:A:23:GLU:HB2	2:A:472:HOH:O	2.16	0.46
1:E:299:LEU:O	1:E:303:ARG:HD3	2.16	0.46
1:E:56:GLY:HA3	1:E:123:SER:HB3	1.98	0.45
1:F:140:ILE:HB	1:F:248:MET:HE2	1.98	0.45
1:G:50:MET:HA	1:G:77:ARG:HB3	1.97	0.45
1:F:245:LYS:HD3	1:F:271:ALA:C	2.42	0.45
1:H:71:LEU:HD23	1:H:71:LEU:HA	1.67	0.45
1:F:154:ARG:O	1:F:158:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:MET:HE3	1:B:266:MET:HB3	1.92	0.45
1:C:264:LEU:HD21	1:C:268:ARG:HH21	1.82	0.45
1:A:123:SER:O	1:A:126:VAL:HG12	2.16	0.45
1:B:268:ARG:NH2	2:B:403:HOH:O	2.33	0.45
1:H:51:VAL:HA	1:H:118:HIS:O	2.17	0.45
1:F:51:VAL:HG23	1:F:76:TYR:HB3	1.99	0.45
1:G:264:LEU:HD13	1:G:276:GLY:HA3	1.99	0.45
1:G:275:ARG:HB3	1:G:275:ARG:NH2	2.32	0.45
1:G:266:MET:HE3	1:G:266:MET:HB3	1.86	0.45
1:H:133:ALA:O	1:H:137:PRO:HG3	2.17	0.45
1:F:264:LEU:O	1:F:268:ARG:HG3	2.17	0.44
1:G:140:ILE:HG22	1:G:248:MET:SD	2.57	0.44
1:H:140:ILE:HD11	1:H:143:LEU:CB	2.47	0.44
1:H:264:LEU:CG	1:H:276:GLY:HA3	2.47	0.44
1:E:264:LEU:HD13	1:E:276:GLY:HA3	2.00	0.44
1:A:39:HIS:CG	1:A:88:GLU:HB2	2.52	0.44
1:B:123:SER:O	1:B:126:VAL:HG12	2.18	0.44
1:H:135:GLN:OE1	1:H:237:ARG:NH2	2.47	0.44
1:A:255:GLY:HA2	1:A:279:ALA:HB3	2.00	0.44
1:D:147:ASP:OD1	2:D:401:HOH:O	2.21	0.44
1:E:176:ARG:HA	1:E:229:ARG:CZ	2.48	0.44
1:E:263:GLU:O	1:E:266:MET:HE3	2.18	0.44
1:G:153:THR:HG22	1:G:242:MET:HE1	2.00	0.44
1:C:36:VAL:HG23	1:C:90:ASP:HB2	2.00	0.44
1:D:296:ARG:HE	1:D:296:ARG:CA	2.30	0.44
1:F:143:LEU:O	1:F:250:VAL:HA	2.18	0.44
1:F:153:THR:HG22	1:F:242:MET:HE1	2.00	0.44
1:D:39:HIS:CG	1:D:88:GLU:HB2	2.53	0.43
1:F:294:LEU:HD11	1:F:298:LEU:HD21	2.00	0.43
1:G:222:ARG:O	1:G:226:GLU:HG2	2.18	0.43
1:G:272:LEU:HA	1:G:272:LEU:HD23	1.56	0.43
1:D:132:TYR:CD1	1:D:140:ILE:HD11	2.53	0.43
1:H:29:ARG:HB2	1:H:40:TYR:CZ	2.53	0.43
1:A:248:MET:HE3	1:A:248:MET:HB3	1.93	0.43
1:F:98:LYS:HG3	1:F:127:MET:HE2	2.01	0.43
1:G:67:VAL:HG21	1:G:294:LEU:HD23	2.01	0.43
1:H:253:LEU:HD13	1:H:293:PHE:HE1	1.83	0.43
1:C:248:MET:HE3	1:C:248:MET:HB3	1.93	0.43
1:H:116:ARG:HG2	1:H:116:ARG:NH2	2.13	0.43
1:B:140:ILE:HB	1:B:248:MET:HE2	2.00	0.43
1:D:266:MET:HE3	1:D:266:MET:HB3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:LYS:HD2	1:F:272:LEU:HG	2.00	0.43
1:F:249:PRO:HB3	1:F:275:ARG:NH2	2.34	0.43
1:H:266:MET:HE3	1:H:266:MET:HB3	1.85	0.43
1:C:29:ARG:NE	2:C:406:HOH:O	2.46	0.43
1:E:108:LEU:HD11	1:E:112:LEU:HD11	2.01	0.43
1:C:39:HIS:CG	1:C:88:GLU:HB2	2.53	0.42
1:B:240:ALA:O	1:B:243:LYS:HG2	2.18	0.42
1:G:26:PHE:CD1	1:G:43:GLY:HA3	2.55	0.42
1:D:188:ARG:NH2	1:D:213:ASP:OD2	2.50	0.42
1:G:132:TYR:C	1:G:132:TYR:CD1	2.97	0.42
1:G:34:ASP:OD2	1:G:34:ASP:N	2.51	0.42
1:E:132:TYR:CD1	1:E:140:ILE:HD11	2.54	0.42
1:E:145:MET:HE1	1:E:270:LEU:HD12	2.01	0.42
1:H:242:MET:HG2	1:H:270:LEU:HD23	2.01	0.42
1:C:266:MET:HE3	1:C:266:MET:HB3	1.82	0.42
1:G:71:LEU:HD23	1:G:71:LEU:HA	1.70	0.42
1:G:226:GLU:HA	1:G:229:ARG:HD2	2.02	0.42
1:G:242:MET:HE2	1:G:270:LEU:HD23	2.00	0.42
1:F:39:HIS:CG	1:F:88:GLU:HB2	2.54	0.42
1:F:152:GLY:O	1:F:239:LYS:HE3	2.19	0.42
1:C:143:LEU:HD21	1:C:145:MET:HE2	2.01	0.42
1:D:176:ARG:HA	1:D:229:ARG:CZ	2.50	0.42
1:G:36:VAL:HG13	1:G:90:ASP:HB2	2.00	0.42
1:G:59:GLN:NE2	1:G:195:TYR:OH	2.38	0.42
1:H:188:ARG:HH21	1:H:213:ASP:CG	2.27	0.42
1:F:118:HIS:HB3	1:F:302:PHE:CZ	2.55	0.41
1:E:71:LEU:HD23	1:E:71:LEU:HA	1.72	0.41
1:F:158:GLU:O	1:F:162:SER:OG	2.29	0.41
1:B:151:PRO:HA	1:B:156:TRP:CG	2.55	0.41
1:B:85:GLY:HA2	1:B:91:LYS:HG3	2.03	0.41
1:D:26:PHE:CD1	1:D:43:GLY:HA3	2.56	0.41
1:G:67:VAL:HA	1:G:295:THR:CG2	2.51	0.41
1:B:247:PRO:O	2:B:401:HOH:O	2.21	0.41
1:C:143:LEU:CD2	1:C:145:MET:HE2	2.51	0.41
1:A:108:LEU:C	1:A:108:LEU:HD23	2.46	0.41
1:E:108:LEU:CD1	1:E:112:LEU:HD11	2.51	0.41
1:F:141:VAL:HG12	1:F:142:LYS:HG3	2.02	0.41
1:F:24:ARG:H	1:F:24:ARG:HG2	1.49	0.41
1:G:130:TYR:CE1	1:G:270:LEU:HD22	2.56	0.41
1:H:140:ILE:HD12	1:H:143:LEU:HB2	2.00	0.41
1:H:264:LEU:HD21	1:H:276:GLY:CA	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HD22	1:D:253:LEU:HB2	2.02	0.40
1:H:68:MET:N	1:H:69:PRO:CD	2.84	0.40
1:F:123:SER:OG	1:F:124:ILE:N	2.49	0.40
1:A:51:VAL:HG22	1:A:118:HIS:HB2	2.02	0.40
1:B:29:ARG:HB3	1:B:40:TYR:CZ	2.56	0.40
1:F:67:VAL:HG21	1:F:294:LEU:HD23	2.03	0.40
1:G:123:SER:OG	1:G:124:ILE:N	2.48	0.40
1:H:116:ARG:CG	1:H:116:ARG:NH2	2.72	0.40
1:A:279:ALA:HA	1:A:280:PRO:HD3	1.98	0.40
1:B:242:MET:HB2	1:B:242:MET:HE3	1.87	0.40
1:G:303:ARG:HD2	1:G:303:ARG:HA	1.81	0.40
1:H:140:ILE:HD11	1:H:142:LYS:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	291/309 (94%)	282 (97%)	8 (3%)	1 (0%)	36	34
1	B	292/309 (94%)	283 (97%)	8 (3%)	1 (0%)	36	34
1	C	291/309 (94%)	282 (97%)	8 (3%)	1 (0%)	36	34
1	D	292/309 (94%)	284 (97%)	7 (2%)	1 (0%)	36	34
1	E	292/309 (94%)	283 (97%)	8 (3%)	1 (0%)	36	34
1	F	291/309 (94%)	281 (97%)	9 (3%)	1 (0%)	36	34
1	G	291/309 (94%)	278 (96%)	12 (4%)	1 (0%)	36	34
1	H	292/309 (94%)	285 (98%)	6 (2%)	1 (0%)	36	34
All	All	2332/2472 (94%)	2258 (97%)	66 (3%)	8 (0%)	36	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	58	PRO
1	D	58	PRO
1	E	58	PRO
1	F	58	PRO
1	H	58	PRO
1	G	58	PRO
1	A	58	PRO
1	B	58	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	228/241 (95%)	226 (99%)	2 (1%)	70	77
1	B	229/241 (95%)	228 (100%)	1 (0%)	84	89
1	C	228/241 (95%)	227 (100%)	1 (0%)	84	89
1	D	229/241 (95%)	224 (98%)	5 (2%)	45	51
1	E	229/241 (95%)	224 (98%)	5 (2%)	45	51
1	F	228/241 (95%)	219 (96%)	9 (4%)	28	28
1	G	228/241 (95%)	218 (96%)	10 (4%)	25	23
1	H	229/241 (95%)	222 (97%)	7 (3%)	35	37
All	All	1828/1928 (95%)	1788 (98%)	40 (2%)	45	51

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	195	TYR
1	B	195	TYR
1	C	195	TYR
1	D	29	ARG
1	D	46	ASP
1	D	126	VAL
1	D	195	TYR

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Mol	Chain	Res	Type
1	D	303	ARG
1	E	35	ASP
1	E	108	LEU
1	E	195	TYR
1	E	275	ARG
1	E	303	ARG
1	F	24	ARG
1	F	29	ARG
1	F	35	ASP
1	F	36	VAL
1	F	53	LEU
1	F	116	ARG
1	F	158	GLU
1	F	195	TYR
1	F	275	ARG
1	G	34	ASP
1	G	35	ASP
1	G	46	ASP
1	G	74	ASP
1	G	111	GLN
1	G	116	ARG
1	G	140	ILE
1	G	195	TYR
1	G	270	LEU
1	G	275	ARG
1	H	116	ARG
1	H	117	ILE
1	H	128	VAL
1	H	140	ILE
1	H	188	ARG
1	H	195	TYR
1	H	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	244	HIS
1	A	281	ASN
1	B	32	GLN
1	B	135	GLN
1	B	200	HIS

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Mol	Chain	Res	Type
1	C	200	HIS
1	C	281	ASN
1	E	66	HIS
1	E	200	HIS
1	E	244	HIS
1	E	290	ASN
1	F	110	HIS
1	F	135	GLN
1	F	281	ASN
1	F	284	HIS
1	G	135	GLN
1	H	166	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	293/309 (94%)	-0.14	3 (1%) 79 82	30, 38, 52, 68	0
1	B	294/309 (95%)	-0.00	4 (1%) 73 77	29, 43, 63, 77	0
1	C	293/309 (94%)	-0.03	2 (0%) 84 85	32, 43, 59, 79	0
1	D	294/309 (95%)	0.41	11 (3%) 45 49	36, 57, 80, 89	0
1	E	294/309 (95%)	0.48	9 (3%) 51 55	36, 58, 80, 93	0
1	F	293/309 (94%)	0.69	15 (5%) 33 37	35, 67, 88, 98	0
1	G	293/309 (94%)	1.31	87 (29%) 1 1	34, 78, 104, 112	0
1	H	294/309 (95%)	0.86	19 (6%) 25 28	38, 72, 96, 110	0
All	All	2348/2472 (94%)	0.45	150 (6%) 25 28	29, 54, 93, 112	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	299	LEU	5.1
1	G	11	PRO	5.1
1	B	11	PRO	4.7
1	A	11	PRO	4.5
1	B	264	LEU	4.3
1	H	11	PRO	4.2
1	G	76	TYR	3.9
1	G	303	ARG	3.8
1	G	138	THR	3.8
1	G	51	VAL	3.7
1	F	250	VAL	3.7
1	G	246	LEU	3.7
1	G	302	PHE	3.6
1	G	72	ALA	3.5
1	E	43	GLY	3.5
1	D	113	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	11	PRO	3.4
1	H	35	ASP	3.4
1	G	114	ALA	3.4
1	H	137	PRO	3.3
1	H	246	LEU	3.2
1	B	35	ASP	3.2
1	F	11	PRO	3.2
1	G	271	ALA	3.1
1	G	79	VAL	3.1
1	G	22	PHE	3.1
1	G	120	VAL	3.1
1	G	133	ALA	3.1
1	G	119	LEU	3.1
1	G	145	MET	3.1
1	G	144	ALA	3.0
1	G	78	VAL	3.0
1	G	248	MET	3.0
1	G	141	VAL	3.0
1	G	20	ALA	2.9
1	F	264	LEU	2.9
1	G	21	GLY	2.9
1	C	12	GLY	2.8
1	G	129	ALA	2.8
1	F	115	THR	2.8
1	G	41	VAL	2.8
1	G	150	VAL	2.8
1	G	140	ILE	2.8
1	G	26	PHE	2.8
1	F	298	LEU	2.8
1	D	11	PRO	2.8
1	G	146	LEU	2.7
1	G	253	LEU	2.7
1	E	29	ARG	2.7
1	G	143	LEU	2.7
1	G	267	ALA	2.7
1	G	274	VAL	2.7
1	G	44	GLY	2.7
1	G	276	GLY	2.7
1	G	142	LYS	2.6
1	G	121	GLY	2.6
1	G	54	LEU	2.6
1	G	298	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	42	THR	2.6
1	E	159	ALA	2.6
1	G	70	ALA	2.6
1	A	35	ASP	2.6
1	H	299	LEU	2.6
1	H	140	ILE	2.6
1	G	117	ILE	2.5
1	G	46	ASP	2.5
1	G	115	THR	2.5
1	H	272	LEU	2.5
1	G	35	ASP	2.5
1	F	236	THR	2.5
1	G	45	PRO	2.5
1	G	252	ALA	2.5
1	G	292	ALA	2.5
1	H	270	LEU	2.4
1	F	303	ARG	2.4
1	G	293	PHE	2.4
1	G	137	PRO	2.4
1	D	112	LEU	2.4
1	G	53	LEU	2.4
1	G	203	LEU	2.4
1	E	304	GLU	2.4
1	D	166	GLN	2.4
1	E	78	VAL	2.4
1	G	52	VAL	2.4
1	D	118	HIS	2.4
1	G	80	ALA	2.3
1	D	272	LEU	2.3
1	H	155	ILE	2.3
1	G	247	PRO	2.3
1	H	252	ALA	2.3
1	G	272	LEU	2.3
1	H	298	LEU	2.3
1	H	268	ARG	2.3
1	G	118	HIS	2.3
1	H	117	ILE	2.3
1	G	81	VAL	2.3
1	A	158	GLU	2.3
1	F	105	ILE	2.3
1	G	36	VAL	2.3
1	G	15	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	251	LEU	2.3
1	G	42	THR	2.2
1	D	296	ARG	2.2
1	E	35	ASP	2.2
1	G	18	LEU	2.2
1	C	304	GLU	2.2
1	G	25	ARG	2.2
1	G	69	PRO	2.2
1	G	126	VAL	2.2
1	G	243	LYS	2.2
1	H	159	ALA	2.2
1	D	299	LEU	2.2
1	F	270	LEU	2.2
1	F	27	SER	2.2
1	G	301	PHE	2.2
1	F	30	TYR	2.2
1	G	132	TYR	2.2
1	G	249	PRO	2.1
1	G	75	GLY	2.1
1	G	277	ALA	2.1
1	B	116	ARG	2.1
1	H	130	TYR	2.1
1	G	238	PHE	2.1
1	D	44	GLY	2.1
1	G	201	VAL	2.1
1	G	107	ALA	2.1
1	G	130	TYR	2.1
1	G	166	GLN	2.1
1	H	51	VAL	2.1
1	G	202	ALA	2.1
1	G	112	LEU	2.1
1	G	251	LEU	2.1
1	H	33	LEU	2.1
1	D	35	ASP	2.1
1	F	141	VAL	2.1
1	E	292	ALA	2.1
1	F	108	LEU	2.0
1	G	71	LEU	2.0
1	G	290	ASN	2.0
1	G	244	HIS	2.0
1	F	243	LYS	2.0
1	G	40	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	245	LYS	2.0
1	D	301	PHE	2.0
1	F	52	VAL	2.0
1	G	240	ALA	2.0
1	G	275	ARG	2.0
1	H	118	HIS	2.0
1	G	280	PRO	2.0
1	G	43	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.