



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:34 AM UTC

PDB ID : 4I46 / pdb_00004i46
Title : Crystal structure of 31kD Heat Shock Protein, VcHsp31 from *Vibrio cholerae*
Authors : Sen, U.; Das, S.
Deposited on : 2012-11-27
Resolution : 2.50 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:

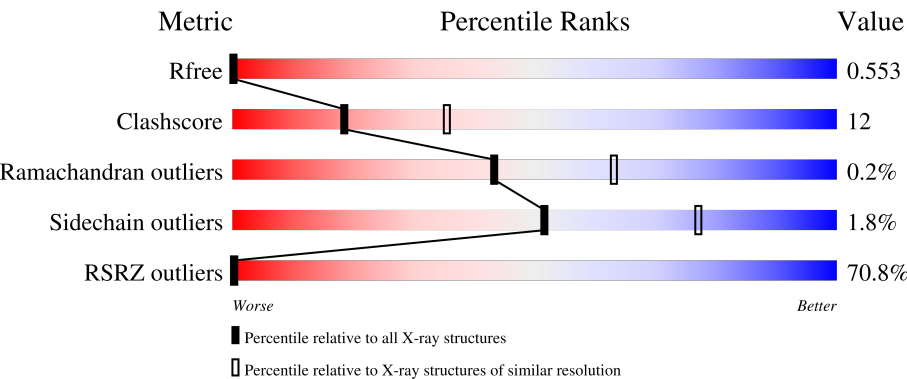
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	72% 69% 28% ..
1	B	286	69% 77% 20% ..
1	C	286	71% 73% 23% ..
1	D	286	66% 74% 23% ..
1	E	286	67% 68% 28% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	286	71% 70%27% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	B	5001	-	X	-	X
2	MPD	F	301	-	-	X	-

2 Entry composition [i](#)

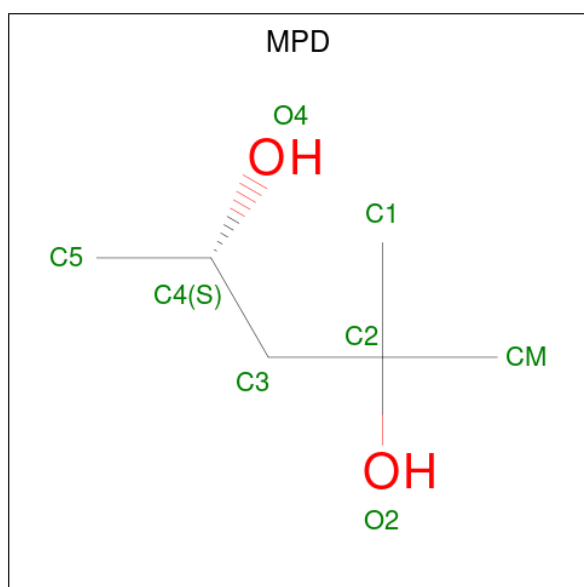
There are 3 unique types of molecules in this entry. The entry contains 13718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Intracellular protease/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	B	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	C	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	D	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	E	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	F	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



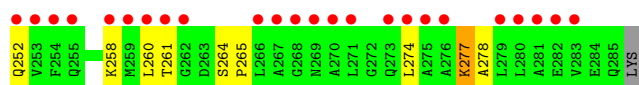
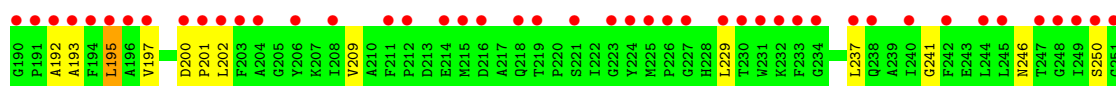
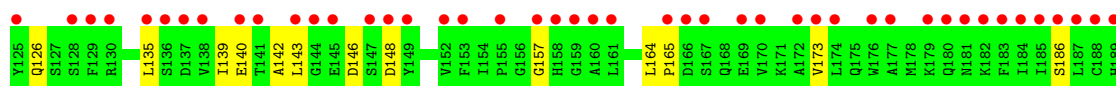
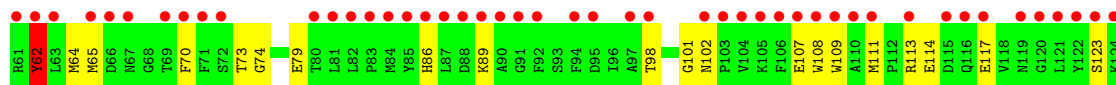
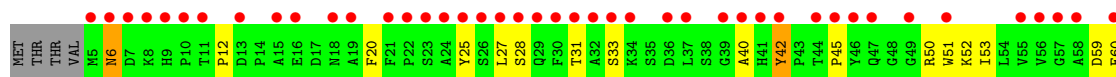
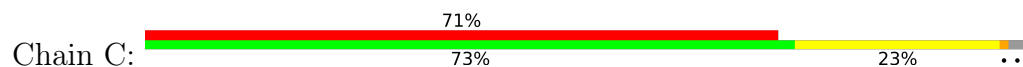
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0

- Molecule 3 is water.

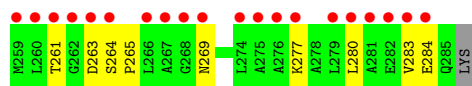
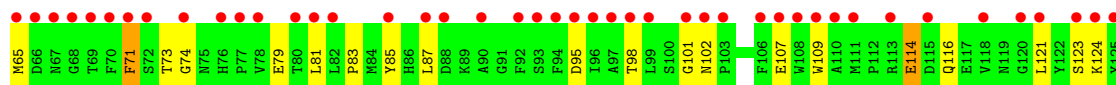
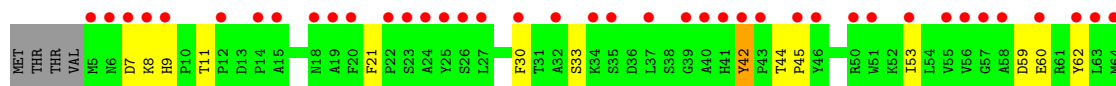
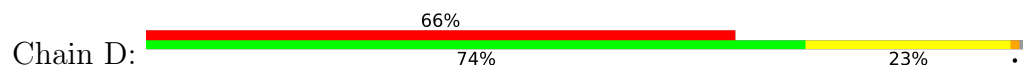
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	131	Total O 131 131	0	0
3	B	131	Total O 131 131	0	0
3	C	113	Total O 113 113	0	0
3	D	123	Total O 123 123	0	0
3	E	91	Total O 91 91	0	0
3	F	103	Total O 103 103	0	0



● Molecule 1: Intracellular protease/amidase

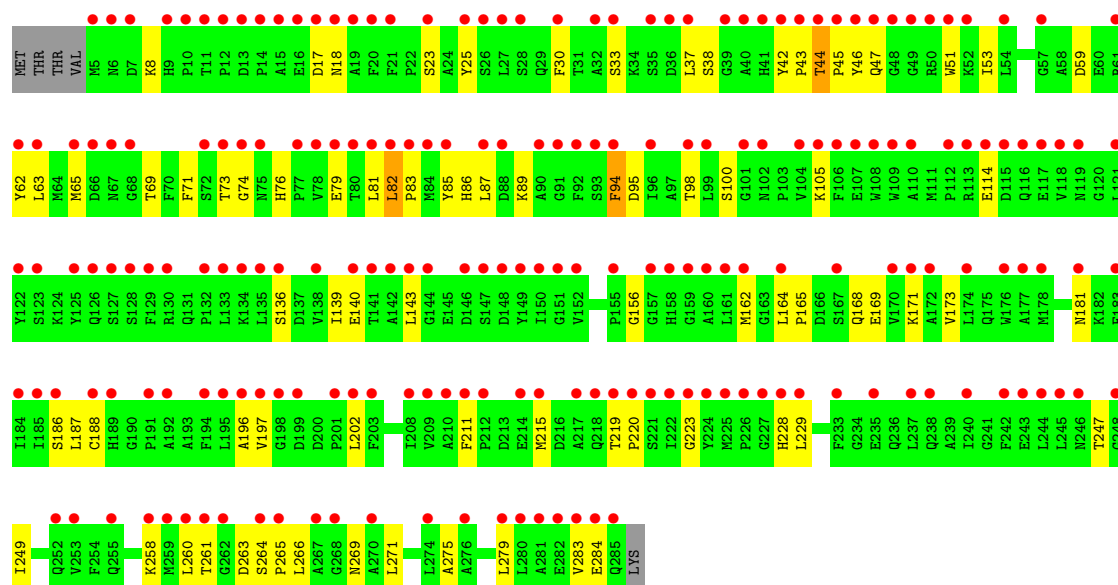


● Molecule 1: Intracellular protease/amidase



● Molecule 1: Intracellular protease/amidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.29Å 80.03Å 133.04Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	29.65 – 2.50 29.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.65-2.50) 44.4 (29.65-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.259 0.558 , 0.553	Depositor DCC
R_{free} test set	1573 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	2.9	Xtriage
Anisotropy	2.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 483.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.28	EDS
Total number of atoms	13718	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MPD

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	0.47	0/2225	0.99	8/3023 (0.3%)
1	B	0.46	0/2225	1.00	8/3023 (0.3%)
1	C	0.44	0/2225	1.00	11/3023 (0.4%)
1	D	0.44	0/2225	0.99	9/3023 (0.3%)
1	E	0.42	0/2225	1.02	12/3023 (0.4%)
1	F	0.43	0/2225	0.90	6/3023 (0.2%)
All	All	0.45	0/13350	0.98	54/18138 (0.3%)

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	157	GLY	N-CA-C	-12.48	100.09	111.95
1	A	131	GLN	CA-C-N	7.80	127.70	120.21
1	A	131	GLN	C-N-CA	7.80	127.70	120.21
1	A	142	ALA	N-CA-C	7.49	122.13	112.92
1	B	241	GLY	N-CA-C	7.20	124.58	115.21
1	D	95	ASP	N-CA-C	-7.12	98.13	109.59
1	E	21	PHE	N-CA-C	-7.03	102.05	110.13
1	A	263	ASP	N-CA-C	6.89	121.69	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	81	LEU	N-CA-C	6.45	118.39	111.36
1	F	263	ASP	N-CA-C	6.42	121.31	112.90
1	D	101	GLY	N-CA-C	-6.40	106.25	115.27
1	E	42	TYR	CA-C-N	6.38	126.59	119.32
1	E	42	TYR	C-N-CA	6.38	126.59	119.32
1	C	157	GLY	N-CA-C	-6.29	103.75	112.18
1	F	30	PHE	N-CA-C	6.09	120.73	112.88
1	E	192	ALA	N-CA-C	-5.99	105.23	112.54
1	E	81	LEU	N-CA-C	5.95	118.72	111.82
1	A	241	GLY	N-CA-C	5.89	121.80	114.37
1	D	71	PHE	N-CA-C	-5.85	99.19	108.73
1	D	81	LEU	N-CA-C	5.83	118.86	111.69
1	A	261	THR	N-CA-C	5.78	118.19	109.23
1	E	188	CYS	CB-CA-C	-5.78	109.92	116.63
1	D	42	TYR	CA-C-N	5.69	126.07	119.47
1	D	42	TYR	C-N-CA	5.69	126.07	119.47
1	B	30	PHE	N-CA-C	5.69	119.91	112.92
1	E	101	GLY	N-CA-C	-5.68	107.26	115.27
1	B	245	LEU	N-CA-C	5.68	120.33	112.90
1	C	258	LYS	N-CA-C	5.63	119.14	112.72
1	B	113	ARG	N-CA-C	5.59	118.14	111.71
1	B	97	ALA	N-CA-C	5.57	117.87	109.23
1	C	142	ALA	N-CA-C	5.57	119.38	112.59
1	C	209	VAL	N-CA-C	-5.57	100.46	108.48
1	D	141	THR	N-CA-C	5.56	122.45	114.39
1	A	202	LEU	N-CA-C	5.54	117.00	111.07
1	B	107	GLU	N-CA-C	-5.53	97.59	107.98
1	E	157	GLY	CA-C-O	-5.45	118.68	122.22
1	C	113	ARG	N-CA-C	5.42	119.00	112.38
1	E	150	ILE	N-CA-C	-5.42	107.70	112.90
1	C	241	GLY	N-CA-C	5.41	121.12	114.69
1	F	188	CYS	CB-CA-C	-5.33	109.98	117.23
1	C	42	TYR	CA-C-N	5.33	124.51	118.97
1	C	42	TYR	C-N-CA	5.33	124.51	118.97
1	A	81	LEU	N-CA-C	5.31	118.92	112.23
1	B	150	ILE	N-CA-C	-5.31	107.57	112.83
1	E	263	ASP	N-CA-C	5.31	118.92	112.23
1	D	247	THR	N-CA-C	-5.30	106.75	114.12
1	F	94	PHE	N-CA-C	5.22	117.75	109.50
1	C	246	ASN	N-CA-C	5.18	118.50	110.17
1	F	62	TYR	N-CA-C	5.16	117.34	107.75
1	C	62	TYR	N-CA-C	5.12	116.66	108.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	ASP	N-CA-C	5.11	119.78	113.50
1	E	216	ASP	N-CA-C	-5.07	105.94	111.82
1	C	101	GLY	N-CA-C	-5.04	108.16	115.27
1	B	81	LEU	N-CA-C	5.01	119.10	112.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	62	TYR	Sidechain
1	D	62	TYR	Sidechain

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	2163	0	2072	54	0
1	B	2163	0	2072	39	0
1	C	2163	0	2072	45	0
1	D	2163	0	2072	50	0
1	E	2163	0	2072	64	0
1	F	2163	0	2072	65	0
2	A	8	0	14	3	0
2	B	16	0	28	3	0
2	D	8	0	14	4	0
2	E	8	0	14	4	0
2	F	8	0	14	6	0
3	A	131	0	0	5	0
3	B	131	0	0	2	0
3	C	113	0	0	1	0
3	D	123	0	0	4	0
3	E	91	0	0	5	0
3	F	103	0	0	6	0
All	All	13718	0	12516	306	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 12.

All (306) 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:D:33:SER:HB2	1:D:114:GLU:HG3	1.42	1.00
1:E:126:GLN:HE21	1:E:130:ARG:NH1	1.66	0.93
1:E:126:GLN:HE21	1:E:130:ARG:CZ	1.85	0.88
2:B:5002:MPD:HM3	3:B:5198:HOH:O	1.74	0.86
1:C:64:MET:HE3	1:D:131:GLN:HE21	1.39	0.85
1:A:64:MET:HE3	1:B:131:GLN:HE21	1.45	0.81
1:A:58:ALA:H	1:A:75:ASN:HD21	1.31	0.79
1:F:249:ILE:CD1	2:F:301:MPD:H31	2.13	0.78
1:C:40:ALA:O	1:C:89:LYS:HD3	1.85	0.76
1:C:140:GLU:HB3	1:F:143:LEU:HB2	1.68	0.76
1:D:85:TYR:HA	1:D:121:LEU:HD13	1.68	0.74
1:C:108:TRP:HZ3	1:C:111:MET:HE2	1.54	0.72
1:E:65:MET:HE1	1:E:229:LEU:HD23	1.74	0.70
1:A:58:ALA:H	1:A:75:ASN:ND2	1.89	0.70
1:D:186:SER:O	1:D:261:THR:HA	1.91	0.70
1:E:10:PRO:HB3	3:E:406:HOH:O	1.93	0.68
1:E:208:ILE:HB	1:E:261:THR:HG21	1.75	0.68
1:C:200:ASP:OD2	1:C:202:LEU:HB2	1.94	0.68
1:D:204:ALA:HA	1:D:241:GLY:HA3	1.74	0.68
1:D:42:TYR:O	1:D:45:PRO:HD3	1.95	0.67
1:B:186:SER:O	1:B:261:THR:HA	1.96	0.66
1:A:229:LEU:HA	3:A:484:HOH:O	1.94	0.66
1:C:264:SER:HB2	1:C:265:PRO:CD	2.26	0.66
1:A:108:TRP:CZ3	1:A:111:MET:HE3	2.31	0.65
1:E:126:GLN:NE2	1:E:130:ARG:NH1	2.42	0.65
1:D:53:ILE:HD13	1:D:87:LEU:HD13	1.78	0.65
1:A:186:SER:O	1:A:261:THR:HA	1.96	0.65
1:D:280:LEU:O	1:D:284:GLU:HG3	1.97	0.65
1:E:188:CYS:O	1:E:191:PRO:HD2	1.95	0.65
1:D:202:LEU:H	1:D:202:LEU:HD23	1.62	0.65
1:A:64:MET:HE3	1:B:131:GLN:NE2	2.12	0.64
1:B:141:THR:HG22	3:B:5132:HOH:O	1.96	0.64
1:E:42:TYR:O	1:E:45:PRO:HD3	1.96	0.64
1:E:134:LYS:HE3	3:F:489:HOH:O	1.96	0.64
1:D:197:VAL:HG11	1:D:202:LEU:HD21	1.80	0.64
1:E:53:ILE:HD13	1:E:87:LEU:HD13	1.79	0.64
1:F:169:GLU:O	1:F:173:VAL:HG23	1.99	0.63
1:F:65:MET:HA	1:F:65:MET:HE2	1.81	0.63
1:B:42:TYR:O	1:B:45:PRO:HD3	1.99	0.63
1:F:65:MET:HE1	1:F:229:LEU:HD23	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:HD3	3:A:480:HOH:O	1.98	0.62
1:E:264:SER:HB2	1:E:265:PRO:CD	2.28	0.62
1:E:37:LEU:HD21	1:E:85:TYR:CE2	2.34	0.62
1:C:277:LYS:HE2	3:C:345:HOH:O	1.98	0.62
1:E:53:ILE:CD1	1:E:87:LEU:HD13	2.30	0.62
1:C:186:SER:O	1:C:261:THR:HA	2.00	0.61
1:D:116:GLN:HG2	3:D:519:HOH:O	2.00	0.61
1:D:264:SER:HB2	1:D:265:PRO:CD	2.31	0.61
1:B:232:LYS:O	1:B:236:GLN:HG2	2.01	0.61
1:E:280:LEU:O	1:E:284:GLU:HG2	2.00	0.61
1:A:108:TRP:HZ3	1:A:111:MET:HE3	1.67	0.60
1:C:192:ALA:O	1:C:195:LEU:HB2	2.02	0.60
1:C:139:ILE:HD11	1:C:173:VAL:CG2	2.33	0.59
1:F:265:PRO:HD2	2:F:301:MPD:H12	1.84	0.59
1:C:200:ASP:C	1:C:202:LEU:H	2.10	0.59
1:C:264:SER:HB2	1:C:265:PRO:HD2	1.84	0.59
1:B:145:GLU:HG3	1:F:284:GLU:C	2.27	0.58
1:F:249:ILE:HD11	2:F:301:MPD:H31	1.85	0.58
1:A:211:PHE:HE1	2:A:301:MPD:C1	2.16	0.58
1:E:126:GLN:NE2	1:E:130:ARG:CZ	2.64	0.58
1:E:277:LYS:HE3	3:E:484:HOH:O	2.02	0.58
1:F:76:HIS:HE1	3:F:499:HOH:O	1.86	0.57
1:B:275:ALA:O	1:B:279:LEU:HD13	2.03	0.57
1:C:108:TRP:CZ3	1:C:111:MET:HE2	2.38	0.57
1:B:18:ASN:ND2	1:B:69:THR:HA	2.19	0.57
1:E:164:LEU:HB2	1:E:165:PRO:HD3	1.88	0.56
1:C:139:ILE:HD11	1:C:173:VAL:HG23	1.88	0.56
1:A:136:SER:O	1:A:140:GLU:HG3	2.06	0.56
1:C:33:SER:HB2	1:C:114:GLU:HG3	1.86	0.56
1:D:59:ASP:HB3	1:D:98:THR:HB	1.86	0.56
1:D:249:ILE:CD1	2:D:301:MPD:HM1	2.35	0.56
1:E:264:SER:HB2	1:E:265:PRO:HD2	1.88	0.56
1:E:85:TYR:HD1	1:E:121:LEU:HD22	1.71	0.56
1:F:37:LEU:HD21	1:F:85:TYR:CE2	2.41	0.56
1:F:187:LEU:HB3	1:F:271:LEU:HD22	1.88	0.55
1:F:53:ILE:CD1	1:F:87:LEU:HD13	2.37	0.55
1:C:164:LEU:HB2	1:C:165:PRO:HD3	1.88	0.55
1:F:171:LYS:HB2	1:F:196:ALA:O	2.06	0.55
1:F:164:LEU:HB2	1:F:165:PRO:HD3	1.87	0.55
1:C:27:LEU:O	1:C:31:THR:HB	2.05	0.55
1:A:130:ARG:HH22	1:B:18:ASN:HD22	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:TYR:O	1:F:45:PRO:HD3	2.07	0.54
1:F:220:PRO:HG2	1:F:228:HIS:CD2	2.43	0.54
1:A:211:PHE:HE1	2:A:301:MPD:H13	1.73	0.54
1:B:76:HIS:CD2	1:B:79:GLU:HG3	2.43	0.54
1:A:59:ASP:HB3	1:A:98:THR:HB	1.89	0.54
1:D:264:SER:HB2	1:D:265:PRO:HD2	1.90	0.54
1:F:249:ILE:HD12	2:F:301:MPD:H31	1.89	0.53
1:D:171:LYS:HG3	1:D:197:VAL:HA	1.90	0.53
1:F:136:SER:O	1:F:140:GLU:HG3	2.08	0.53
1:B:96:ILE:HD12	1:B:128:SER:CB	2.38	0.53
1:A:279:LEU:O	1:A:283:VAL:HG22	2.09	0.53
1:E:63:LEU:O	1:E:70:PHE:HA	2.08	0.53
1:A:87:LEU:HB2	1:A:94:PHE:HZ	1.74	0.52
1:B:140:GLU:HB3	3:F:416:HOH:O	2.09	0.52
1:F:18:ASN:ND2	1:F:69:THR:HA	2.25	0.52
1:A:189:HIS:HE1	1:A:216:ASP:OD2	1.93	0.52
1:E:186:SER:O	1:E:261:THR:HA	2.09	0.52
1:D:171:LYS:HB2	1:D:196:ALA:O	2.10	0.52
1:E:37:LEU:HD11	1:E:85:TYR:CD2	2.44	0.52
1:D:215:MET:O	1:D:219:THR:HG23	2.10	0.52
1:C:135:LEU:O	1:C:139:ILE:HG12	2.10	0.51
3:A:464:HOH:O	1:B:17:ASP:HB2	2.10	0.51
1:F:82:LEU:HD23	1:F:269:ASN:N	2.25	0.51
1:A:211:PHE:CE1	2:A:301:MPD:H13	2.45	0.51
1:A:253:VAL:HG12	1:A:262:GLY:HA2	1.93	0.51
1:D:249:ILE:HD11	2:D:301:MPD:HM1	1.92	0.51
1:F:46:TYR:O	1:F:47:GLN:HG3	2.11	0.51
1:F:82:LEU:HB3	1:F:83:PRO:HD3	1.93	0.51
1:A:8:LYS:O	1:A:223:GLY:HA3	2.11	0.51
1:E:115:ASP:OD1	1:E:117:GLU:HB2	2.11	0.51
1:E:168:GLN:HB3	3:E:482:HOH:O	2.11	0.51
1:E:195:LEU:HD23	1:E:240:ILE:HD13	1.92	0.51
1:E:258:LYS:NZ	1:E:282:GLU:OE2	2.41	0.50
1:F:186:SER:O	1:F:261:THR:HA	2.12	0.50
1:F:47:GLN:NE2	3:F:490:HOH:O	2.45	0.50
1:B:207:LYS:HE3	1:B:243:GLU:OE1	2.11	0.50
1:C:73:THR:OG1	1:C:74:GLY:N	2.45	0.50
1:A:42:TYR:OH	1:A:86:HIS:HD2	1.94	0.50
1:C:277:LYS:HG3	1:C:278:ALA:N	2.26	0.49
1:B:107:GLU:HB3	1:B:109:TRP:CE2	2.47	0.49
1:E:79:GLU:OE1	1:E:156:GLY:HA3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:THR:N	1:F:220:PRO:CD	2.75	0.49
1:E:30:PHE:CG	2:E:301:MPD:H11	2.48	0.49
1:F:187:LEU:N	1:F:187:LEU:HD23	2.28	0.49
1:F:171:LYS:HG3	1:F:197:VAL:HA	1.94	0.49
1:F:264:SER:HB2	1:F:265:PRO:CD	2.42	0.49
1:E:65:MET:HE2	1:E:65:MET:HA	1.94	0.49
1:A:65:MET:HG3	1:A:226:PRO:HG2	1.95	0.49
1:C:42:TYR:OH	1:C:86:HIS:HD2	1.96	0.49
1:B:96:ILE:HD12	1:B:128:SER:HB3	1.93	0.48
1:C:65:MET:HE1	1:C:229:LEU:HD23	1.93	0.48
1:A:171:LYS:O	1:A:175:GLN:HG3	2.12	0.48
1:B:199:ASP:OD1	1:B:200:ASP:N	2.46	0.48
1:B:51:TRP:HA	1:B:51:TRP:CE3	2.48	0.48
1:D:7:ASP:OD2	1:D:9:HIS:HB2	2.14	0.48
1:A:79:GLU:OE2	1:A:265:PRO:HG3	2.13	0.48
1:F:264:SER:HB2	1:F:265:PRO:HD2	1.95	0.48
1:F:275:ALA:O	1:F:279:LEU:HD13	2.13	0.48
1:F:73:THR:OG1	1:F:74:GLY:N	2.47	0.48
1:F:95:ASP:HA	3:F:425:HOH:O	2.12	0.48
1:C:60:GLU:OE1	1:D:102:ASN:HB3	2.13	0.48
1:F:197:VAL:HG11	1:F:202:LEU:HD21	1.96	0.48
1:E:167:SER:OG	1:E:170:VAL:HG23	2.13	0.47
1:E:167:SER:CB	1:E:170:VAL:HG23	2.45	0.47
1:F:266:LEU:HD21	2:F:301:MPD:H51	1.96	0.47
1:C:59:ASP:HB3	1:C:98:THR:HB	1.96	0.47
1:E:11:THR:O	1:E:20:PHE:HA	2.14	0.47
1:E:167:SER:HB3	1:E:170:VAL:CG2	2.45	0.47
1:F:63:LEU:HB2	1:F:162:MET:HE2	1.95	0.47
1:A:96:ILE:HD13	1:A:129:PHE:CE1	2.49	0.47
1:D:79:GLU:O	1:D:83:PRO:HG2	2.14	0.47
1:D:157:GLY:C	1:D:159:GLY:H	2.23	0.47
1:D:187:LEU:N	1:D:187:LEU:HD23	2.29	0.47
1:A:200:ASP:C	1:A:202:LEU:H	2.21	0.47
1:A:275:ALA:O	1:A:279:LEU:HD13	2.15	0.47
1:D:107:GLU:HB3	1:D:109:TRP:CE2	2.49	0.47
1:E:235:GLU:HB3	3:E:440:HOH:O	2.15	0.47
1:D:8:LYS:O	1:D:223:GLY:HA3	2.14	0.47
1:C:52:LYS:C	1:C:53:ILE:HD12	2.40	0.47
1:E:85:TYR:CD1	1:E:121:LEU:HD22	2.50	0.46
1:B:264:SER:HB2	1:B:265:PRO:CD	2.46	0.46
1:C:42:TYR:O	1:C:45:PRO:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:TYR:HA	1:D:121:LEU:CD1	2.41	0.46
1:E:30:PHE:HB3	2:E:301:MPD:H31	1.98	0.46
1:F:82:LEU:CB	1:F:83:PRO:HD3	2.45	0.46
1:F:71:PHE:CD1	1:F:73:THR:HB	2.51	0.46
1:A:61:ARG:HH12	1:B:16:GLU:HG2	1.80	0.46
1:A:264:SER:HB2	1:A:265:PRO:CD	2.46	0.46
1:B:194:PHE:O	1:B:197:VAL:HG22	2.16	0.46
1:C:140:GLU:HA	1:F:140:GLU:HA	1.97	0.46
1:D:150:ILE:HG12	1:D:150:ILE:O	2.16	0.46
1:D:212:PRO:HG2	1:D:215:MET:HG3	1.98	0.46
1:D:30:PHE:CD1	2:D:301:MPD:H11	2.51	0.46
1:E:204:ALA:HA	1:E:241:GLY:HA3	1.98	0.46
1:F:8:LYS:HE2	1:F:25:TYR:CD2	2.50	0.46
1:A:42:TYR:O	1:A:45:PRO:HD3	2.16	0.46
1:A:73:THR:OG1	1:A:74:GLY:N	2.49	0.46
1:C:195:LEU:HD13	1:C:237:LEU:HD23	1.97	0.46
1:F:44:THR:HG23	3:F:421:HOH:O	2.16	0.46
1:A:76:HIS:CE1	1:A:78:VAL:HB	2.51	0.45
1:A:191:PRO:O	1:A:237:LEU:HD21	2.16	0.45
1:C:51:TRP:HA	1:C:148:ASP:O	2.16	0.45
1:D:197:VAL:CG1	1:D:202:LEU:HD21	2.46	0.45
1:F:105:LYS:HA	1:F:105:LYS:HD3	1.69	0.45
1:E:30:PHE:O	2:E:301:MPD:H52	2.16	0.45
1:E:143:LEU:HB3	1:E:144:GLY:H	1.51	0.45
1:D:200:ASP:CG	1:D:202:LEU:HD22	2.41	0.45
1:F:89:LYS:HD3	1:F:89:LYS:HA	1.79	0.45
1:F:139:ILE:HG22	1:F:173:VAL:HG22	1.98	0.45
1:A:96:ILE:HD13	1:A:129:PHE:CD1	2.52	0.45
1:F:53:ILE:HD13	1:F:87:LEU:HD13	1.98	0.45
1:E:86:HIS:NE2	1:E:273:GLN:HG2	2.32	0.45
1:A:79:GLU:OE1	1:A:156:GLY:HA3	2.17	0.45
1:C:260:LEU:HD22	1:C:274:LEU:HD21	1.98	0.45
1:D:141:THR:HB	3:D:505:HOH:O	2.16	0.45
1:E:79:GLU:OE2	1:E:265:PRO:HG3	2.17	0.45
1:F:211:PHE:CE1	2:F:301:MPD:H11	2.52	0.45
1:A:43:PRO:HG2	3:A:494:HOH:O	2.15	0.45
1:E:30:PHE:CD1	2:E:301:MPD:H11	2.51	0.45
1:F:37:LEU:HD12	1:F:38:SER:N	2.32	0.45
1:F:87:LEU:HB2	1:F:94:PHE:HZ	1.82	0.45
1:A:102:ASN:HB3	1:A:103:PRO:HD2	1.99	0.45
1:B:171:LYS:O	1:B:175:GLN:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:N	1:B:187:LEU:HD23	2.32	0.44
1:E:100:SER:HB2	1:F:100:SER:HB3	1.99	0.44
1:A:104:VAL:HG23	1:A:132:PRO:HG3	1.98	0.44
1:A:227:GLY:HA2	3:A:513:HOH:O	2.16	0.44
1:A:269:ASN:O	1:A:273:GLN:HG3	2.18	0.44
1:F:23:SER:HB3	1:F:223:GLY:HA3	1.98	0.44
1:A:74:GLY:HA2	1:A:159:GLY:HA3	2.00	0.44
1:E:59:ASP:HB3	1:E:98:THR:HB	1.98	0.44
1:A:236:GLN:O	1:A:239:ALA:HB3	2.17	0.44
1:E:27:LEU:HD12	3:E:424:HOH:O	2.18	0.44
1:B:44:THR:O	1:B:44:THR:HG23	2.18	0.44
1:B:234:GLY:O	1:B:238:GLN:HG3	2.18	0.44
1:D:178:MET:HG3	1:D:202:LEU:HD12	2.00	0.44
1:E:197:VAL:HG11	1:E:202:LEU:HD21	2.00	0.44
1:B:203:PHE:CG	1:B:242:PHE:CZ	3.06	0.44
1:B:265:PRO:HB2	2:B:5001:MPD:H53	2.00	0.44
1:E:275:ALA:O	1:E:279:LEU:HD13	2.18	0.44
1:C:62:TYR:HB3	1:C:70:PHE:CD1	2.53	0.44
1:D:277:LYS:HB2	3:D:473:HOH:O	2.17	0.44
1:E:73:THR:HG23	1:E:74:GLY:N	2.33	0.44
1:A:123:SER:O	1:A:126:GLN:HG2	2.18	0.43
1:B:96:ILE:HD12	1:B:128:SER:HB2	2.00	0.43
1:A:115:ASP:HB3	1:A:118:VAL:HB	1.99	0.43
1:D:65:MET:HG3	1:D:226:PRO:HG2	2.00	0.43
1:E:171:LYS:HG3	1:E:197:VAL:HA	1.99	0.43
1:B:16:GLU:HB2	1:B:62:TYR:CE1	2.54	0.43
1:F:53:ILE:HB	1:F:94:PHE:CD1	2.54	0.43
1:D:73:THR:HG23	1:D:74:GLY:N	2.34	0.43
1:C:107:GLU:HB3	1:C:109:TRP:CE2	2.54	0.43
1:D:73:THR:OG1	1:D:74:GLY:N	2.52	0.43
1:A:231:TRP:CZ3	1:A:233:PHE:HA	2.54	0.43
1:C:79:GLU:OE2	1:C:265:PRO:HG3	2.19	0.43
1:D:79:GLU:OE1	1:D:156:GLY:HA3	2.18	0.43
1:B:79:GLU:OE2	1:B:265:PRO:HG3	2.18	0.43
1:D:249:ILE:O	1:D:249:ILE:HG13	2.19	0.43
1:D:11:THR:HB	1:D:21:PHE:HB2	2.01	0.42
1:E:219:THR:N	1:E:220:PRO:CD	2.82	0.42
1:A:42:TYR:HA	1:A:43:PRO:HD2	1.85	0.42
1:A:256:ASP:O	1:A:257:ARG:HB2	2.18	0.42
1:B:6:ASN:HB3	1:B:9:HIS:NE2	2.34	0.42
1:C:6:ASN:HD22	1:C:6:ASN:HA	1.56	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:PHE:O	1:D:206:TYR:HB2	2.19	0.42
1:D:280:LEU:HA	1:D:283:VAL:HG22	2.01	0.42
1:C:50:ARG:HG3	1:C:148:ASP:OD1	2.19	0.42
1:E:35:SER:HB3	1:E:118:VAL:HG21	2.00	0.42
1:E:167:SER:HB3	1:E:170:VAL:HG23	2.02	0.42
1:A:108:TRP:CZ3	1:A:111:MET:CE	3.01	0.42
1:A:259:MET:C	1:A:260:LEU:HD12	2.44	0.42
1:D:71:PHE:CD1	1:D:73:THR:HB	2.54	0.42
1:A:82:LEU:HD23	1:A:269:ASN:HB2	2.02	0.42
1:E:7:ASP:OD2	1:E:9:HIS:HB2	2.19	0.42
1:E:139:ILE:HD11	1:E:169:GLU:O	2.20	0.42
1:F:215:MET:HE2	1:F:215:MET:HB3	1.90	0.42
1:A:52:LYS:HB3	1:A:93:SER:HB2	2.02	0.42
1:C:197:VAL:HG11	1:C:202:LEU:HD23	2.02	0.42
1:D:265:PRO:HG2	2:D:301:MPD:O4	2.19	0.42
1:F:79:GLU:OE1	1:F:156:GLY:HA3	2.20	0.42
1:D:157:GLY:C	1:D:159:GLY:N	2.76	0.42
1:E:75:ASN:HD22	1:E:75:ASN:HA	1.74	0.42
1:F:42:TYR:OH	1:F:86:HIS:HD2	2.01	0.42
1:F:51:TRP:HA	1:F:51:TRP:CE3	2.55	0.42
1:A:260:LEU:N	1:A:260:LEU:CD1	2.83	0.41
1:C:25:TYR:O	1:C:28:SER:HB3	2.20	0.41
1:E:214:GLU:CD	1:E:214:GLU:H	2.27	0.41
1:D:123:SER:O	1:D:124:LYS:C	2.63	0.41
1:E:73:THR:OG1	1:E:74:GLY:N	2.50	0.41
1:F:37:LEU:HD12	1:F:38:SER:H	1.85	0.41
1:B:22:PRO:HG2	1:B:109:TRP:CZ3	2.54	0.41
1:B:179:LYS:HG3	1:B:180:GLN:NE2	2.35	0.41
1:D:269:ASN:HB3	3:D:416:HOH:O	2.21	0.41
1:E:19:ALA:HA	1:E:70:PHE:O	2.21	0.41
1:E:187:LEU:HB3	1:E:271:LEU:HD22	2.02	0.41
1:E:263:ASP:OD1	1:E:264:SER:N	2.53	0.41
1:C:140:GLU:HA	1:F:139:ILE:O	2.21	0.41
1:C:123:SER:O	1:C:126:GLN:HG2	2.20	0.41
1:E:42:TYR:OH	1:E:86:HIS:HD2	2.03	0.41
1:E:234:GLY:O	1:E:244:LEU:HD11	2.21	0.41
1:F:59:ASP:HB3	1:F:98:THR:HB	2.02	0.41
1:F:136:SER:O	1:F:139:ILE:HG12	2.21	0.41
1:B:236:GLN:O	1:B:239:ALA:HB3	2.21	0.41
1:C:143:LEU:HB2	1:F:140:GLU:HB3	2.03	0.41
1:F:53:ILE:HD12	1:F:94:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HG12	1:A:150:ILE:O	2.21	0.41
1:F:33:SER:OG	1:F:114:GLU:HB2	2.20	0.41
1:F:43:PRO:C	1:F:45:PRO:HD3	2.45	0.41
1:B:59:ASP:HB3	1:B:98:THR:HB	2.03	0.41
1:B:252:GLN:HE21	1:B:252:GLN:HB2	1.76	0.41
1:C:102:ASN:HB3	1:D:60:GLU:OE1	2.21	0.41
1:C:193:ALA:C	1:C:195:LEU:N	2.79	0.41
1:C:12:PRO:HG3	1:C:20:PHE:HE1	1.85	0.41
1:C:200:ASP:O	1:C:202:LEU:N	2.45	0.41
1:A:207:LYS:HB3	1:A:245:LEU:HD11	2.03	0.40
1:E:82:LEU:HB2	1:E:83:PRO:HD3	2.03	0.40
1:B:200:ASP:C	1:B:202:LEU:H	2.29	0.40
1:F:168:GLN:HE22	1:F:171:LYS:HD3	1.86	0.40
2:B:5001:MPD:O4	2:B:5001:MPD:C1	2.69	0.40
1:F:181:ASN:ND2	1:F:258:LYS:NZ	2.70	0.40
1:B:73:THR:HG23	1:B:74:GLY:N	2.36	0.40
1:C:40:ALA:HA	1:C:86:HIS:CD2	2.56	0.40
1:D:219:THR:N	1:D:220:PRO:CD	2.84	0.40
1:E:202:LEU:N	1:E:202:LEU:HD23	2.35	0.40
1:F:42:TYR:HA	1:F:43:PRO:HD2	1.95	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	279/286 (98%)	267 (96%)	12 (4%)	0	100	100
1	B	279/286 (98%)	262 (94%)	17 (6%)	0	100	100
1	C	279/286 (98%)	262 (94%)	15 (5%)	2 (1%)	18	34
1	D	279/286 (98%)	262 (94%)	17 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	279/286 (98%)	264 (95%)	15 (5%)	0	100	100
1	F	279/286 (98%)	259 (93%)	19 (7%)	1 (0%)	30	49
All	All	1674/1716 (98%)	1576 (94%)	95 (6%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	250	SER
1	C	201	PRO
1	F	283	VAL

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	226/233 (97%)	222 (98%)	4 (2%)	51	77
1	B	226/233 (97%)	223 (99%)	3 (1%)	61	82
1	C	226/233 (97%)	220 (97%)	6 (3%)	39	67
1	D	226/233 (97%)	223 (99%)	3 (1%)	61	82
1	E	226/233 (97%)	222 (98%)	4 (2%)	51	77
1	F	226/233 (97%)	221 (98%)	5 (2%)	45	73
All	All	1356/1398 (97%)	1331 (98%)	25 (2%)	51	77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	82	LEU
1	A	146	ASP
1	A	238	GLN
1	B	16	GLU
1	B	169	GLU
1	B	252	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	6	ASN
1	C	117	GLU
1	C	146	ASP
1	C	195	LEU
1	C	252	GLN
1	C	277	LYS
1	D	44	THR
1	D	114	GLU
1	D	209	VAL
1	E	75	ASN
1	E	145	GLU
1	E	179	LYS
1	E	277	LYS
1	F	17	ASP
1	F	44	THR
1	F	82	LEU
1	F	247	THR
1	F	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	86	HIS
1	A	116	GLN
1	A	181	ASN
1	A	236	GLN
1	A	255	GLN
1	B	18	ASN
1	B	29	GLN
1	B	76	HIS
1	B	86	HIS
1	B	102	ASN
1	B	126	GLN
1	B	131	GLN
1	B	180	GLN
1	B	236	GLN
1	B	252	GLN
1	B	273	GLN
1	C	6	ASN
1	C	9	HIS
1	C	29	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	86	HIS
1	C	273	GLN
1	D	41	HIS
1	D	76	HIS
1	D	86	HIS
1	D	102	ASN
1	D	131	GLN
1	D	168	GLN
1	D	255	GLN
1	E	18	ASN
1	E	47	GLN
1	E	76	HIS
1	E	86	HIS
1	E	126	GLN
1	F	9	HIS
1	F	18	ASN
1	F	76	HIS
1	F	86	HIS
1	F	168	GLN
1	F	181	ASN
1	F	189	HIS
1	F	273	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	F	301	-	7,7,7	0.74	0	9,10,10	0.38	0
2	MPD	D	301	-	7,7,7	0.44	0	9,10,10	0.26	0
2	MPD	B	5002	-	7,7,7	0.52	0	9,10,10	0.70	0
2	MPD	A	301	-	7,7,7	0.51	0	9,10,10	0.44	0
2	MPD	B	5001	-	7,7,7	1.31	1 (14%)	9,10,10	5.78	7 (77%)
2	MPD	E	301	-	7,7,7	0.51	0	9,10,10	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	F	301	-	-	0/5/5/5	-
2	MPD	D	301	-	-	0/5/5/5	-
2	MPD	B	5002	-	-	0/5/5/5	-
2	MPD	A	301	-	-	0/5/5/5	-
2	MPD	B	5001	-	-	1/5/5/5	-
2	MPD	E	301	-	-	0/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	MPD	CM-C2	-2.30	1.45	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5001	MPD	O2-C2-C3	-10.85	68.69	109.27
2	B	5001	MPD	O2-C2-CM	-9.48	78.45	107.99
2	B	5001	MPD	CM-C2-C3	7.93	144.39	110.20
2	B	5001	MPD	C1-C2-C3	-3.67	94.35	110.20
2	B	5001	MPD	CM-C2-C1	-2.38	105.30	110.63
2	B	5001	MPD	O4-C4-C3	2.31	120.54	111.35
2	B	5001	MPD	O2-C2-C1	-2.24	101.02	107.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5001	MPD	O2-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	MPD	6	0
2	D	301	MPD	4	0
2	B	5002	MPD	1	0
2	A	301	MPD	3	0
2	B	5001	MPD	2	0
2	E	301	MPD	4	0

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	281/286 (98%)	3.23	207 (73%) 0 0	22, 32, 48, 66	0
1	B	281/286 (98%)	3.29	198 (70%) 0 0	19, 31, 48, 84	0
1	C	281/286 (98%)	3.47	204 (72%) 0 0	22, 35, 51, 85	0
1	D	281/286 (98%)	3.29	189 (67%) 0 0	20, 33, 53, 95	0
1	E	281/286 (98%)	2.99	192 (68%) 0 0	26, 40, 58, 84	0
1	F	281/286 (98%)	3.54	204 (72%) 0 0	25, 37, 58, 79	0
All	All	1686/1716 (98%)	3.30	1194 (70%) 0 0	19, 35, 55, 95	0

All (1194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	PHE	37.4
1	F	147	SER	20.6
1	C	191	PRO	17.3
1	C	15	ALA	17.0
1	A	174	LEU	16.1
1	F	74	GLY	14.9
1	D	222	ILE	14.7
1	A	189	HIS	14.7
1	C	184	ILE	14.6
1	C	104	VAL	14.5
1	F	224	TYR	14.1
1	B	97	ALA	13.9
1	D	81	LEU	13.9
1	B	49	GLY	13.6
1	B	210	ALA	13.2
1	E	40	ALA	12.8
1	C	193	ALA	11.7
1	F	94	PHE	11.7
1	D	98	THR	11.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	283	VAL	11.4
1	F	75	ASN	11.3
1	B	67	ASN	11.3
1	E	106	PHE	11.1
1	F	159	GLY	11.1
1	B	197	VAL	11.1
1	D	211	PHE	10.9
1	B	270	ALA	10.7
1	F	107	GLU	10.7
1	F	93	SER	10.6
1	B	65	MET	10.5
1	E	114	GLU	10.5
1	C	143	LEU	10.4
1	B	28	SER	10.3
1	D	99	LEU	10.2
1	B	30	PHE	10.1
1	F	40	ALA	10.1
1	F	73	THR	10.1
1	D	147	SER	10.1
1	D	5	MET	10.0
1	D	107	GLU	9.8
1	D	217	ALA	9.8
1	E	184	ILE	9.5
1	B	66	ASP	9.4
1	B	212	PRO	9.4
1	C	275	ALA	9.2
1	C	37	LEU	9.1
1	D	262	GLY	9.1
1	D	70	PHE	9.1
1	D	130	ARG	9.1
1	C	231	TRP	9.0
1	F	152	VAL	9.0
1	C	106	PHE	8.9
1	A	147	SER	8.9
1	A	233	PHE	8.9
1	C	192	ALA	8.8
1	B	266	LEU	8.6
1	C	255	GLN	8.6
1	F	133	LEU	8.6
1	E	44	THR	8.6
1	D	194	PHE	8.6
1	A	176	TRP	8.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	68	GLY	8.4
1	B	81	LEU	8.4
1	F	37	LEU	8.3
1	A	149	TYR	8.3
1	F	148	ASP	8.3
1	D	78	VAL	8.3
1	B	224	TYR	8.2
1	D	193	ALA	8.2
1	F	242	PHE	8.2
1	D	77	PRO	8.2
1	C	197	VAL	8.2
1	C	280	LEU	8.1
1	C	88	ASP	8.1
1	F	219	THR	8.1
1	D	135	LEU	8.0
1	E	55	VAL	8.0
1	F	170	VAL	7.9
1	D	151	GLY	7.9
1	F	88	ASP	7.8
1	E	75	ASN	7.7
1	C	185	ILE	7.7
1	F	265	PRO	7.7
1	A	26	SER	7.7
1	D	166	ASP	7.6
1	B	72	SER	7.6
1	D	42	TYR	7.6
1	F	63	LEU	7.6
1	D	69	THR	7.6
1	D	191	PRO	7.4
1	F	253	VAL	7.3
1	E	136	SER	7.3
1	B	57	GLY	7.3
1	B	231	TRP	7.2
1	E	16	GLU	7.2
1	A	86	HIS	7.1
1	A	274	LEU	7.1
1	E	212	PRO	7.1
1	F	132	PRO	7.1
1	A	102	ASN	7.0
1	D	40	ALA	7.0
1	C	63	LEU	7.0
1	F	35	SER	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	149	TYR	6.9
1	B	86	HIS	6.9
1	C	181	ASN	6.9
1	B	27	LEU	6.9
1	D	96	ILE	6.9
1	C	70	PHE	6.9
1	E	91	GLY	6.9
1	F	183	PHE	6.8
1	F	19	ALA	6.8
1	F	197	VAL	6.8
1	F	49	GLY	6.7
1	A	183	PHE	6.7
1	B	185	ILE	6.6
1	C	174	LEU	6.6
1	B	61	ARG	6.6
1	A	38	SER	6.6
1	A	29	GLN	6.6
1	E	240	ILE	6.5
1	B	216	ASP	6.5
1	E	132	PRO	6.5
1	D	276	ALA	6.5
1	B	42	TYR	6.5
1	C	252	GLN	6.5
1	C	121	LEU	6.4
1	F	283	VAL	6.4
1	A	262	GLY	6.4
1	B	95	ASP	6.4
1	C	138	VAL	6.4
1	B	166	ASP	6.4
1	D	90	ALA	6.4
1	A	199	ASP	6.4
1	B	152	VAL	6.4
1	A	272	GLY	6.3
1	F	174	LEU	6.3
1	B	106	PHE	6.3
1	C	194	PHE	6.3
1	C	195	LEU	6.3
1	C	129	PHE	6.3
1	D	35	SER	6.3
1	F	199	ASP	6.3
1	B	96	ILE	6.2
1	C	87	LEU	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	229	LEU	6.2
1	D	229	LEU	6.2
1	D	30	PHE	6.2
1	E	245	LEU	6.1
1	A	187	LEU	6.1
1	E	265	PRO	6.1
1	A	227	GLY	6.1
1	F	48	GLY	6.1
1	B	176	TRP	6.1
1	A	270	ALA	6.1
1	F	66	ASP	6.1
1	C	124	LYS	6.0
1	F	227	GLY	6.0
1	E	244	LEU	6.0
1	F	143	LEU	6.0
1	A	65	MET	6.0
1	D	259	MET	6.0
1	B	56	VAL	6.0
1	E	151	GLY	5.9
1	D	176	TRP	5.9
1	E	69	THR	5.9
1	A	97	ALA	5.9
1	C	224	TYR	5.8
1	A	127	SER	5.8
1	A	170	VAL	5.8
1	C	204	ALA	5.8
1	D	143	LEU	5.8
1	F	160	ALA	5.8
1	D	282	GLU	5.8
1	C	136	SER	5.8
1	F	84	MET	5.8
1	B	183	PHE	5.8
1	D	94	PHE	5.8
1	C	9	HIS	5.7
1	F	85	TYR	5.7
1	C	5	MET	5.7
1	F	14	PRO	5.7
1	C	249	ILE	5.7
1	C	212	PRO	5.7
1	F	46	TYR	5.7
1	F	82	LEU	5.7
1	F	146	ASP	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	159	GLY	5.7
1	E	227	GLY	5.7
1	D	197	VAL	5.7
1	C	41	HIS	5.6
1	A	30	PHE	5.6
1	B	227	GLY	5.6
1	B	132	PRO	5.6
1	D	138	VAL	5.6
1	D	246	ASN	5.6
1	A	200	ASP	5.5
1	B	32	ALA	5.5
1	C	268	GLY	5.5
1	C	56	VAL	5.5
1	A	217	ALA	5.5
1	C	71	PHE	5.5
1	C	6	ASN	5.5
1	D	226	PRO	5.5
1	E	237	LEU	5.5
1	B	58	ALA	5.5
1	D	124	LYS	5.5
1	D	269	ASN	5.5
1	B	252	GLN	5.4
1	E	238	GLN	5.4
1	D	260	LEU	5.4
1	E	196	ALA	5.3
1	A	136	SER	5.3
1	B	177	ALA	5.3
1	F	141	THR	5.3
1	B	194	PHE	5.3
1	B	233	PHE	5.3
1	D	125	TYR	5.3
1	D	261	THR	5.3
1	B	278	ALA	5.3
1	B	198	GLY	5.2
1	A	206	TYR	5.2
1	B	77	PRO	5.2
1	F	223	GLY	5.2
1	F	81	LEU	5.2
1	D	129	PHE	5.2
1	B	205	GLY	5.2
1	E	268	GLY	5.2
1	F	209	VAL	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	163	GLY	5.1
1	E	174	LEU	5.1
1	C	245	LEU	5.1
1	E	82	LEU	5.1
1	D	255	GLN	5.1
1	C	223	GLY	5.1
1	B	202	LEU	5.1
1	A	171	LYS	5.1
1	D	128	SER	5.1
1	F	78	VAL	5.1
1	C	10	PRO	5.1
1	A	284	GLU	5.0
1	E	6	ASN	5.0
1	B	108	TRP	5.0
1	B	155	PRO	5.0
1	D	245	LEU	5.0
1	C	19	ALA	5.0
1	B	219	THR	5.0
1	E	33	SER	5.0
1	D	6	ASN	5.0
1	F	134	LYS	5.0
1	A	280	LEU	5.0
1	B	249	ILE	5.0
1	A	115	ASP	5.0
1	C	109	TRP	5.0
1	E	121	LEU	5.0
1	F	39	GLY	5.0
1	C	40	ALA	5.0
1	D	46	TYR	5.0
1	D	146	ASP	5.0
1	E	42	TYR	5.0
1	D	219	THR	4.9
1	C	153	PHE	4.9
1	F	21	PHE	4.9
1	F	135	LEU	4.9
1	A	180	GLN	4.9
1	F	90	ALA	4.9
1	D	280	LEU	4.9
1	E	183	PHE	4.9
1	E	119	ASN	4.9
1	C	49	GLY	4.9
1	D	250	SER	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	58	ALA	4.8
1	E	11	THR	4.8
1	E	54	LEU	4.8
1	B	276	ALA	4.8
1	A	254	PHE	4.8
1	C	32	ALA	4.8
1	F	210	ALA	4.8
1	D	103	PRO	4.8
1	D	220	PRO	4.8
1	C	182	LYS	4.8
1	D	149	TYR	4.8
1	B	75	ASN	4.8
1	E	262	GLY	4.8
1	B	129	PHE	4.8
1	F	233	PHE	4.8
1	E	135	LEU	4.7
1	E	56	VAL	4.7
1	C	208	ILE	4.7
1	A	112	PRO	4.7
1	E	105	LYS	4.7
1	B	135	LEU	4.7
1	B	237	LEU	4.7
1	F	20	PHE	4.7
1	F	92	PHE	4.7
1	F	186	SER	4.7
1	F	68	GLY	4.7
1	F	208	ILE	4.7
1	C	206	TYR	4.7
1	F	259	MET	4.7
1	E	228	HIS	4.7
1	C	233	PHE	4.7
1	E	209	VAL	4.7
1	F	149	TYR	4.7
1	C	103	PRO	4.7
1	F	10	PRO	4.7
1	E	41	HIS	4.6
1	B	285	GLN	4.6
1	B	169	GLU	4.6
1	A	226	PRO	4.6
1	F	91	GLY	4.6
1	A	28	SER	4.6
1	C	107	GLU	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	136	SER	4.6
1	A	106	PHE	4.6
1	F	248	GLY	4.6
1	E	231	TRP	4.6
1	B	31	THR	4.6
1	A	173	VAL	4.5
1	C	282	GLU	4.5
1	E	128	SER	4.5
1	B	267	ALA	4.5
1	F	116	GLN	4.5
1	C	105	LYS	4.5
1	C	60	GLU	4.5
1	B	139	ILE	4.5
1	F	184	ILE	4.5
1	E	43	PRO	4.5
1	C	102	ASN	4.5
1	E	37	LEU	4.5
1	E	99	LEU	4.5
1	F	113	ARG	4.5
1	F	108	TRP	4.5
1	C	242	PHE	4.5
1	F	45	PRO	4.5
1	C	232	LYS	4.5
1	E	255	GLN	4.5
1	E	24	ALA	4.5
1	F	65	MET	4.5
1	A	17	ASP	4.5
1	D	88	ASP	4.5
1	F	237	LEU	4.5
1	B	186	SER	4.5
1	B	274	LEU	4.5
1	B	104	VAL	4.4
1	B	211	PHE	4.4
1	C	260	LEU	4.4
1	C	137	ASP	4.4
1	B	103	PRO	4.4
1	B	71	PHE	4.4
1	E	92	PHE	4.4
1	F	67	ASN	4.4
1	A	141	THR	4.4
1	A	96	ILE	4.4
1	E	30	PHE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	217	ALA	4.4
1	A	213	ASP	4.4
1	F	226	PRO	4.4
1	D	199	ASP	4.4
1	C	247	THR	4.3
1	C	259	MET	4.3
1	B	40	ALA	4.3
1	C	117	GLU	4.3
1	F	117	GLU	4.3
1	A	158	HIS	4.3
1	B	10	PRO	4.3
1	A	119	ASN	4.3
1	D	97	ALA	4.3
1	A	222	ILE	4.3
1	D	284	GLU	4.3
1	E	192	ALA	4.3
1	F	177	ALA	4.3
1	F	112	PRO	4.3
1	E	215	MET	4.3
1	E	140	GLU	4.3
1	B	122	TYR	4.3
1	D	186	SER	4.3
1	E	264	SER	4.3
1	A	185	ILE	4.2
1	E	96	ILE	4.2
1	D	192	ALA	4.2
1	F	142	ALA	4.2
1	B	148	ASP	4.2
1	D	216	ASP	4.2
1	F	215	MET	4.2
1	A	251	GLY	4.2
1	D	248	GLY	4.2
1	F	101	GLY	4.2
1	C	240	ILE	4.2
1	C	214	GLU	4.2
1	C	267	ALA	4.2
1	C	270	ALA	4.2
1	A	225	MET	4.2
1	E	178	MET	4.2
1	B	226	PRO	4.2
1	A	166	ASP	4.2
1	D	159	GLY	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	4.2
1	E	90	ALA	4.2
1	E	172	ALA	4.2
1	B	15	ALA	4.1
1	E	165	PRO	4.1
1	E	20	PHE	4.1
1	E	194	PHE	4.1
1	F	51	TRP	4.1
1	F	201	PRO	4.1
1	A	85	TYR	4.1
1	C	122	TYR	4.1
1	A	184	ILE	4.1
1	D	184	ILE	4.1
1	E	81	LEU	4.1
1	F	280	LEU	4.1
1	E	88	ASP	4.1
1	D	150	ILE	4.1
1	B	121	LEU	4.1
1	B	242	PHE	4.1
1	C	279	LEU	4.0
1	C	173	VAL	4.0
1	A	218	GLN	4.0
1	C	218	GLN	4.0
1	B	239	ALA	4.0
1	C	90	ALA	4.0
1	A	108	TRP	4.0
1	D	39	GLY	4.0
1	D	66	ASP	4.0
1	B	153	PHE	4.0
1	D	275	ALA	4.0
1	F	270	ALA	4.0
1	A	67	ASN	4.0
1	A	268	GLY	4.0
1	A	164	LEU	4.0
1	A	212	PRO	4.0
1	D	15	ALA	4.0
1	E	188	CYS	4.0
1	E	213	ASP	4.0
1	D	87	LEU	4.0
1	F	44	THR	4.0
1	B	62	TYR	4.0
1	F	104	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	74	GLY	3.9
1	C	190	GLY	3.9
1	B	164	LEU	3.9
1	D	82	LEU	3.9
1	A	98	THR	3.9
1	A	219	THR	3.9
1	F	79	GLU	3.9
1	A	24	ALA	3.9
1	F	172	ALA	3.9
1	C	18	ASN	3.9
1	F	188	CYS	3.9
1	B	51	TRP	3.9
1	B	170	VAL	3.9
1	D	196	ALA	3.9
1	F	225	MET	3.9
1	A	241	GLY	3.9
1	D	268	GLY	3.9
1	B	17	ASP	3.9
1	A	188	CYS	3.9
1	A	197	VAL	3.9
1	D	14	PRO	3.9
1	E	10	PRO	3.9
1	D	108	TRP	3.9
1	B	206	TYR	3.9
1	C	85	TYR	3.9
1	C	276	ALA	3.9
1	B	261	THR	3.9
1	C	225	MET	3.8
1	C	7	ASP	3.8
1	C	148	ASP	3.8
1	A	105	LYS	3.8
1	C	157	GLY	3.8
1	C	26	SER	3.8
1	C	80	THR	3.8
1	C	170	VAL	3.8
1	D	20	PHE	3.8
1	A	269	ASN	3.8
1	D	190	GLY	3.8
1	C	274	LEU	3.8
1	F	36	ASP	3.8
1	F	123	SER	3.8
1	A	283	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	215	MET	3.8
1	F	194	PHE	3.8
1	A	39	GLY	3.8
1	D	279	LEU	3.8
1	F	7	ASP	3.8
1	F	12	PRO	3.8
1	C	31	THR	3.7
1	E	152	VAL	3.7
1	B	208	ILE	3.7
1	F	243	GLU	3.7
1	C	82	LEU	3.7
1	A	23	SER	3.7
1	E	127	SER	3.7
1	E	203	PHE	3.7
1	A	144	GLY	3.7
1	B	268	GLY	3.7
1	A	271	LEU	3.7
1	C	202	LEU	3.7
1	E	208	ILE	3.7
1	C	62	TYR	3.7
1	E	22	PRO	3.7
1	F	52	LYS	3.7
1	F	128	SER	3.7
1	F	32	ALA	3.7
1	C	21	PHE	3.7
1	C	244	LEU	3.7
1	E	185	ILE	3.7
1	F	118	VAL	3.7
1	C	227	GLY	3.7
1	E	57	GLY	3.7
1	B	269	ASN	3.7
1	C	55	VAL	3.6
1	C	72	SER	3.6
1	C	128	SER	3.6
1	F	214	GLU	3.6
1	A	153	PHE	3.6
1	E	45	PRO	3.6
1	A	216	ASP	3.6
1	A	109	TRP	3.6
1	C	11	THR	3.6
1	A	114	GLU	3.6
1	B	250	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	19	ALA	3.6
1	A	160	ALA	3.6
1	A	194	PHE	3.6
1	B	255	GLN	3.6
1	C	47	GLN	3.6
1	F	87	LEU	3.6
1	F	229	LEU	3.6
1	F	268	GLY	3.6
1	B	41	HIS	3.6
1	F	125	TYR	3.6
1	B	23	SER	3.6
1	D	127	SER	3.6
1	C	281	ALA	3.6
1	E	97	ALA	3.6
1	A	82	LEU	3.6
1	C	271	LEU	3.6
1	F	220	PRO	3.6
1	E	224	TYR	3.6
1	A	55	VAL	3.6
1	C	23	SER	3.6
1	C	28	SER	3.6
1	D	123	SER	3.6
1	A	168	GLN	3.6
1	A	177	ALA	3.6
1	A	242	PHE	3.6
1	C	115	ASP	3.6
1	F	158	HIS	3.5
1	C	152	VAL	3.5
1	E	149	TYR	3.5
1	A	72	SER	3.5
1	C	61	ARG	3.5
1	D	109	TRP	3.5
1	B	150	ILE	3.5
1	B	18	ASN	3.5
1	D	95	ASP	3.5
1	F	102	ASN	3.5
1	E	235	GLU	3.5
1	D	111	MET	3.5
1	D	113	ARG	3.5
1	A	229	LEU	3.5
1	D	19	ALA	3.5
1	E	195	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	198	GLY	3.5
1	D	240	ILE	3.5
1	A	129	PHE	3.5
1	C	119	ASN	3.5
1	E	61	ARG	3.5
1	A	25	TYR	3.5
1	A	135	LEU	3.5
1	A	195	LEU	3.5
1	F	99	LEU	3.5
1	A	275	ALA	3.5
1	C	36	ASP	3.5
1	D	188	CYS	3.5
1	C	24	ALA	3.5
1	E	15	ALA	3.5
1	E	129	PHE	3.5
1	C	216	ASP	3.4
1	F	285	GLN	3.4
1	E	31	THR	3.4
1	A	83	PRO	3.4
1	D	74	GLY	3.4
1	D	120	GLY	3.4
1	F	77	PRO	3.4
1	B	26	SER	3.4
1	E	267	ALA	3.4
1	D	254	PHE	3.4
1	E	9	HIS	3.4
1	A	231	TRP	3.4
1	B	178	MET	3.4
1	F	11	THR	3.4
1	A	43	PRO	3.4
1	C	226	PRO	3.4
1	D	45	PRO	3.4
1	B	223	GLY	3.4
1	B	251	GLY	3.4
1	C	39	GLY	3.4
1	A	172	ALA	3.4
1	E	53	ILE	3.4
1	F	150	ILE	3.4
1	E	76	HIS	3.4
1	F	50	ARG	3.4
1	D	115	ASP	3.4
1	F	202	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	157	GLY	3.4
1	A	142	ALA	3.4
1	F	26	SER	3.4
1	A	282	GLU	3.4
1	C	183	PHE	3.4
1	F	203	PHE	3.4
1	B	59	ASP	3.4
1	A	18	ASN	3.4
1	B	280	LEU	3.4
1	E	201	PRO	3.4
1	B	234	GLY	3.4
1	B	160	ALA	3.4
1	F	192	ALA	3.4
1	F	28	SER	3.4
1	D	65	MET	3.3
1	A	209	VAL	3.3
1	D	55	VAL	3.3
1	D	209	VAL	3.3
1	E	98	THR	3.3
1	E	141	THR	3.3
1	E	170	VAL	3.3
1	F	212	PRO	3.3
1	A	53	ILE	3.3
1	E	193	ALA	3.3
1	F	114	GLU	3.3
1	D	64	MET	3.3
1	F	167	SER	3.3
1	A	21	PHE	3.3
1	F	42	TYR	3.3
1	D	63	LEU	3.3
1	E	51	TRP	3.3
1	E	202	LEU	3.3
1	B	241	GLY	3.3
1	D	228	HIS	3.3
1	B	154	ILE	3.3
1	A	167	SER	3.3
1	B	38	SER	3.3
1	A	258	LYS	3.3
1	B	254	PHE	3.3
1	E	71	PHE	3.3
1	A	130	ARG	3.3
1	F	191	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	8	LYS	3.3
1	E	100	SER	3.3
1	E	147	SER	3.3
1	F	23	SER	3.3
1	F	30	PHE	3.3
1	D	218	GLN	3.3
1	E	236	GLN	3.3
1	B	188	CYS	3.3
1	E	67	ASN	3.3
1	A	27	LEU	3.3
1	A	266	LEU	3.3
1	C	81	LEU	3.3
1	E	79	GLU	3.3
1	A	73	THR	3.3
1	C	91	GLY	3.3
1	C	262	GLY	3.3
1	C	176	TRP	3.3
1	F	185	ILE	3.3
1	B	207	LYS	3.3
1	A	285	GLN	3.2
1	F	106	PHE	3.2
1	A	263	ASP	3.2
1	C	200	ASP	3.2
1	D	121	LEU	3.2
1	A	74	GLY	3.2
1	B	215	MET	3.2
1	A	264	SER	3.2
1	C	123	SER	3.2
1	E	130	ARG	3.2
1	C	42	TYR	3.2
1	D	224	TYR	3.2
1	F	25	TYR	3.2
1	E	158	HIS	3.2
1	F	16	GLU	3.2
1	B	34	LYS	3.2
1	B	209	VAL	3.2
1	E	104	VAL	3.2
1	D	160	ALA	3.2
1	C	95	ASP	3.2
1	C	67	ASN	3.2
1	C	16	GLU	3.2
1	E	133	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	258	LYS	3.2
1	A	71	PHE	3.2
1	F	115	ASP	3.2
1	B	14	PRO	3.2
1	B	191	PRO	3.2
1	C	140	GLU	3.2
1	E	164	LEU	3.2
1	F	140	GLU	3.2
1	E	85	TYR	3.2
1	F	198	GLY	3.2
1	B	240	ILE	3.2
1	C	219	THR	3.2
1	D	53	ILE	3.2
1	B	92	PHE	3.1
1	B	179	LYS	3.1
1	C	13	ASP	3.1
1	F	105	LYS	3.1
1	B	201	PRO	3.1
1	F	161	LEU	3.1
1	F	244	LEU	3.1
1	C	269	ASN	3.1
1	A	48	GLY	3.1
1	B	25	TYR	3.1
1	E	144	GLY	3.1
1	E	251	GLY	3.1
1	A	154	ILE	3.1
1	F	98	THR	3.1
1	B	90	ALA	3.1
1	E	89	LYS	3.1
1	A	132	PRO	3.1
1	B	221	SER	3.1
1	E	250	SER	3.1
1	F	129	PHE	3.1
1	D	22	PRO	3.1
1	F	43	PRO	3.1
1	B	271	LEU	3.1
1	E	63	LEU	3.1
1	F	260	LEU	3.1
1	B	78	VAL	3.1
1	C	283	VAL	3.1
1	E	120	GLY	3.1
1	A	31	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	139	ILE	3.1
1	A	182	LYS	3.1
1	A	243	GLU	3.1
1	A	70	PHE	3.1
1	A	63	LEU	3.1
1	A	88	ASP	3.1
1	D	106	PHE	3.1
1	E	186	SER	3.1
1	E	271	LEU	3.1
1	B	39	GLY	3.1
1	A	122	TYR	3.1
1	A	196	ALA	3.1
1	F	281	ALA	3.1
1	E	86	HIS	3.1
1	D	165	PRO	3.1
1	B	55	VAL	3.1
1	D	230	THR	3.0
1	A	46	TYR	3.0
1	D	267	ALA	3.0
1	A	87	LEU	3.0
1	E	254	PHE	3.0
1	E	28	SER	3.0
1	E	78	VAL	3.0
1	C	97	ALA	3.0
1	D	85	TYR	3.0
1	B	256	ASP	3.0
1	D	263	ASP	3.0
1	E	146	ASP	3.0
1	B	144	GLY	3.0
1	B	272	GLY	3.0
1	B	53	ILE	3.0
1	A	204	ALA	3.0
1	F	41	HIS	3.0
1	A	99	LEU	3.0
1	E	115	ASP	3.0
1	B	93	SER	3.0
1	D	26	SER	3.0
1	F	127	SER	3.0
1	F	181	ASN	3.0
1	C	120	GLY	3.0
1	E	205	GLY	3.0
1	A	152	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	64	MET	3.0
1	F	178	MET	3.0
1	C	160	ALA	3.0
1	D	76	HIS	3.0
1	E	206	TYR	3.0
1	A	7	ASP	3.0
1	A	13	ASP	3.0
1	E	52	LYS	3.0
1	A	221	SER	3.0
1	C	186	SER	3.0
1	D	136	SER	3.0
1	A	138	VAL	2.9
1	B	24	ALA	2.9
1	C	58	ALA	2.9
1	E	32	ALA	2.9
1	F	228	HIS	2.9
1	B	112	PRO	2.9
1	E	113	ARG	2.9
1	E	25	TYR	2.9
1	D	71	PHE	2.9
1	A	100	SER	2.9
1	E	197	VAL	2.9
1	A	80	THR	2.9
1	A	20	PHE	2.9
1	A	273	GLN	2.9
1	A	5	MET	2.9
1	A	181	ASN	2.9
1	C	111	MET	2.9
1	C	144	GLY	2.9
1	A	208	ILE	2.9
1	F	261	THR	2.9
1	A	179	LYS	2.9
1	D	37	LEU	2.9
1	F	54	LEU	2.9
1	D	51	TRP	2.9
1	F	17	ASP	2.9
1	C	180	GLN	2.9
1	D	264	SER	2.9
1	A	78	VAL	2.9
1	D	56	VAL	2.9
1	D	118	VAL	2.9
1	A	81	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	266	LEU	2.9
1	B	46	TYR	2.9
1	D	225	MET	2.9
1	E	125	TYR	2.9
1	F	162	MET	2.9
1	B	140	GLU	2.9
1	B	222	ILE	2.8
1	F	110	ALA	2.8
1	F	121	LEU	2.8
1	F	62	TYR	2.8
1	A	49	GLY	2.8
1	A	101	GLY	2.8
1	A	139	ILE	2.8
1	F	240	ILE	2.8
1	E	220	PRO	2.8
1	A	259	MET	2.8
1	B	182	LYS	2.8
1	F	9	HIS	2.8
1	A	118	VAL	2.8
1	B	281	ALA	2.8
1	D	133	LEU	2.8
1	D	266	LEU	2.8
1	A	47	GLN	2.8
1	E	153	PHE	2.8
1	D	43	PRO	2.8
1	E	112	PRO	2.8
1	A	161	LEU	2.8
1	B	80	THR	2.8
1	B	275	ALA	2.8
1	C	172	ALA	2.8
1	C	237	LEU	2.8
1	D	187	LEU	2.8
1	E	266	LEU	2.8
1	B	145	GLU	2.8
1	F	126	GLN	2.8
1	D	7	ASP	2.8
1	E	21	PHE	2.8
1	E	211	PHE	2.8
1	E	248	GLY	2.7
1	E	246	ASN	2.7
1	D	167	SER	2.7
1	B	253	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	204	ALA	2.7
1	E	278	ALA	2.7
1	C	65	MET	2.7
1	A	134	LYS	2.7
1	E	134	LYS	2.7
1	F	258	LYS	2.7
1	A	113	ARG	2.7
1	D	50	ARG	2.7
1	B	20	PHE	2.7
1	B	156	GLY	2.7
1	B	102	ASN	2.7
1	C	155	PRO	2.7
1	B	127	SER	2.7
1	A	143	LEU	2.7
1	D	195	LEU	2.7
1	A	15	ALA	2.7
1	A	69	THR	2.7
1	D	8	LYS	2.7
1	A	145	GLU	2.7
1	F	252	GLN	2.7
1	E	189	HIS	2.7
1	C	188	CYS	2.7
1	F	13	ASP	2.7
1	B	265	PRO	2.7
1	D	67	ASN	2.7
1	B	37	LEU	2.7
1	E	87	LEU	2.7
1	F	171	LYS	2.7
1	B	84	MET	2.7
1	F	196	ALA	2.7
1	C	169	GLU	2.7
1	F	284	GLU	2.7
1	A	238	GLN	2.7
1	D	213	ASP	2.7
1	D	57	GLY	2.7
1	F	151	GLY	2.7
1	A	207	LYS	2.7
1	A	237	LEU	2.7
1	C	221	SER	2.7
1	F	61	ARG	2.7
1	A	32	ALA	2.7
1	A	169	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	109	TRP	2.7
1	B	114	GLU	2.7
1	C	108	TRP	2.7
1	A	36	ASP	2.6
1	C	203	PHE	2.6
1	D	171	LYS	2.6
1	D	203	PHE	2.6
1	D	257	ARG	2.6
1	B	133	LEU	2.6
1	D	60	GLU	2.6
1	F	282	GLU	2.6
1	A	40	ALA	2.6
1	A	131	GLN	2.6
1	E	73	THR	2.6
1	F	80	THR	2.6
1	C	22	PRO	2.6
1	B	260	LEU	2.6
1	C	161	LEU	2.6
1	E	161	LEU	2.6
1	E	260	LEU	2.6
1	B	284	GLU	2.6
1	D	238	GLN	2.6
1	E	180	GLN	2.6
1	F	122	TYR	2.6
1	F	176	TRP	2.6
1	A	95	ASP	2.6
1	B	190	GLY	2.6
1	D	101	GLY	2.6
1	E	263	ASP	2.6
1	A	265	PRO	2.6
1	F	155	PRO	2.6
1	B	184	ILE	2.6
1	D	249	ILE	2.6
1	D	183	PHE	2.6
1	B	229	LEU	2.6
1	F	47	GLN	2.6
1	A	239	ALA	2.6
1	A	281	ALA	2.6
1	C	34	LYS	2.6
1	C	179	LYS	2.6
1	B	13	ASP	2.6
1	B	22	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	211	PHE	2.6
1	A	236	GLN	2.6
1	A	123	SER	2.6
1	A	267	ALA	2.6
1	E	123	SER	2.6
1	C	141	THR	2.6
1	D	34	LYS	2.6
1	E	34	LYS	2.6
1	C	201	PRO	2.5
1	C	234	GLY	2.5
1	F	144	GLY	2.5
1	A	150	ILE	2.5
1	F	96	ILE	2.5
1	F	245	LEU	2.5
1	D	9	HIS	2.5
1	B	204	ALA	2.5
1	F	264	SER	2.5
1	B	113	ARG	2.5
1	C	130	ARG	2.5
1	E	272	GLY	2.5
1	A	107	GLU	2.5
1	A	54	LEU	2.5
1	B	82	LEU	2.5
1	C	92	PHE	2.5
1	D	233	PHE	2.5
1	B	126	GLN	2.5
1	C	238	GLN	2.5
1	E	38	SER	2.5
1	B	262	GLY	2.5
1	D	154	ILE	2.5
1	E	176	TRP	2.5
1	F	211	PHE	2.5
1	C	8	LYS	2.5
1	B	9	HIS	2.5
1	C	158	HIS	2.5
1	A	110	ALA	2.5
1	A	193	ALA	2.5
1	B	192	ALA	2.5
1	B	64	MET	2.5
1	D	25	TYR	2.5
1	D	206	TYR	2.5
1	B	143	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	162	MET	2.5
1	B	111	MET	2.5
1	C	230	THR	2.5
1	A	205	GLY	2.4
1	B	159	GLY	2.4
1	B	163	GLY	2.4
1	B	235	GLU	2.4
1	D	205	GLY	2.4
1	E	46	TYR	2.4
1	C	29	GLN	2.4
1	B	94	PHE	2.4
1	D	92	PHE	2.4
1	B	193	ALA	2.4
1	C	84	MET	2.4
1	D	281	ALA	2.4
1	E	210	ALA	2.4
1	B	69	THR	2.4
1	A	77	PRO	2.4
1	D	144	GLY	2.4
1	A	37	LEU	2.4
1	C	135	LEU	2.4
1	D	244	LEU	2.4
1	E	279	LEU	2.4
1	F	164	LEU	2.4
1	F	218	GLN	2.4
1	F	279	LEU	2.4
1	E	233	PHE	2.4
1	D	18	ASN	2.4
1	D	173	VAL	2.4
1	E	108	TRP	2.4
1	B	162	MET	2.4
1	E	225	MET	2.4
1	C	177	ALA	2.4
1	D	142	ALA	2.4
1	E	270	ALA	2.4
1	E	275	ALA	2.4
1	D	12	PRO	2.4
1	D	157	GLY	2.4
1	E	95	ASP	2.4
1	D	161	LEU	2.4
1	F	274	LEU	2.4
1	C	25	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	2.4
1	E	118	VAL	2.4
1	C	51	TRP	2.4
1	D	110	ALA	2.4
1	C	44	THR	2.4
1	B	123	SER	2.4
1	C	66	ASP	2.4
1	C	166	ASP	2.4
1	A	42	TYR	2.4
1	C	253	VAL	2.4
1	A	246	ASN	2.4
1	F	119	ASN	2.4
1	E	58	ALA	2.4
1	E	281	ALA	2.4
1	B	141	THR	2.3
1	C	261	THR	2.3
1	D	80	THR	2.3
1	C	187	LEU	2.3
1	F	222	ILE	2.3
1	C	189	HIS	2.3
1	D	256	ASP	2.3
1	D	178	MET	2.3
1	D	62	TYR	2.3
1	A	6	ASN	2.3
1	F	6	ASN	2.3
1	A	103	PRO	2.3
1	C	83	PRO	2.3
1	F	57	GLY	2.3
1	C	116	GLN	2.3
1	E	218	GLN	2.3
1	B	187	LEU	2.3
1	B	279	LEU	2.3
1	F	195	LEU	2.3
1	B	115	ASP	2.3
1	A	92	PHE	2.3
1	A	79	GLU	2.3
1	A	155	PRO	2.3
1	B	217	ALA	2.3
1	E	177	ALA	2.3
1	B	230	THR	2.3
1	E	230	THR	2.3
1	D	215	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	242	PHE	2.3
1	B	214	GLU	2.3
1	A	125	TYR	2.3
1	F	138	VAL	2.3
1	C	69	THR	2.3
1	C	57	GLY	2.3
1	A	33	SER	2.3
1	A	41	HIS	2.3
1	A	120	GLY	2.3
1	A	126	GLN	2.3
1	D	41	HIS	2.3
1	E	175	GLN	2.3
1	D	202	LEU	2.3
1	E	229	LEU	2.3
1	F	5	MET	2.3
1	A	34	LYS	2.3
1	C	254	PHE	2.3
1	A	201	PRO	2.3
1	C	46	TYR	2.3
1	D	102	ASN	2.2
1	F	15	ALA	2.2
1	F	18	ASN	2.2
1	F	130	ARG	2.3
1	C	196	ALA	2.2
1	B	101	GLY	2.2
1	E	47	GLN	2.2
1	E	163	GLY	2.2
1	E	252	GLN	2.2
1	B	174	LEU	2.2
1	B	232	LYS	2.2
1	C	250	SER	2.2
1	D	23	SER	2.2
1	A	50	ARG	2.2
1	E	155	PRO	2.2
1	B	85	TYR	2.2
1	E	122	TYR	2.2
1	A	84	MET	2.2
1	E	171	LYS	2.2
1	C	27	LEU	2.2
1	C	147	SER	2.2
1	C	145	GLU	2.2
1	F	235	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	PRO	2.2
1	E	160	ALA	2.2
1	F	267	ALA	2.2
1	B	73	THR	2.2
1	B	273	GLN	2.2
1	D	277	LYS	2.2
1	E	249	ILE	2.2
1	C	33	SER	2.2
1	E	72	SER	2.2
1	C	273	GLN	2.2
1	F	255	GLN	2.2
1	B	264	SER	2.2
1	A	12	PRO	2.2
1	C	165	PRO	2.2
1	E	109	TRP	2.2
1	E	94	PHE	2.2
1	F	276	ALA	2.1
1	A	159	GLY	2.1
1	A	202	LEU	2.1
1	B	161	LEU	2.1
1	D	27	LEU	2.1
1	D	274	LEU	2.1
1	F	27	LEU	2.1
1	E	139	ILE	2.1
1	D	72	SER	2.1
1	D	93	SER	2.1
1	A	8	LYS	2.1
1	A	191	PRO	2.1
1	C	94	PHE	2.1
1	E	19	ALA	2.1
1	B	6	ASN	2.1
1	A	245	LEU	2.1
1	C	251	GLY	2.1
1	E	74	GLY	2.1
1	E	222	ILE	2.1
1	C	113	ARG	2.1
1	D	200	ASP	2.1
1	B	105	LYS	2.1
1	E	124	LYS	2.1
1	B	225	MET	2.1
1	E	111	MET	2.1
1	D	32	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	262	GLY	2.1
1	D	145	GLU	2.1
1	E	150	ILE	2.1
1	C	125	TYR	2.1
1	B	171	LYS	2.1
1	C	89	LYS	2.1
1	C	167	SER	2.1
1	D	132	PRO	2.1
1	D	162	MET	2.1
1	B	180	GLN	2.1
1	F	246	ASN	2.1
1	C	248	GLY	2.1
1	E	219	THR	2.1
1	D	207	LYS	2.1
1	F	221	SER	2.1
1	A	111	MET	2.1
1	C	86	HIS	2.1
1	F	189	HIS	2.1
1	D	153	PHE	2.0
1	B	245	LEU	2.0
1	B	68	GLY	2.0
1	D	234	GLY	2.0
1	E	117	GLU	2.0
1	F	109	TRP	2.0
1	E	154	ILE	2.0
1	B	200	ASP	2.0
1	A	165	PRO	2.0
1	D	212	PRO	2.0
1	F	72	SER	2.0
1	B	47	GLN	2.0
1	F	238	GLN	2.0
1	C	30	PHE	2.0
1	B	172	ALA	2.0
1	C	110	ALA	2.0
1	D	24	ALA	2.0
1	D	68	GLY	2.0
1	C	98	THR	2.0
1	F	83	PRO	2.0
1	A	224	TYR	2.0
1	B	76	HIS	2.0
1	F	33	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	B	5002	8/8	0.21	0.18	49,50,52,54	0
2	MPD	D	301	8/8	0.27	0.23	58,59,60,60	0
2	MPD	A	301	8/8	0.36	0.40	51,52,53,54	0
2	MPD	B	5001	8/8	0.40	0.47	53,54,55,55	0
2	MPD	F	301	8/8	0.56	0.22	63,64,65,65	0
2	MPD	E	301	8/8	0.67	0.13	53,56,57,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.