



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 5B6N / pdb_00005b6n
Title : Crystal structures of human peroxiredoxin 6 in sulfinic acid state
Authors : Kim, K.H.; Lee, W.T.; Kim, E.E.
Deposited on : 2016-05-30
Resolution : 2.90 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

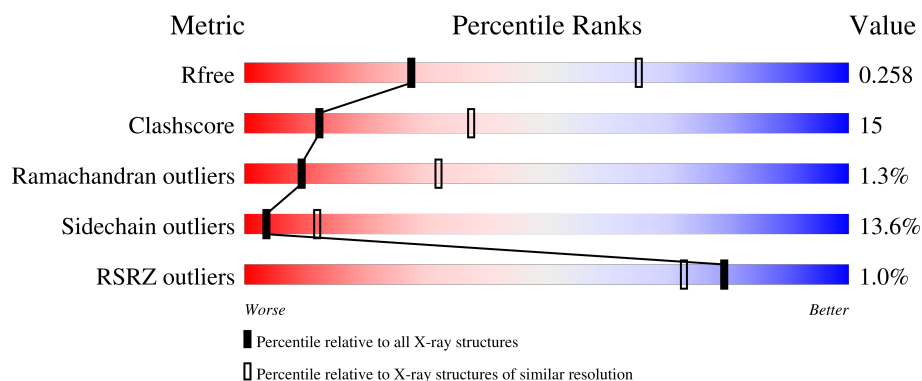
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	224	
1	B	224	
1	C	224	
1	D	224	
1	E	224	

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Mol	Chain	Length	Quality of chain
1	F	224	 59% 33% 8%

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
1	CSD	B	47	-	-	X	-
1	CSD	E	47	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10576 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 Peroxiredoxin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1749	1127	293	324	5			
1	B	221	Total	C	N	O	S	0	0	0
			1749	1127	293	324	5			
1	C	217	Total	C	N	O	S	0	0	0
			1723	1111	288	319	5			
1	D	213	Total	C	N	O	S	0	0	0
			1690	1092	285	309	4			
1	E	221	Total	C	N	O	S	0	0	0
			1749	1127	293	324	5			
1	F	223	Total	C	N	O	S	0	0	0
			1760	1134	295	326	5			

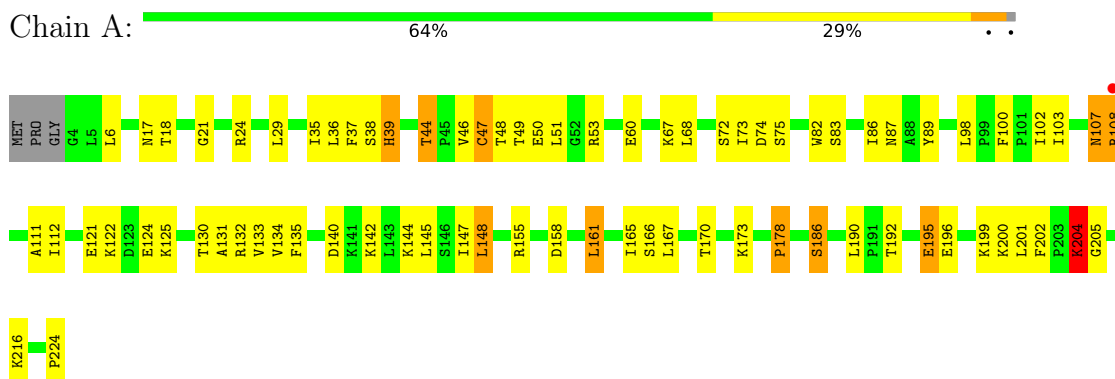
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total	O	0	0
			28	28		
2	B	22	Total	O	0	0
			22	22		
2	C	29	Total	O	0	0
			29	29		
2	D	21	Total	O	0	0
			21	21		
2	E	27	Total	O	0	0
			27	27		
2	F	29	Total	O	0	0
			29	29		

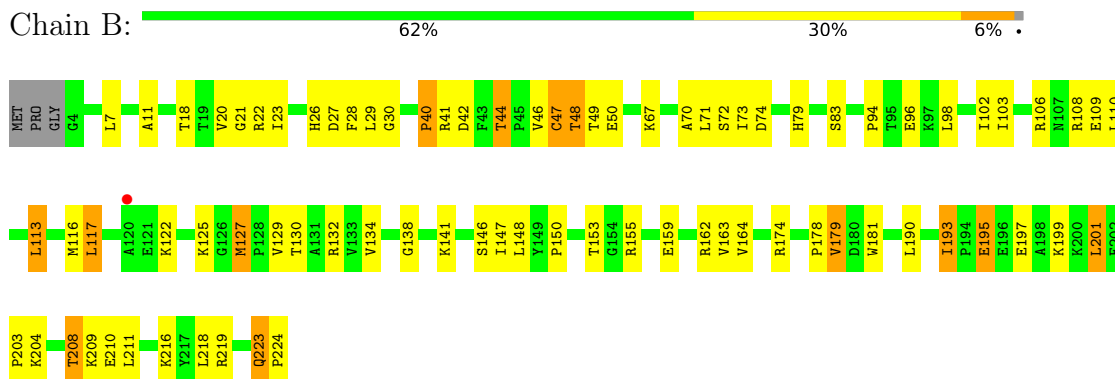
3 Residue-property plots

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

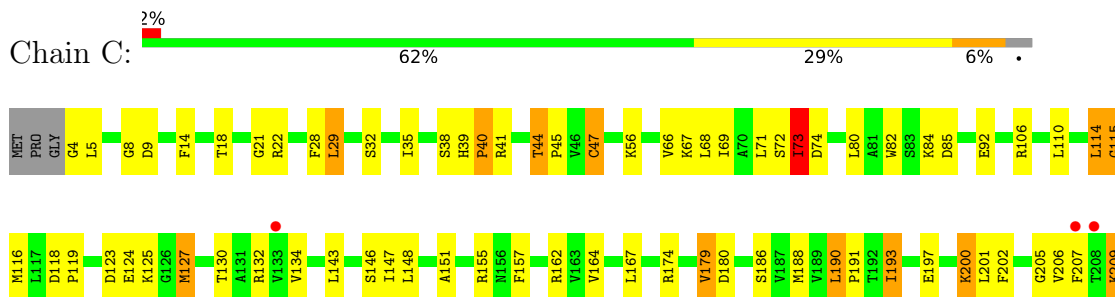
• Molecule 1: Peroxiredoxin-6

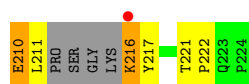


• Molecule 1: Peroxiredoxin-6

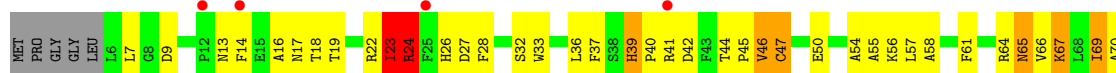


• Molecule 1: Peroxiredoxin-6

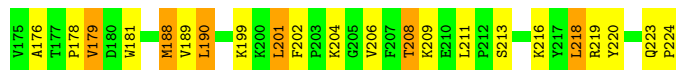




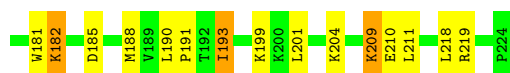
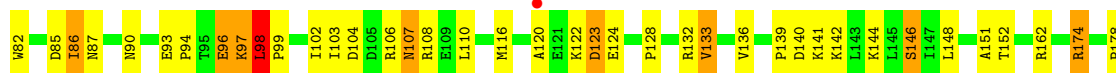
● Molecule 1: Peroxiredoxin-6



● Molecule 1: Peroxiredoxin-6



● Molecule 1: Peroxiredoxin-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.42Å 106.54Å 167.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.90 29.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.99-2.90) 97.7 (29.99-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.248 , 0.304 0.250 , 0.258	Depositor DCC
R_{free} test set	1887 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 1.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10576	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: CSD

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	0.81	0/1783	0.96	12/2420 (0.5%)
1	B	0.78	0/1783	0.93	9/2420 (0.4%)
1	C	0.74	0/1755	0.94	5/2381 (0.2%)
1	D	0.64	0/1722	1.00	14/2335 (0.6%)
1	E	0.69	0/1783	0.94	11/2420 (0.5%)
1	F	0.75	0/1795	0.92	4/2436 (0.2%)
All	All	0.74	0/10621	0.95	55/14412 (0.4%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	ARG	N-CA-C	-8.34	96.12	107.88
1	A	44	THR	CA-C-N	7.97	128.05	119.28
1	A	44	THR	C-N-CA	7.97	128.05	119.28
1	E	202	PHE	CA-C-N	7.82	127.10	118.97
1	E	202	PHE	C-N-CA	7.82	127.10	118.97
1	F	39	HIS	CA-C-N	7.73	129.51	119.84
1	F	39	HIS	C-N-CA	7.73	129.51	119.84
1	D	89	TYR	N-CA-C	-7.60	103.80	113.23
1	A	202	PHE	CA-C-N	7.45	127.09	119.19
1	A	202	PHE	C-N-CA	7.45	127.09	119.19
1	A	100	PHE	CA-C-N	7.03	127.00	119.76
1	A	100	PHE	C-N-CA	7.03	127.00	119.76
1	B	190	LEU	CA-C-N	7.02	126.70	119.82
1	B	190	LEU	C-N-CA	7.02	126.70	119.82
1	C	190	LEU	CA-C-N	6.76	127.31	119.47
1	C	190	LEU	C-N-CA	6.76	127.31	119.47
1	E	211	LEU	CA-C-N	6.68	128.20	119.84
1	E	211	LEU	C-N-CA	6.68	128.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	LEU	CA-C-N	6.52	126.10	119.19
1	A	190	LEU	C-N-CA	6.52	126.10	119.19
1	F	98	LEU	CA-C-N	6.49	127.32	120.12
1	F	98	LEU	C-N-CA	6.49	127.32	120.12
1	C	73	ILE	N-CA-C	-6.45	106.95	113.47
1	D	23	ILE	N-CA-C	6.35	117.92	108.46
1	D	177	THR	CA-C-N	6.17	127.55	119.84
1	D	177	THR	C-N-CA	6.17	127.55	119.84
1	D	39	HIS	CA-C-N	6.15	127.53	119.84
1	D	39	HIS	C-N-CA	6.15	127.53	119.84
1	B	44	THR	CA-C-N	6.11	125.83	119.05
1	B	44	THR	C-N-CA	6.11	125.83	119.05
1	E	127	MET	CA-C-N	6.06	127.42	119.84
1	E	127	MET	C-N-CA	6.06	127.42	119.84
1	D	202	PHE	CA-C-N	5.85	125.47	119.56
1	D	202	PHE	C-N-CA	5.85	125.47	119.56
1	C	202	PHE	CA-C-N	5.79	125.47	119.05
1	C	202	PHE	C-N-CA	5.79	125.47	119.05
1	A	204	LYS	N-CA-C	-5.75	102.40	110.50
1	A	205	GLY	N-CA-C	5.73	118.06	111.36
1	A	39	HIS	CA-C-N	5.55	126.78	119.84
1	A	39	HIS	C-N-CA	5.55	126.78	119.84
1	B	96	GLU	N-CA-C	-5.49	106.63	113.38
1	B	211	LEU	CA-C-N	5.47	126.67	119.84
1	B	211	LEU	C-N-CA	5.47	126.67	119.84
1	E	19	THR	N-CA-C	-5.47	106.61	113.28
1	E	98	LEU	CA-C-N	5.40	125.22	119.28
1	E	98	LEU	C-N-CA	5.40	125.22	119.28
1	D	211	LEU	CA-C-N	5.35	124.99	119.05
1	D	211	LEU	C-N-CA	5.35	124.99	119.05
1	E	190	LEU	CA-C-N	5.33	125.00	119.56
1	E	190	LEU	C-N-CA	5.33	125.00	119.56
1	D	79	HIS	N-CA-C	-5.29	105.65	112.68
1	B	193	ILE	CA-C-N	5.23	125.21	120.03
1	B	193	ILE	C-N-CA	5.23	125.21	120.03
1	D	127	MET	CA-C-N	5.03	126.13	119.84
1	D	127	MET	C-N-CA	5.03	126.13	119.84

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	1749	0	1778	44	1
1	B	1749	0	1778	53	0
1	C	1723	0	1749	51	0
1	D	1690	0	1726	80	0
1	E	1749	0	1778	63	0
1	F	1760	0	1789	58	1
2	A	28	0	0	0	0
2	B	22	0	0	0	0
2	C	29	0	0	0	0
2	D	21	0	0	0	0
2	E	27	0	0	0	0
2	F	29	0	0	0	0
All	All	10576	0	10598	324	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 15.

All (324) 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:C:28:PHE:O	1:C:67:LYS:NZ	2.10	0.85
1:D:108:ARG:HG2	1:D:128:PRO:HB2	1.59	0.83
1:C:41:ARG:O	1:C:44:THR:OG1	1.99	0.81
1:A:204:LYS:H	1:A:204:LYS:HE3	1.49	0.78
1:B:44:THR:O	1:B:48:THR:OG1	2.02	0.78
1:E:39:HIS:NE2	1:E:42:ASP:OD2	2.16	0.77
1:D:205:GLY:O	1:D:221:THR:OG1	2.03	0.74
1:B:208:THR:HB	1:B:219:ARG:HG2	1.68	0.74
1:A:83:SER:O	1:A:87:ASN:ND2	2.20	0.73
1:B:174:ARG:NH1	1:B:197:GLU:OE1	2.22	0.73
1:C:197:GLU:O	1:C:200:LYS:NZ	2.21	0.73
1:F:96:GLU:O	1:F:98:LEU:N	2.20	0.73
1:C:186:SER:HA	1:C:222:PRO:HA	1.70	0.72
1:F:193:ILE:O	1:F:219:ARG:NH2	2.18	0.72
1:F:35:ILE:HG13	1:F:136:VAL:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LEU:HD22	1:E:116:MET:HE1	1.72	0.71
1:A:6:LEU:HD13	1:B:117:LEU:HD21	1.72	0.71
1:A:50:GLU:HG2	1:B:179:VAL:HG13	1.72	0.71
1:E:162:ARG:HD3	1:E:181:TRP:O	1.91	0.70
1:D:32:SER:HB3	1:D:65:ASN:HD21	1.56	0.70
1:A:38:SER:OG	1:A:131:ALA:O	2.09	0.70
1:A:166:SER:O	1:A:170:THR:OG1	2.08	0.70
1:A:37:PHE:HB2	1:A:155:ARG:HH12	1.56	0.69
1:D:106:ARG:NH1	1:D:107:ASN:OD1	2.25	0.69
1:D:111:ALA:O	1:D:115:GLY:N	2.24	0.68
1:E:11:ALA:O	1:E:26:HIS:NE2	2.23	0.68
1:B:47:CSD:OD1	1:B:132:ARG:NH1	2.27	0.68
1:A:44:THR:O	1:A:48:THR:OG1	2.13	0.67
1:F:33:TRP:HB2	1:F:66:VAL:HG22	1.75	0.67
1:F:52:GLY:O	1:F:90:ASN:ND2	2.27	0.66
1:C:167:LEU:HD21	1:D:150:PRO:HG3	1.78	0.66
1:D:159:GLU:OE1	1:D:162:ARG:NE	2.29	0.66
1:B:11:ALA:O	1:B:26:HIS:NE2	2.22	0.66
1:E:130:THR:OG1	1:E:131:ALA:N	2.27	0.66
1:D:18:THR:OG1	1:D:19:THR:N	2.25	0.65
1:E:47:CSD:OD2	1:E:132:ARG:NH1	2.28	0.65
1:F:162:ARG:NH1	1:F:181:TRP:O	2.26	0.65
1:C:18:THR:OG1	1:C:21:GLY:O	2.13	0.65
1:E:208:THR:HG23	1:E:219:ARG:HG2	1.77	0.65
1:C:72:SER:OG	1:C:73:ILE:N	2.22	0.65
1:D:33:TRP:HB2	1:D:65:ASN:O	1.97	0.64
1:E:38:SER:OG	1:E:131:ALA:O	2.16	0.64
1:D:72:SER:HB3	1:D:79:HIS:HE1	1.60	0.64
1:B:46:VAL:O	1:B:49:THR:OG1	2.15	0.64
1:B:71:LEU:HD12	1:B:103:ILE:HD12	1.80	0.64
1:C:56:LYS:NZ	1:C:92:GLU:OE2	2.28	0.64
1:E:129:VAL:HG12	1:E:130:THR:H	1.63	0.62
1:D:61:PHE:HD1	1:D:66:VAL:HG21	1.64	0.62
1:F:116:MET:HB2	1:F:133:VAL:HG11	1.81	0.62
1:A:18:THR:OG1	1:A:21:GLY:O	2.18	0.61
1:E:122:LYS:HB3	1:E:126:GLY:HA2	1.81	0.61
1:E:39:HIS:HB2	1:E:47:CSD:HB2	1.83	0.61
1:E:47:CSD:HD2	1:E:132:ARG:HH12	1.48	0.61
1:E:31:ASP:HA	1:E:141:LYS:HE3	1.82	0.61
1:B:44:THR:HG1	1:B:47:CSD:HD2	1.39	0.61
1:F:139:PRO:O	1:F:141:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:CSD:OD2	1:D:47:CSD:N	2.34	0.60
1:A:39:HIS:NE2	1:A:72:SER:HB2	2.16	0.60
1:B:44:THR:OG1	1:B:47:CSD:OD2	2.14	0.60
1:C:35:ILE:HD11	1:C:164:VAL:HG21	1.83	0.60
1:D:54:ALA:HA	1:D:57:LEU:HD12	1.83	0.60
1:A:29:LEU:HA	1:A:67:LYS:HD2	1.83	0.60
1:A:47:CSD:OD2	1:A:47:CSD:N	2.33	0.60
1:A:145:LEU:HD12	1:B:150:PRO:HD3	1.82	0.60
1:D:156:ASN:OD1	1:D:159:GLU:N	2.35	0.60
1:F:48:THR:HG23	1:F:86:ILE:HG22	1.83	0.60
1:E:44:THR:HG23	1:F:191:PRO:HG3	1.84	0.60
1:A:133:VAL:HG22	1:A:148:LEU:HG	1.83	0.59
1:C:188:MET:SD	1:C:188:MET:N	2.75	0.59
1:D:98:LEU:HD23	1:D:99:PRO:HD2	1.83	0.59
1:F:18:THR:HG22	1:F:103:ILE:HG23	1.83	0.59
1:F:120:ALA:O	1:F:122:LYS:NZ	2.24	0.59
1:A:196:GLU:HA	1:A:199:LYS:HE2	1.85	0.59
1:B:150:PRO:HD2	1:B:153:THR:HB	1.85	0.58
1:F:11:ALA:O	1:F:26:HIS:NE2	2.30	0.58
1:B:30:GLY:O	1:B:141:LYS:NZ	2.36	0.58
1:E:40:PRO:HA	1:E:130:THR:HG23	1.85	0.58
1:A:167:LEU:HD21	1:B:150:PRO:HG2	1.84	0.58
1:B:42:ASP:OD2	1:B:79:HIS:ND1	2.36	0.58
1:A:36:LEU:HD23	1:A:135:PHE:HD2	1.67	0.57
1:A:148:LEU:HD23	1:B:7:LEU:HG	1.87	0.57
1:C:134:VAL:HB	1:C:147:ILE:HG12	1.86	0.57
1:D:69:ILE:HD11	1:D:103:ILE:HG13	1.85	0.57
1:D:129:VAL:HG22	1:D:130:THR:H	1.69	0.57
1:A:46:VAL:O	1:A:49:THR:OG1	2.22	0.57
1:B:108:ARG:CZ	1:B:127:MET:HB3	2.34	0.57
1:F:35:ILE:HB	1:F:68:LEU:HD23	1.85	0.56
1:D:41:ARG:HG2	1:D:42:ASP:H	1.70	0.56
1:D:71:LEU:HD22	1:D:116:MET:HE3	1.86	0.56
1:D:79:HIS:O	1:D:83:SER:N	2.31	0.56
1:E:61:PHE:HB3	1:E:66:VAL:HB	1.87	0.56
1:D:18:THR:HG1	1:D:19:THR:H	1.51	0.56
1:D:24:ARG:HG3	1:D:26:HIS:HB2	1.87	0.56
1:F:41:ARG:NH2	1:F:123:ASP:HB2	2.21	0.55
1:F:53:ARG:HH11	1:F:56:LYS:HE3	1.70	0.55
1:C:8:GLY:HA3	1:D:119:PRO:HG2	1.88	0.55
1:D:64:ARG:O	1:D:66:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PHE:O	1:B:67:LYS:NZ	2.38	0.55
1:C:179:VAL:HG13	1:D:50:GLU:HG2	1.89	0.55
1:D:58:ALA:HA	1:D:61:PHE:HB2	1.89	0.55
1:F:122:LYS:HA	1:F:128:PRO:HA	1.89	0.55
1:F:151:ALA:O	1:F:152:THR:OG1	2.18	0.55
1:D:105:ASP:C	1:D:107:ASN:H	2.15	0.55
1:F:136:VAL:HG23	1:F:144:LYS:HB2	1.89	0.55
1:A:178:PRO:HA	1:B:46:VAL:HG13	1.88	0.54
1:D:193:ILE:O	1:D:219:ARG:NH2	2.40	0.54
1:E:70:ALA:HB3	1:E:102:ILE:HG23	1.89	0.54
1:E:71:LEU:HA	1:E:103:ILE:HG22	1.89	0.54
1:F:8:GLY:O	1:F:142:LYS:HE3	2.07	0.54
1:A:46:VAL:HG13	1:B:178:PRO:HA	1.88	0.54
1:F:70:ALA:O	1:F:103:ILE:HG13	2.07	0.54
1:E:174:ARG:HD3	1:E:201:LEU:HD11	1.88	0.54
1:D:22:ARG:CZ	1:D:22:ARG:HA	2.37	0.54
1:A:140:ASP:OD1	1:A:140:ASP:N	2.36	0.54
1:C:47:CSD:OD2	1:C:132:ARG:NH1	2.41	0.53
1:D:42:ASP:HA	1:D:82:TRP:CZ3	2.43	0.53
1:A:53:ARG:NH2	1:A:158:ASP:OD1	2.39	0.53
1:D:18:THR:HG22	1:D:23:ILE:HG21	1.91	0.53
1:A:37:PHE:HB2	1:A:155:ARG:NH1	2.23	0.53
1:D:28:PHE:O	1:D:67:LYS:NZ	2.37	0.53
1:E:121:GLU:O	1:E:129:VAL:HG23	2.09	0.53
1:F:53:ARG:HA	1:F:56:LYS:HE2	1.90	0.53
1:A:108:ARG:HG2	1:A:111:ALA:HB3	1.91	0.53
1:C:191:PRO:HG3	1:D:45:PRO:HD2	1.90	0.53
1:E:41:ARG:HH12	1:E:124:GLU:HG3	1.74	0.53
1:B:79:HIS:O	1:B:83:SER:OG	2.26	0.52
1:D:16:ALA:H	1:D:23:ILE:HD11	1.74	0.52
1:C:216:LYS:HG3	1:C:217:TYR:HD2	1.74	0.52
1:C:29:LEU:O	1:C:32:SER:OG	2.27	0.52
1:E:73:ILE:HG13	1:E:108:ARG:HG2	1.91	0.52
1:E:189:VAL:HB	1:E:219:ARG:HB2	1.90	0.52
1:A:35:ILE:HB	1:A:68:LEU:HD23	1.90	0.52
1:D:197:GLU:HA	1:D:200:LYS:HD2	1.91	0.52
1:E:133:VAL:HG22	1:E:148:LEU:HD23	1.90	0.52
1:A:140:ASP:O	1:A:142:LYS:HG3	2.10	0.51
1:C:134:VAL:HG22	1:C:155:ARG:HH11	1.76	0.51
1:F:60:GLU:OE1	1:F:64:ARG:NH1	2.43	0.51
1:E:81:ALA:HA	1:E:84:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LEU:HD11	1:C:114:LEU:HD23	1.93	0.51
1:D:50:GLU:OE2	1:D:155:ARG:HG2	2.11	0.51
1:D:133:VAL:N	1:D:155:ARG:HH12	2.07	0.51
1:E:138:GLY:HA3	1:E:144:LYS:NZ	2.26	0.51
1:E:178:PRO:HA	1:F:46:VAL:HG13	1.91	0.51
1:F:45:PRO:O	1:F:49:THR:HG23	2.10	0.51
1:D:162:ARG:HD2	1:D:181:TRP:O	2.10	0.51
1:D:111:ALA:HB1	1:D:117:LEU:HB2	1.91	0.50
1:C:35:ILE:HB	1:C:68:LEU:HD23	1.94	0.50
1:D:36:LEU:HD11	1:D:71:LEU:HD13	1.94	0.50
1:F:86:ILE:HD11	1:F:98:LEU:HD11	1.94	0.50
1:A:38:SER:O	1:A:155:ARG:NH2	2.38	0.50
1:F:29:LEU:HB2	1:F:141:LYS:HE3	1.94	0.50
1:D:178:PRO:HG3	1:D:188:MET:SD	2.52	0.50
1:E:84:LYS:HB3	1:E:95:THR:HA	1.92	0.50
1:A:173:LYS:HG3	1:A:224:PRO:HB2	1.95	0.49
1:B:40:PRO:HD2	1:B:47:CSD:SG	2.52	0.49
1:B:193:ILE:O	1:B:219:ARG:NH2	2.37	0.49
1:D:64:ARG:HB3	1:D:168:GLN:HE22	1.76	0.49
1:E:148:LEU:HD13	1:F:7:LEU:HG	1.95	0.49
1:E:121:GLU:O	1:E:128:PRO:HA	2.12	0.49
1:D:18:THR:HB	1:D:103:ILE:HA	1.95	0.49
1:B:108:ARG:NH2	1:B:127:MET:HB3	2.27	0.49
1:D:14:PHE:HD1	1:D:23:ILE:HD12	1.77	0.49
1:D:73:ILE:HD12	1:D:106:ARG:HA	1.95	0.49
1:E:116:MET:HB3	1:E:133:VAL:HG21	1.95	0.49
1:C:197:GLU:HG2	1:C:200:LYS:HZ2	1.78	0.48
1:D:166:SER:O	1:D:170:THR:OG1	2.17	0.48
1:D:223:GLN:HA	1:D:224:PRO:HD3	1.71	0.48
1:F:93:GLU:H	1:F:97:LYS:HZ1	1.60	0.48
1:B:18:THR:OG1	1:B:21:GLY:O	2.30	0.48
1:D:55:ALA:C	1:D:57:LEU:H	2.21	0.48
1:F:44:THR:OG1	1:F:47:CSD:OD2	2.05	0.48
1:B:210:GLU:CD	1:B:216:LYS:HZ2	2.21	0.48
1:D:197:GLU:O	1:D:200:LYS:HB2	2.14	0.47
1:F:174:ARG:HG3	1:F:201:LEU:HD21	1.97	0.47
1:B:108:ARG:NH2	1:B:127:MET:O	2.48	0.47
1:D:111:ALA:HA	1:D:116:MET:HB2	1.95	0.47
1:C:66:VAL:HG21	1:C:164:VAL:HG11	1.95	0.47
1:F:82:TRP:O	1:F:86:ILE:HG23	2.14	0.47
1:E:47:CSD:HD2	1:E:132:ARG:NH1	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:H	1:A:107:ASN:HD22	1.62	0.47
1:A:144:LYS:O	1:B:150:PRO:HG3	2.14	0.47
1:B:159:GLU:OE2	1:B:162:ARG:NH2	2.31	0.47
1:B:209:LYS:HB3	1:B:218:LEU:HD23	1.97	0.47
1:F:47:CSD:SG	1:F:132:ARG:NH1	2.83	0.47
1:B:127:MET:HB2	1:B:127:MET:HE2	1.73	0.47
1:E:148:LEU:N	1:F:146:SER:O	2.34	0.47
1:D:57:LEU:O	1:D:61:PHE:N	2.47	0.47
1:E:213:SER:OG	1:F:85:ASP:OD2	2.20	0.47
1:B:71:LEU:HG	1:B:103:ILE:HB	1.97	0.46
1:B:73:ILE:HD12	1:B:108:ARG:HG3	1.96	0.46
1:C:82:TRP:O	1:C:85:ASP:N	2.42	0.46
1:C:38:SER:O	1:C:155:ARG:NH2	2.46	0.46
1:B:110:LEU:HA	1:B:113:LEU:HB2	1.96	0.46
1:C:148:LEU:HD12	1:D:146:SER:OG	2.15	0.46
1:C:14:PHE:CG	1:C:110:LEU:HD21	2.51	0.46
1:E:84:LYS:H	1:E:84:LYS:HG2	1.54	0.46
1:E:110:LEU:HA	1:E:113:LEU:HB2	1.97	0.46
1:C:38:SER:HB3	1:C:116:MET:HE3	1.98	0.46
1:D:108:ARG:H	1:D:108:ARG:HD2	1.81	0.46
1:E:179:VAL:CG1	1:F:50:GLU:HG3	2.46	0.46
1:E:93:GLU:HA	1:E:94:PRO:HA	1.75	0.46
1:C:114:LEU:O	1:C:116:MET:N	2.49	0.46
1:E:116:MET:HB2	1:E:116:MET:HE3	1.68	0.46
1:A:195:GLU:H	1:A:195:GLU:CD	2.23	0.45
1:C:74:ASP:OD2	1:C:74:ASP:N	2.49	0.45
1:E:136:VAL:HG23	1:E:144:LYS:HB2	1.98	0.45
1:B:72:SER:OG	1:B:73:ILE:N	2.47	0.45
1:D:14:PHE:CD1	1:D:23:ILE:HD12	2.51	0.45
1:A:18:THR:HG22	1:A:103:ILE:HA	1.98	0.45
1:B:26:HIS:O	1:B:30:GLY:N	2.46	0.45
1:E:138:GLY:HA3	1:E:144:LYS:HZ2	1.81	0.45
1:F:193:ILE:H	1:F:193:ILE:HG12	1.41	0.45
1:D:115:GLY:C	1:D:117:LEU:H	2.24	0.45
1:D:203:PRO:HG2	1:D:204:LYS:HE2	1.99	0.45
1:F:15:GLU:HA	1:F:23:ILE:O	2.17	0.45
1:C:197:GLU:HG2	1:C:200:LYS:NZ	2.32	0.44
1:F:96:GLU:H	1:F:96:GLU:HG3	1.61	0.44
1:B:134:VAL:O	1:B:146:SER:HA	2.17	0.44
1:C:45:PRO:HD3	1:D:191:PRO:HB3	1.99	0.44
1:D:9:ASP:C	1:D:142:LYS:HG2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:NH2	1:C:151:ALA:O	2.44	0.44
1:F:15:GLU:HB3	1:F:24:ARG:HD2	2.00	0.44
1:F:93:GLU:HA	1:F:94:PRO:HD3	1.89	0.44
1:E:33:TRP:CE3	1:E:138:GLY:HA2	2.53	0.44
1:F:69:ILE:HG12	1:F:103:ILE:HD11	2.00	0.44
1:F:107:ASN:OD1	1:F:107:ASN:N	2.51	0.44
1:A:161:LEU:O	1:A:165:ILE:HG13	2.17	0.44
1:D:46:VAL:O	1:D:132:ARG:NH2	2.51	0.44
1:E:45:PRO:HB3	1:F:218:LEU:HA	1.99	0.44
1:C:134:VAL:CG2	1:C:155:ARG:HH11	2.31	0.44
1:E:223:GLN:HA	1:E:224:PRO:HD3	1.76	0.44
1:B:41:ARG:HD2	1:B:74:ASP:OD2	2.18	0.44
1:C:39:HIS:NE2	1:C:72:SER:HB2	2.33	0.44
1:B:70:ALA:HB3	1:B:102:ILE:HG23	2.00	0.43
1:C:71:LEU:HD22	1:C:116:MET:HE1	2.00	0.43
1:D:56:LYS:NZ	1:D:90:ASN:HA	2.32	0.43
1:E:24:ARG:HG2	1:E:27:ASP:HB2	2.00	0.43
1:D:108:ARG:NH1	1:D:127:MET:HB3	2.33	0.43
1:D:178:PRO:HD2	1:D:181:TRP:CD1	2.53	0.43
1:D:211:LEU:HD21	1:D:218:LEU:HD12	1.99	0.43
1:A:49:THR:HB	1:B:179:VAL:HG22	2.01	0.43
1:C:5:LEU:HB3	1:C:143:LEU:HD22	1.98	0.43
1:C:84:LYS:O	1:D:212:PRO:HG2	2.18	0.43
1:C:190:LEU:O	1:C:193:ILE:HG23	2.18	0.43
1:F:76:VAL:HG22	1:F:104:ASP:HB2	2.00	0.43
1:B:110:LEU:HD23	1:B:110:LEU:H	1.83	0.43
1:F:71:LEU:HD21	1:F:116:MET:HE1	2.00	0.43
1:F:209:LYS:HE3	1:F:210:GLU:N	2.34	0.43
1:B:71:LEU:HD13	1:B:116:MET:HE1	2.01	0.43
1:C:72:SER:OG	1:C:74:ASP:OD2	2.35	0.43
1:F:41:ARG:NH2	1:F:124:GLU:HG2	2.33	0.43
1:B:22:ARG:NH2	1:C:66:VAL:O	2.52	0.43
1:C:47:CSD:N	1:C:47:CSD:OD1	2.52	0.43
1:C:179:VAL:HB	1:C:180:ASP:OD1	2.19	0.43
1:E:188:MET:HE1	1:E:220:TYR:CZ	2.53	0.43
1:F:23:ILE:H	1:F:23:ILE:HG13	1.53	0.43
1:C:4:GLY:HA3	1:C:115:GLY:H	1.83	0.43
1:D:209:LYS:O	1:D:211:LEU:HD22	2.18	0.43
1:A:98:LEU:HD12	1:A:102:ILE:HD11	2.01	0.42
1:C:209:LYS:HE3	1:C:209:LYS:HA	2.01	0.42
1:E:18:THR:HG22	1:E:103:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:LEU:HA	1:E:99:PRO:HD3	1.85	0.42
1:F:42:ASP:O	1:F:82:TRP:CD2	2.72	0.42
1:D:72:SER:OG	1:D:73:ILE:N	2.52	0.42
1:E:134:VAL:HG23	1:E:147:ILE:HD11	2.02	0.42
1:D:132:ARG:HH11	1:D:151:ALA:HA	1.84	0.42
1:D:204:LYS:HA	1:D:204:LYS:HD3	1.71	0.42
1:B:195:GLU:O	1:B:199:LYS:HE2	2.20	0.42
1:F:182:LYS:NZ	1:F:185:ASP:OD2	2.38	0.42
1:C:110:LEU:O	1:C:114:LEU:HD12	2.20	0.42
1:E:199:LYS:HB3	1:E:199:LYS:HE2	1.71	0.42
1:A:72:SER:OG	1:A:74:ASP:OD2	2.37	0.42
1:B:223:GLN:HA	1:B:224:PRO:HD3	1.86	0.42
1:E:100:PHE:HA	1:E:101:PRO:HD3	1.87	0.42
1:B:162:ARG:HD2	1:B:181:TRP:O	2.19	0.42
1:E:44:THR:HB	1:E:47:CSD:SG	2.60	0.42
1:F:56:LYS:HE2	1:F:56:LYS:HB2	1.77	0.42
1:A:51:LEU:HD22	1:A:82:TRP:CZ3	2.54	0.41
1:D:41:ARG:HG2	1:D:42:ASP:N	2.34	0.41
1:E:28:PHE:CZ	1:E:67:LYS:HB3	2.55	0.41
1:B:201:LEU:C	1:B:203:PRO:HD3	2.44	0.41
1:D:195:GLU:O	1:D:199:LYS:HG2	2.20	0.41
1:E:76:VAL:HG23	1:E:104:ASP:HB2	2.02	0.41
1:A:134:VAL:CG2	1:A:155:ARG:HH11	2.32	0.41
1:A:134:VAL:HG22	1:A:155:ARG:HH11	1.84	0.41
1:E:127:MET:SD	1:E:128:PRO:HD2	2.60	0.41
1:F:16:ALA:HB2	1:F:110:LEU:HD11	2.01	0.41
1:F:98:LEU:HA	1:F:99:PRO:HD2	1.78	0.41
1:D:210:GLU:CD	1:D:210:GLU:H	2.28	0.41
1:E:132:ARG:HB3	1:E:155:ARG:NE	2.34	0.41
1:E:190:LEU:HD12	1:E:190:LEU:H	1.84	0.41
1:A:124:GLU:HG2	1:A:125:LYS:HG3	2.03	0.41
1:D:50:GLU:OE2	1:D:155:ARG:N	2.53	0.41
1:D:76:VAL:HA	1:D:79:HIS:HD2	1.85	0.41
1:A:132:ARG:HB3	1:A:155:ARG:NE	2.35	0.41
1:B:134:VAL:HB	1:B:147:ILE:HG12	2.03	0.41
1:C:123:ASP:N	1:C:127:MET:O	2.47	0.41
1:C:200:LYS:HZ3	1:C:201:LEU:HB2	1.85	0.41
1:A:47:CSD:OD2	1:A:132:ARG:NH1	2.44	0.41
1:F:73:ILE:H	1:F:73:ILE:HG13	1.62	0.41
1:F:140:ASP:OD2	1:F:142:LYS:HB2	2.21	0.41
1:B:138:GLY:O	1:B:141:LYS:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLU:O	1:C:211:LEU:HD23	2.20	0.41
1:D:33:TRP:HB3	1:D:66:VAL:HG12	2.03	0.41
1:D:39:HIS:NE2	1:D:72:SER:HB2	2.36	0.41
1:E:144:LYS:HB3	1:E:167:LEU:HD13	2.03	0.41
1:B:125:LYS:HD2	1:B:125:LYS:HA	1.98	0.41
1:A:86:ILE:O	1:A:89:TYR:HB3	2.20	0.40
1:D:72:SER:HB3	1:D:79:HIS:CE1	2.48	0.40
1:D:211:LEU:HD21	1:D:218:LEU:HB2	2.01	0.40
1:D:42:ASP:HA	1:D:82:TRP:CE3	2.57	0.40
1:E:16:ALA:HB3	1:E:103:ILE:HD11	2.03	0.40
1:E:209:LYS:HB3	1:E:218:LEU:HB3	2.03	0.40
1:F:87:ASN:HD22	1:F:87:ASN:HA	1.74	0.40
1:F:106:ARG:O	1:F:108:ARG:NH1	2.51	0.40
1:B:27:ASP:OD2	1:B:27:ASP:N	2.52	0.40
1:C:119:PRO:HG2	1:D:7:LEU:O	2.20	0.40
1:D:37:PHE:O	1:D:70:ALA:HA	2.21	0.40
1:E:118:ASP:HB3	1:E:121:GLU:HB2	2.03	0.40
1:B:49:THR:OG1	1:B:50:GLU:N	2.54	0.40
1:C:118:ASP:HA	1:C:119:PRO:HD3	1.85	0.40
1:C:200:LYS:NZ	1:C:201:LEU:HB2	2.37	0.40
1:E:57:LEU:HD23	1:E:57:LEU:HA	1.97	0.40
1:E:176:ALA:O	1:E:188:MET:HB2	2.21	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)
1:A:186:SER:OG	1:F:204:LYS:O[1_655]	2.13	0.07

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	218/224 (97%)	204 (94%)	13 (6%)	1 (0%)	24	54
1	B	218/224 (97%)	199 (91%)	17 (8%)	2 (1%)	14	41
1	C	212/224 (95%)	186 (88%)	23 (11%)	3 (1%)	9	30
1	D	208/224 (93%)	171 (82%)	32 (15%)	5 (2%)	4	18
1	E	218/224 (97%)	185 (85%)	30 (14%)	3 (1%)	9	30
1	F	220/224 (98%)	193 (88%)	24 (11%)	3 (1%)	9	30
All	All	1294/1344 (96%)	1138 (88%)	139 (11%)	17 (1%)	9	32

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	97	LYS
1	C	205	GLY
1	D	40	PRO
1	D	65	ASN
1	C	115	GLY
1	D	128	PRO
1	E	125	LYS
1	F	178	PRO
1	E	25	PHE
1	E	94	PRO
1	D	140	ASP
1	F	3	GLY
1	A	178	PRO
1	B	94	PRO
1	D	178	PRO
1	C	40	PRO
1	B	40	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	191/193 (99%)	170 (89%)	21 (11%)	6	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	191/193 (99%)	168 (88%)	23 (12%)	5	16
1	C	188/193 (97%)	161 (86%)	27 (14%)	3	11
1	D	184/193 (95%)	154 (84%)	30 (16%)	2	8
1	E	191/193 (99%)	161 (84%)	30 (16%)	2	9
1	F	192/193 (100%)	168 (88%)	24 (12%)	4	15
All	All	1137/1158 (98%)	982 (86%)	155 (14%)	3	12

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	24	ARG
1	A	60	GLU
1	A	73	ILE
1	A	75	SER
1	A	107	ASN
1	A	108	ARG
1	A	112	ILE
1	A	121	GLU
1	A	122	LYS
1	A	130	THR
1	A	147	ILE
1	A	148	LEU
1	A	161	LEU
1	A	186	SER
1	A	192	THR
1	A	195	GLU
1	A	200	LYS
1	A	201	LEU
1	A	204	LYS
1	A	216	LYS
1	B	20	VAL
1	B	23	ILE
1	B	29	LEU
1	B	48	THR
1	B	98	LEU
1	B	106	ARG
1	B	109	GLU
1	B	113	LEU
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	122	LYS
1	B	127	MET
1	B	129	VAL
1	B	130	THR
1	B	148	LEU
1	B	155	ARG
1	B	163	VAL
1	B	164	VAL
1	B	179	VAL
1	B	195	GLU
1	B	201	LEU
1	B	204	LYS
1	B	208	THR
1	B	223	GLN
1	C	9	ASP
1	C	22	ARG
1	C	29	LEU
1	C	40	PRO
1	C	44	THR
1	C	69	ILE
1	C	73	ILE
1	C	80	LEU
1	C	106	ARG
1	C	114	LEU
1	C	124	GLU
1	C	125	LYS
1	C	127	MET
1	C	130	THR
1	C	146	SER
1	C	157	PHE
1	C	162	ARG
1	C	174	ARG
1	C	179	VAL
1	C	193	ILE
1	C	200	LYS
1	C	206	VAL
1	C	207	PHE
1	C	209	LYS
1	C	210	GLU
1	C	216	LYS
1	C	221	THR
1	D	13	ASN

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Mol	Chain	Res	Type
1	D	17	ASN
1	D	23	ILE
1	D	24	ARG
1	D	27	ASP
1	D	44	THR
1	D	46	VAL
1	D	67	LYS
1	D	69	ILE
1	D	71	LEU
1	D	77	GLU
1	D	87	ASN
1	D	89	TYR
1	D	98	LEU
1	D	105	ASP
1	D	106	ARG
1	D	108	ARG
1	D	112	ILE
1	D	113	LEU
1	D	127	MET
1	D	133	VAL
1	D	148	LEU
1	D	159	GLU
1	D	164	VAL
1	D	170	THR
1	D	182	LYS
1	D	206	VAL
1	D	210	GLU
1	D	211	LEU
1	D	218	LEU
1	E	7	LEU
1	E	53	ARG
1	E	56	LYS
1	E	73	ILE
1	E	84	LYS
1	E	87	ASN
1	E	98	LEU
1	E	103	ILE
1	E	105	ASP
1	E	107	ASN
1	E	114	LEU
1	E	116	MET
1	E	121	GLU

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Mol	Chain	Res	Type
1	E	127	MET
1	E	129	VAL
1	E	130	THR
1	E	136	VAL
1	E	142	LYS
1	E	147	ILE
1	E	148	LEU
1	E	161	LEU
1	E	173	LYS
1	E	179	VAL
1	E	188	MET
1	E	201	LEU
1	E	204	LYS
1	E	206	VAL
1	E	208	THR
1	E	216	LYS
1	E	218	LEU
1	F	6	LEU
1	F	23	ILE
1	F	41	ARG
1	F	42	ASP
1	F	50	GLU
1	F	63	LYS
1	F	73	ILE
1	F	86	ILE
1	F	96	GLU
1	F	98	LEU
1	F	102	ILE
1	F	107	ASN
1	F	123	ASP
1	F	133	VAL
1	F	146	SER
1	F	148	LEU
1	F	174	ARG
1	F	182	LYS
1	F	188	MET
1	F	190	LEU
1	F	193	ILE
1	F	199	LYS
1	F	209	LYS
1	F	211	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	B	223	GLN
1	D	13	ASN
1	D	65	ASN
1	D	79	HIS
1	D	168	GLN
1	E	90	ASN
1	F	65	ASN
1	F	87	ASN
1	F	156	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSD	C	47	1	4,7,8	1.92	1 (25%)	1,8,10	1.53	0
1	CSD	F	47	1	4,7,8	2.05	1 (25%)	1,8,10	1.80	0
1	CSD	D	47	1	4,7,8	1.78	1 (25%)	1,8,10	0.06	0
1	CSD	E	47	1	4,7,8	2.15	1 (25%)	1,8,10	0.17	0
1	CSD	A	47	1	4,7,8	2.20	1 (25%)	1,8,10	0.70	0
1	CSD	B	47	1	4,7,8	1.93	1 (25%)	1,8,10	0.33	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
1	CSD	C	47	1	-	0/2/6/8	-
1	CSD	F	47	1	-	1/2/6/8	-
1	CSD	D	47	1	-	1/2/6/8	-
1	CSD	E	47	1	-	2/2/6/8	-
1	CSD	A	47	1	-	1/2/6/8	-
1	CSD	B	47	1	-	1/2/6/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	CSD	OD1-SG	-4.04	1.44	1.47
1	E	47	CSD	OD1-SG	-3.84	1.44	1.47
1	F	47	CSD	OD1-SG	-3.54	1.44	1.47
1	C	47	CSD	OD1-SG	-3.47	1.44	1.47
1	B	47	CSD	OD1-SG	-3.33	1.44	1.47
1	D	47	CSD	OD1-SG	-3.22	1.44	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	47	CSD	CA-CB-SG-OD1
1	B	47	CSD	CA-CB-SG-OD1
1	D	47	CSD	CA-CB-SG-OD1
1	E	47	CSD	N-CA-CB-SG
1	E	47	CSD	CA-CB-SG-OD1
1	F	47	CSD	CA-CB-SG-OD1

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	47	CSD	2	0
1	F	47	CSD	2	0
1	D	47	CSD	1	0
1	E	47	CSD	5	0
1	A	47	CSD	2	0
1	B	47	CSD	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	220/224 (98%)	-0.46	1 (0%) 87 83	0, 9, 29, 44	0
1	B	220/224 (98%)	-0.41	1 (0%) 87 83	0, 11, 33, 59	0
1	C	216/224 (96%)	-0.38	4 (1%) 66 58	0, 13, 46, 59	0
1	D	212/224 (94%)	0.07	5 (2%) 59 50	2, 33, 64, 71	0
1	E	220/224 (98%)	-0.16	1 (0%) 87 83	1, 24, 54, 76	0
1	F	222/224 (99%)	-0.32	1 (0%) 87 83	0, 15, 35, 64	0
All	All	1310/1344 (97%)	-0.28	13 (0%) 79 73	0, 16, 52, 76	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	ALA	6.9
1	D	12	PRO	3.6
1	D	14	PHE	3.1
1	D	41	ARG	2.6
1	D	112	ILE	2.6
1	D	25	PHE	2.6
1	E	112	ILE	2.4
1	C	208	THR	2.3
1	C	216	LYS	2.3
1	F	120	ALA	2.2
1	A	108	ARG	2.1
1	C	133	VAL	2.0
1	C	207	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSD	D	47	8/9	0.84	0.11	43,43,43,43	0
1	CSD	A	47	8/9	0.94	0.08	5,5,5,5	0
1	CSD	E	47	8/9	0.95	0.09	16,16,16,16	0
1	CSD	B	47	8/9	0.96	0.07	15,15,15,15	0
1	CSD	C	47	8/9	0.97	0.06	8,8,8,8	0
1	CSD	F	47	8/9	0.98	0.05	11,11,11,11	0

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.