



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:21 AM UTC

PDB ID : 2BHN / pdb_00002bhn
Title : XPF from *Aeropyrum pernix*
Authors : Newman, M.; Murray-Rust, J.; Lally, J.; Rudolf, J.; Fadden, A.; Knowles, P.P.; White, M.F.; McDonald, N.Q.
Deposited on : 2005-01-14
Resolution : 3.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

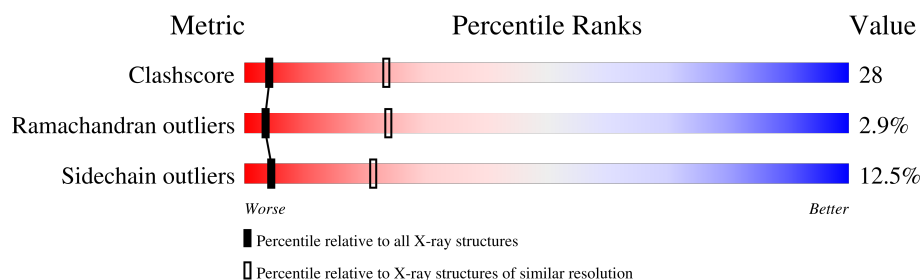
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
1	B	214	
1	C	214	
1	D	214	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5905 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 XPF ENDONUCLEASE.

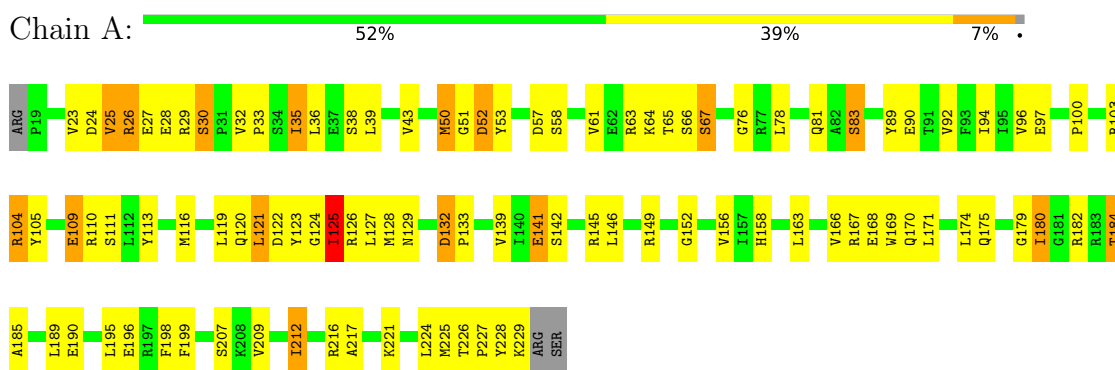
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1551	1001	258	287	5			
1	B	199	Total	C	N	O	S	0	0	0
			1442	934	230	273	5			
1	C	194	Total	C	N	O	S	0	0	0
			1375	886	222	262	5			
1	D	211	Total	C	N	O	S	0	0	0
			1537	985	259	289	4			

3 Residue-property plots

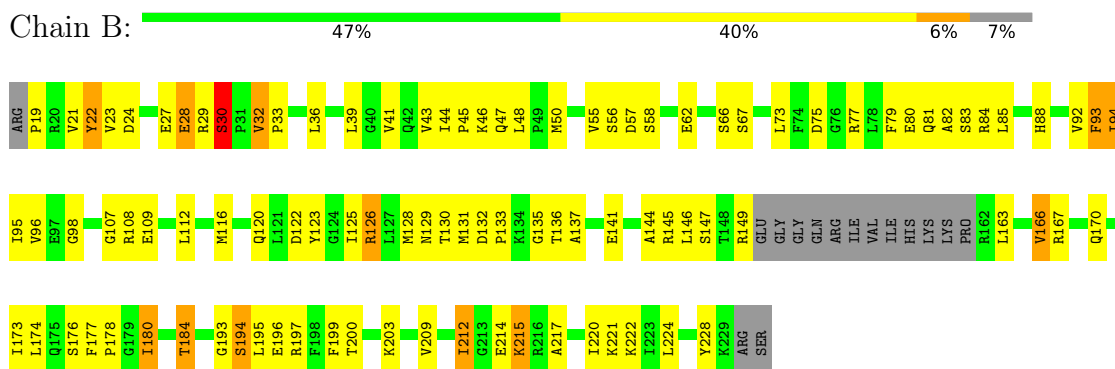
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

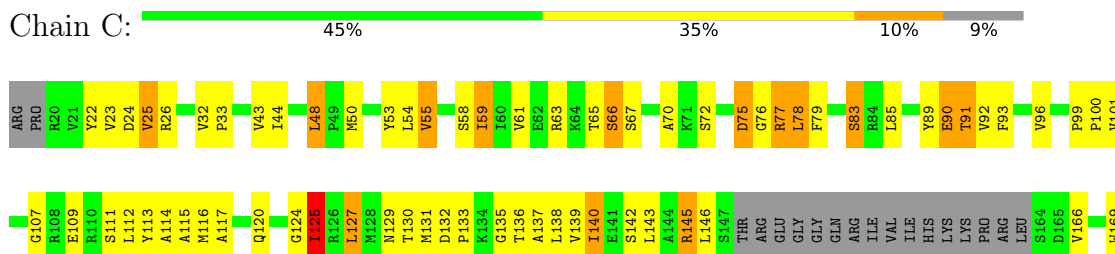
• Molecule 1: XPF ENDONUCLEASE

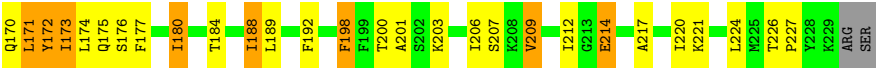


• Molecule 1: XPF ENDONUCLEASE

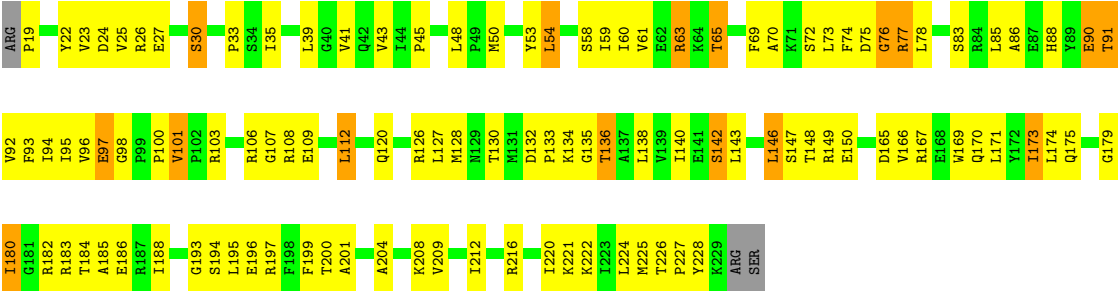


• Molecule 1: XPF ENDONUCLEASE





● Molecule 1: XPF ENDONUCLEASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.32Å 42.75Å 118.74Å 90.00° 121.42° 90.00°	Depositor
Resolution (Å)	25.00 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (25.00-3.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5905	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

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	0.90	0/1582	1.25	12/2153 (0.6%)
1	B	0.95	0/1469	1.25	13/2002 (0.6%)
1	C	1.05	8/1401 (0.6%)	1.16	13/1917 (0.7%)
1	D	0.78	0/1566	1.11	4/2133 (0.2%)
All	All	0.92	8/6018 (0.1%)	1.19	42/8205 (0.5%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	172	TYR	CA-C	13.27	1.70	1.52
1	C	172	TYR	C-O	11.69	1.37	1.24
1	C	171	LEU	C-N	8.55	1.45	1.33
1	C	171	LEU	CA-CB	-7.53	1.40	1.53
1	C	172	TYR	CA-CB	-5.94	1.44	1.53
1	C	171	LEU	CA-C	-5.51	1.45	1.52
1	C	171	LEU	CB-CG	5.46	1.64	1.53
1	C	209	VAL	CA-CB	5.10	1.60	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	LEU	O-C-N	8.32	131.69	122.20
1	A	78	LEU	N-CA-C	7.08	118.69	110.97
1	B	180	ILE	N-CA-C	7.05	118.73	107.73
1	C	99	PRO	CA-C-N	6.84	128.40	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	PRO	C-N-CA	6.84	128.40	119.84
1	A	152	GLY	N-CA-C	-6.76	104.04	115.80
1	B	212	ILE	CB-CA-C	-6.75	102.21	110.99
1	D	222	LYS	N-CA-C	-6.75	103.85	111.07
1	C	180	ILE	N-CA-C	6.27	117.82	108.54
1	A	103	ARG	N-CA-C	-6.03	104.03	111.33
1	B	203	LYS	N-CA-C	-5.99	104.08	111.33
1	B	80	GLU	N-CA-C	-5.94	103.78	111.02
1	B	30	SER	CA-C-N	-5.86	113.71	120.04
1	B	30	SER	C-N-CA	-5.86	113.71	120.04
1	C	172	TYR	O-C-N	-5.82	115.95	122.12
1	D	48	LEU	N-CA-C	5.78	116.68	109.57
1	A	190	GLU	N-CA-C	-5.78	104.89	111.07
1	C	173	ILE	N-CA-C	5.68	115.87	110.42
1	A	30	SER	N-CA-C	5.62	118.15	110.01
1	A	76	GLY	N-CA-C	-5.44	100.28	113.18
1	C	214	GLU	N-CA-C	-5.41	105.30	111.14
1	B	126	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	B	137	ALA	N-CA-C	-5.28	105.42	111.07
1	B	94	ILE	N-CA-CB	5.28	117.39	111.21
1	A	226	THR	CA-C-N	5.28	126.44	119.84
1	A	226	THR	C-N-CA	5.28	126.44	119.84
1	C	59	ILE	N-CA-C	5.26	116.28	107.18
1	D	97	GLU	N-CA-C	5.22	117.75	109.24
1	A	121	LEU	N-CA-C	5.20	116.94	111.28
1	B	32	VAL	CA-C-N	-5.16	113.44	119.32
1	B	32	VAL	C-N-CA	-5.16	113.44	119.32
1	C	171	LEU	CA-C-O	-5.11	114.48	120.20
1	B	93	PHE	CA-C-N	-5.10	116.37	122.90
1	B	93	PHE	C-N-CA	-5.10	116.37	122.90
1	C	171	LEU	CA-C-N	-5.09	113.46	120.28
1	C	171	LEU	C-N-CA	-5.09	113.46	120.28
1	C	226	THR	CA-C-N	5.08	125.80	120.11
1	C	226	THR	C-N-CA	5.08	125.80	120.11
1	A	30	SER	CA-C-N	5.05	124.65	119.05
1	A	30	SER	C-N-CA	5.05	124.65	119.05
1	A	25	VAL	N-CA-C	5.03	115.46	110.23
1	D	59	ILE	CB-CA-C	-5.01	104.89	110.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	172	TYR	Mainchain

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	1551	0	1485	91	0
1	B	1442	0	1354	83	0
1	C	1375	0	1247	78	0
1	D	1537	0	1458	92	0
All	All	5905	0	5544	316	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 28.

All (316) 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:B:95:ILE:HG21	1:B:136:THR:HG23	1.36	1.01
1:D:50:MET:HE1	1:D:88:HIS:HB2	1.49	0.94
1:A:207:SER:HB3	1:A:217:ALA:HB2	1.52	0.90
1:A:24:ASP:OD1	1:A:26:ARG:HG2	1.71	0.90
1:A:128:MET:HE1	1:B:116:MET:HB3	1.51	0.89
1:B:112:LEU:O	1:B:116:MET:HG3	1.72	0.89
1:B:62:GLU:CD	1:B:81:GLN:HE22	1.81	0.89
1:D:23:VAL:HG21	1:D:43:VAL:HG13	1.59	0.84
1:D:90:GLU:HG3	1:D:91:THR:H	1.44	0.82
1:B:180:ILE:HD11	1:B:220:ILE:HD11	1.60	0.81
1:A:128:MET:HE1	1:B:116:MET:CB	2.11	0.81
1:B:50:MET:HE3	1:B:85:LEU:HA	1.62	0.81
1:D:23:VAL:HG21	1:D:43:VAL:CG1	2.10	0.81
1:D:221:LYS:O	1:D:225:MET:HG2	1.81	0.80
1:C:130:THR:HG21	1:C:136:THR:HA	1.64	0.80
1:D:50:MET:CE	1:D:85:LEU:HA	2.11	0.79
1:D:221:LYS:HE3	1:D:225:MET:CE	2.12	0.79
1:C:23:VAL:HG21	1:C:43:VAL:HG13	1.65	0.78
1:A:179:GLY:HA3	1:A:216:ARG:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:VAL:HG22	1:D:93:PHE:HB2	1.67	0.76
1:D:221:LYS:HE3	1:D:225:MET:HE1	1.67	0.76
1:D:109:GLU:HA	1:D:112:LEU:HB2	1.68	0.76
1:D:75:ASP:O	1:D:77:ARG:N	2.18	0.75
1:C:50:MET:HE3	1:C:85:LEU:HA	1.70	0.74
1:C:180:ILE:HD11	1:C:220:ILE:HD11	1.69	0.74
1:D:90:GLU:HG3	1:D:91:THR:N	2.03	0.73
1:D:169:TRP:O	1:D:173:ILE:HG13	1.89	0.73
1:C:132:ASP:HB2	1:C:133:PRO:HD2	1.71	0.72
1:D:35:ILE:O	1:D:39:LEU:HG	1.90	0.72
1:D:50:MET:HB3	1:D:85:LEU:HD22	1.70	0.72
1:B:19:PRO:HB2	1:B:41:VAL:HG22	1.72	0.71
1:A:33:PRO:O	1:A:36:LEU:HB2	1.91	0.71
1:C:23:VAL:CG2	1:C:43:VAL:HG13	2.21	0.70
1:D:50:MET:HE3	1:D:85:LEU:HA	1.71	0.70
1:D:175:GLN:NE2	1:D:182:ARG:HG2	2.05	0.70
1:D:27:GLU:OE2	1:D:63:ARG:HD3	1.90	0.70
1:A:120:GLN:OE1	1:B:93:PHE:HE2	1.74	0.70
1:A:221:LYS:HE3	1:A:225:MET:HE1	1.72	0.70
1:B:22:TYR:HD1	1:B:22:TYR:N	1.90	0.70
1:B:75:ASP:C	1:B:77:ARG:H	2.00	0.69
1:B:46:LYS:C	1:B:47:GLN:CA	2.65	0.69
1:A:221:LYS:HE3	1:A:225:MET:CE	2.22	0.69
1:C:23:VAL:HG21	1:C:43:VAL:CG1	2.22	0.68
1:C:48:LEU:HD21	1:C:54:LEU:HB2	1.74	0.68
1:B:98:GLY:O	1:B:129:ASN:ND2	2.24	0.68
1:A:225:MET:HE2	1:B:196:GLU:OE1	1.93	0.67
1:C:145:ARG:HH11	1:C:145:ARG:HB3	1.60	0.67
1:B:22:TYR:N	1:B:22:TYR:CD1	2.61	0.66
1:A:182:ARG:O	1:A:185:ALA:HB3	1.95	0.66
1:B:173:ILE:O	1:B:176:SER:HB2	1.96	0.65
1:A:120:GLN:OE1	1:B:93:PHE:CE2	2.47	0.65
1:C:92:VAL:HB	1:C:125:ILE:HD12	1.79	0.65
1:A:100:PRO:HG2	1:B:131:MET:HG3	1.77	0.65
1:D:179:GLY:HA3	1:D:216:ARG:HD3	1.78	0.65
1:B:96:VAL:O	1:B:129:ASN:ND2	2.29	0.64
1:D:69:PHE:CE1	1:D:78:LEU:HD21	2.32	0.64
1:D:73:LEU:HA	1:D:78:LEU:HD22	1.80	0.64
1:D:171:LEU:O	1:D:175:GLN:HG3	1.97	0.64
1:C:22:TYR:HD1	1:C:54:LEU:HD23	1.63	0.64
1:D:76:GLY:C	1:D:78:LEU:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:OD1	1:A:26:ARG:CG	2.44	0.63
1:B:180:ILE:HG23	1:B:184:THR:HG22	1.80	0.63
1:C:209:VAL:HB	1:C:212:ILE:HD12	1.81	0.62
1:C:117:ALA:HB1	1:D:143:LEU:HD23	1.81	0.62
1:C:22:TYR:HA	1:C:44:ILE:O	1.98	0.62
1:C:135:GLY:HA2	1:C:138:LEU:HD12	1.80	0.62
1:C:140:ILE:HA	1:C:143:LEU:HD12	1.82	0.62
1:B:46:LYS:O	1:B:47:GLN:CA	2.47	0.62
1:A:92:VAL:HG11	1:A:125:ILE:HD13	1.81	0.61
1:C:227:PRO:HA	1:D:193:GLY:O	2.00	0.61
1:B:33:PRO:HB3	1:B:43:VAL:HG11	1.81	0.61
1:A:124:GLY:O	1:B:126:ARG:NH2	2.33	0.61
1:B:209:VAL:HB	1:B:212:ILE:HD12	1.81	0.61
1:A:94:ILE:HB	1:A:127:LEU:HD23	1.82	0.61
1:B:50:MET:CE	1:B:85:LEU:HA	2.29	0.60
1:C:72:SER:HA	1:C:75:ASP:HB2	1.82	0.60
1:A:23:VAL:HG12	1:A:27:GLU:HB3	1.83	0.60
1:A:25:VAL:O	1:A:26:ARG:C	2.45	0.60
1:C:76:GLY:O	1:C:77:ARG:C	2.45	0.60
1:A:50:MET:HE2	1:A:89:TYR:HE1	1.66	0.59
1:A:50:MET:CE	1:A:89:TYR:HE1	2.15	0.59
1:C:189:LEU:HD13	1:D:228:TYR:CD1	2.36	0.59
1:D:76:GLY:C	1:D:78:LEU:N	2.58	0.59
1:C:79:PHE:O	1:C:83:SER:OG	2.21	0.59
1:D:101:VAL:HG11	1:D:109:GLU:HB3	1.83	0.59
1:D:50:MET:HE2	1:D:85:LEU:HA	1.85	0.58
1:C:135:GLY:O	1:C:139:VAL:HG23	2.04	0.58
1:A:221:LYS:O	1:A:225:MET:HG2	2.02	0.58
1:B:79:PHE:HA	1:B:82:ALA:HB3	1.85	0.58
1:A:126:ARG:HG2	1:A:126:ARG:HH11	1.69	0.58
1:C:207:SER:HB3	1:C:217:ALA:HB2	1.86	0.58
1:B:180:ILE:HD12	1:B:180:ILE:N	2.19	0.58
1:D:175:GLN:HE22	1:D:182:ARG:HG2	1.67	0.58
1:D:73:LEU:CA	1:D:78:LEU:HD22	2.34	0.57
1:B:50:MET:HE1	1:B:88:HIS:HB2	1.85	0.57
1:C:58:SER:CB	1:C:90:GLU:HG2	2.35	0.57
1:C:50:MET:CE	1:C:85:LEU:HA	2.35	0.56
1:A:126:ARG:HG2	1:A:126:ARG:NH1	2.20	0.56
1:A:126:ARG:NH1	1:B:120:GLN:OE1	2.37	0.56
1:D:76:GLY:O	1:D:78:LEU:N	2.39	0.56
1:A:39:LEU:O	1:A:145:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:CE	1:A:225:MET:HE1	2.35	0.55
1:B:214:GLU:O	1:B:215:LYS:C	2.48	0.55
1:C:177:PHE:HB2	1:C:180:ILE:HD12	1.89	0.55
1:A:128:MET:HG3	1:A:139:VAL:HG11	1.87	0.55
1:C:221:LYS:HA	1:C:224:LEU:HD12	1.87	0.55
1:A:196:GLU:HB2	1:B:224:LEU:O	2.06	0.55
1:D:221:LYS:HE3	1:D:225:MET:HE3	1.87	0.55
1:A:27:GLU:C	1:A:29:ARG:N	2.65	0.55
1:A:83:SER:HB3	1:A:123:TYR:HE2	1.73	0.54
1:B:21:VAL:HG12	1:B:55:VAL:HA	1.89	0.54
1:D:19:PRO:HG2	1:D:41:VAL:HG22	1.90	0.54
1:D:30:SER:HB2	1:D:33:PRO:HD3	1.88	0.54
1:C:171:LEU:O	1:C:175:GLN:HG3	2.06	0.54
1:D:70:ALA:O	1:D:74:PHE:HD1	1.90	0.54
1:A:32:VAL:O	1:A:33:PRO:C	2.49	0.54
1:D:72:SER:OG	1:D:78:LEU:HD13	2.07	0.54
1:D:103:ARG:HA	1:D:106:ARG:CB	2.39	0.54
1:C:92:VAL:CB	1:C:125:ILE:HD12	2.37	0.53
1:D:130:THR:HG21	1:D:136:THR:N	2.23	0.53
1:D:134:LYS:O	1:D:138:LEU:N	2.34	0.53
1:A:116:MET:HB3	1:B:128:MET:CE	2.37	0.53
1:D:23:VAL:CG2	1:D:43:VAL:HG13	2.36	0.53
1:D:95:ILE:HG21	1:D:136:THR:HG23	1.90	0.53
1:C:133:PRO:HA	1:C:136:THR:HB	1.89	0.53
1:C:63:ARG:HD2	1:C:136:THR:HG21	1.89	0.53
1:C:136:THR:O	1:C:140:ILE:HG13	2.08	0.53
1:B:36:LEU:O	1:B:39:LEU:HB2	2.09	0.52
1:B:141:GLU:O	1:B:144:ALA:HB3	2.09	0.52
1:A:132:ASP:HB2	1:A:133:PRO:CD	2.39	0.52
1:D:221:LYS:HB3	1:D:225:MET:HE3	1.91	0.52
1:A:53:TYR:HB2	1:A:61:VAL:HB	1.90	0.52
1:A:124:GLY:O	1:A:125:ILE:C	2.52	0.52
1:D:23:VAL:O	1:D:45:PRO:HA	2.09	0.52
1:B:194:SER:HB3	1:B:197:ARG:H	1.74	0.52
1:D:195:LEU:HB3	1:D:199:PHE:CE1	2.45	0.52
1:D:60:ILE:HG13	1:D:61:VAL:N	2.23	0.52
1:D:69:PHE:CD1	1:D:78:LEU:HD11	2.45	0.52
1:A:120:GLN:HE21	1:A:127:LEU:HD12	1.74	0.52
1:D:175:GLN:HA	1:D:180:ILE:HG22	1.92	0.52
1:D:23:VAL:HG13	1:D:53:TYR:CE2	2.46	0.51
1:A:52:ASP:OD2	1:A:63:ARG:N	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:VAL:O	1:B:170:GLN:HG3	2.10	0.51
1:D:130:THR:HG21	1:D:135:GLY:C	2.36	0.50
1:B:163:LEU:O	1:B:166:VAL:HB	2.11	0.50
1:C:192:PHE:CD1	1:C:198:PHE:HB2	2.47	0.50
1:D:133:PRO:O	1:D:136:THR:HB	2.11	0.50
1:D:180:ILE:HG13	1:D:184:THR:HG21	1.92	0.50
1:A:207:SER:HB3	1:A:217:ALA:CB	2.35	0.50
1:B:132:ASP:HB2	1:B:133:PRO:CD	2.41	0.50
1:D:24:ASP:OD1	1:D:26:ARG:HG2	2.12	0.50
1:D:98:GLY:N	1:D:130:THR:O	2.43	0.50
1:B:146:LEU:HD23	1:B:149:ARG:NH1	2.28	0.49
1:C:23:VAL:HG22	1:C:53:TYR:CE2	2.48	0.49
1:C:32:VAL:HG13	1:C:137:ALA:HB2	1.95	0.49
1:D:180:ILE:HG13	1:D:184:THR:CG2	2.42	0.49
1:C:77:ARG:O	1:C:78:LEU:C	2.55	0.49
1:A:26:ARG:NH1	1:A:52:ASP:OD1	2.42	0.49
1:B:96:VAL:O	1:B:129:ASN:HA	2.13	0.49
1:A:64:LYS:O	1:A:96:VAL:HA	2.13	0.49
1:B:27:GLU:O	1:B:29:ARG:N	2.46	0.49
1:B:107:GLY:C	1:B:109:GLU:H	2.21	0.49
1:A:128:MET:CE	1:B:116:MET:HB3	2.34	0.49
1:B:195:LEU:HD13	1:B:199:PHE:HE1	1.78	0.49
1:C:180:ILE:HD11	1:C:220:ILE:CD1	2.38	0.49
1:D:93:PHE:HA	1:D:126:ARG:O	2.12	0.48
1:B:30:SER:HB2	1:B:32:VAL:H	1.77	0.48
1:D:149:ARG:HG3	1:D:149:ARG:O	2.13	0.48
1:A:156:VAL:HG11	1:A:158:HIS:CE1	2.48	0.48
1:C:90:GLU:HG3	1:C:91:THR:N	2.28	0.48
1:D:27:GLU:CD	1:D:30:SER:OG	2.57	0.48
1:C:131:MET:HG3	1:D:100:PRO:HD2	1.95	0.48
1:C:22:TYR:HB2	1:C:54:LEU:HB3	1.95	0.48
1:D:70:ALA:O	1:D:74:PHE:CD1	2.66	0.48
1:C:220:ILE:HG22	1:C:224:LEU:HD11	1.96	0.48
1:C:130:THR:HG21	1:C:136:THR:CA	2.39	0.48
1:D:72:SER:C	1:D:78:LEU:HB2	2.39	0.48
1:B:123:TYR:HB3	1:B:125:ILE:HG13	1.95	0.48
1:D:169:TRP:O	1:D:170:GLN:C	2.57	0.48
1:D:188:ILE:HD11	1:D:212:ILE:HD11	1.96	0.48
1:A:65:THR:HA	1:A:97:GLU:HB3	1.96	0.47
1:A:94:ILE:HD12	1:A:125:ILE:HG21	1.95	0.47
1:B:75:ASP:C	1:B:77:ARG:N	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:VAL:O	1:B:167:ARG:C	2.56	0.47
1:D:201:ALA:O	1:D:221:LYS:NZ	2.45	0.47
1:A:50:MET:CE	1:A:89:TYR:CE1	2.97	0.47
1:B:177:PHE:CB	1:B:180:ILE:HD13	2.44	0.47
1:D:74:PHE:CZ	1:D:108:ARG:HB3	2.50	0.47
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.73	0.47
1:A:179:GLY:C	1:A:216:ARG:NH1	2.72	0.47
1:C:116:MET:HB3	1:D:128:MET:HE1	1.97	0.47
1:C:166:VAL:O	1:C:170:GLN:HG3	2.14	0.47
1:A:92:VAL:HG12	1:A:125:ILE:HG23	1.96	0.47
1:A:149:ARG:HH22	1:B:122:ASP:CG	2.22	0.47
1:C:66:SER:HB3	1:C:96:VAL:CG1	2.45	0.47
1:C:66:SER:HB3	1:C:96:VAL:HG13	1.96	0.47
1:C:133:PRO:O	1:C:136:THR:HB	2.14	0.47
1:C:177:PHE:CB	1:C:180:ILE:HD12	2.44	0.47
1:D:194:SER:HB2	1:D:197:ARG:HB2	1.96	0.47
1:C:61:VAL:HG22	1:C:93:PHE:HB2	1.96	0.47
1:D:74:PHE:HZ	1:D:108:ARG:HB3	1.79	0.47
1:B:132:ASP:HB2	1:B:133:PRO:HD2	1.96	0.47
1:C:170:GLN:O	1:C:173:ILE:HB	2.14	0.47
1:B:141:GLU:O	1:B:145:ARG:HG3	2.14	0.46
1:A:27:GLU:C	1:A:29:ARG:H	2.23	0.46
1:C:24:ASP:OD1	1:C:26:ARG:HG3	2.15	0.46
1:C:96:VAL:HB	1:C:129:ASN:OD1	2.14	0.46
1:A:125:ILE:H	1:A:125:ILE:HG12	1.59	0.46
1:B:23:VAL:CG2	1:B:43:VAL:HG13	2.45	0.46
1:A:132:ASP:OD2	1:A:132:ASP:N	2.48	0.46
1:B:24:ASP:HB2	1:B:48:LEU:HB2	1.97	0.46
1:D:166:VAL:O	1:D:170:GLN:HG3	2.16	0.46
1:B:27:GLU:O	1:B:28:GLU:C	2.59	0.46
1:A:25:VAL:C	1:A:27:GLU:N	2.72	0.45
1:B:73:LEU:C	1:B:75:ASP:H	2.24	0.45
1:A:225:MET:HE2	1:A:225:MET:HB3	1.83	0.45
1:B:83:SER:O	1:B:84:ARG:C	2.60	0.45
1:C:67:SER:O	1:C:70:ALA:HB3	2.16	0.45
1:D:182:ARG:NH1	1:D:186:GLU:OE2	2.48	0.45
1:A:167:ARG:O	1:A:170:GLN:HB2	2.16	0.45
1:C:93:PHE:HE2	1:D:120:GLN:OE1	1.99	0.45
1:B:62:GLU:HB3	1:B:94:ILE:HG12	1.98	0.45
1:D:86:ALA:HA	1:D:92:VAL:HG21	1.98	0.45
1:A:109:GLU:O	1:A:110:ARG:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ASP:HB3	1:D:167:ARG:H	1.82	0.45
1:A:35:ILE:O	1:A:38:SER:HB2	2.17	0.44
1:C:192:PHE:CG	1:C:198:PHE:HB2	2.51	0.44
1:C:201:ALA:HB3	1:C:206:ILE:HD11	1.99	0.44
1:C:50:MET:CE	1:C:89:TYR:HE1	2.30	0.44
1:D:94:ILE:HG22	1:D:96:VAL:HG23	1.99	0.44
1:A:227:PRO:HA	1:B:193:GLY:O	2.17	0.44
1:A:168:GLU:HA	1:A:171:LEU:HD12	1.99	0.44
1:B:23:VAL:HG23	1:B:43:VAL:HG13	1.98	0.44
1:C:120:GLN:NE2	1:C:127:LEU:HB2	2.33	0.44
1:D:22:TYR:O	1:D:53:TYR:HA	2.18	0.44
1:A:104:ARG:HG2	1:A:105:TYR:CE1	2.52	0.44
1:A:198:PHE:HD2	1:A:199:PHE:CD1	2.36	0.44
1:A:224:LEU:HA	1:A:224:LEU:HD23	1.70	0.44
1:A:228:TYR:CG	1:A:229:LYS:N	2.85	0.44
1:A:113:TYR:CE1	1:B:135:GLY:HA2	2.53	0.43
1:A:141:GLU:OE2	1:A:145:ARG:NE	2.51	0.43
1:A:189:LEU:HD13	1:B:228:TYR:CD1	2.53	0.43
1:B:44:ILE:HA	1:B:45:PRO:HD3	1.90	0.43
1:D:167:ARG:O	1:D:171:LEU:HG	2.18	0.43
1:A:166:VAL:HG21	1:B:222:LYS:HZ2	1.82	0.43
1:A:96:VAL:O	1:A:129:ASN:ND2	2.51	0.43
1:A:174:LEU:HG	1:A:195:LEU:HD21	2.00	0.43
1:D:220:ILE:HG22	1:D:224:LEU:HD12	2.01	0.43
1:C:124:GLY:O	1:C:125:ILE:C	2.61	0.43
1:A:179:GLY:O	1:A:216:ARG:NH1	2.51	0.43
1:D:75:ASP:C	1:D:77:ARG:H	2.17	0.43
1:A:175:GLN:HA	1:A:180:ILE:HG22	2.00	0.43
1:B:123:TYR:CB	1:B:125:ILE:HG13	2.49	0.43
1:C:184:THR:O	1:C:188:ILE:HD12	2.17	0.43
1:B:23:VAL:HG12	1:B:27:GLU:HB3	2.00	0.43
1:C:120:GLN:NE2	1:D:128:MET:SD	2.86	0.43
1:A:179:GLY:C	1:A:216:ARG:HH11	2.27	0.43
1:A:189:LEU:HB3	1:B:228:TYR:CD1	2.53	0.43
1:D:142:SER:O	1:D:146:LEU:HG	2.18	0.43
1:A:63:ARG:HH21	1:A:97:GLU:CD	2.26	0.43
1:B:214:GLU:O	1:B:217:ALA:N	2.51	0.43
1:A:120:GLN:HE22	1:B:128:MET:HG2	1.83	0.43
1:B:200:THR:HG22	1:B:200:THR:O	2.18	0.43
1:C:116:MET:HG2	1:C:127:LEU:HD11	2.01	0.43
1:B:130:THR:HG21	1:B:136:THR:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:O	1:A:27:GLU:HB3	2.19	0.42
1:C:173:ILE:O	1:C:176:SER:HB2	2.19	0.42
1:D:136:THR:O	1:D:140:ILE:HG13	2.20	0.42
1:A:166:VAL:HG21	1:B:222:LYS:NZ	2.34	0.42
1:B:195:LEU:HD13	1:B:199:PHE:CE1	2.55	0.42
1:D:65:THR:HA	1:D:97:GLU:HB3	2.01	0.42
1:D:194:SER:HB2	1:D:197:ARG:H	1.84	0.42
1:A:50:MET:HE2	1:A:50:MET:HB2	1.72	0.42
1:A:122:ASP:OD1	1:B:149:ARG:NH2	2.50	0.42
1:A:169:TRP:CZ2	1:B:178:PRO:HB3	2.54	0.42
1:C:50:MET:HE2	1:C:89:TYR:HE1	1.84	0.42
1:D:226:THR:HA	1:D:227:PRO:HD3	1.87	0.42
1:C:53:TYR:HB2	1:C:61:VAL:HB	2.01	0.42
1:C:59:ILE:HG12	1:C:91:THR:HB	2.02	0.42
1:D:209:VAL:HB	1:D:212:ILE:HD12	2.02	0.42
1:A:66:SER:O	1:A:67:SER:C	2.62	0.42
1:B:174:LEU:HG	1:B:195:LEU:HD21	2.01	0.42
1:B:95:ILE:HG21	1:B:136:THR:CG2	2.27	0.41
1:B:177:PHE:HB2	1:B:180:ILE:HD13	2.01	0.41
1:C:169:TRP:O	1:C:173:ILE:HG13	2.19	0.41
1:C:59:ILE:HG12	1:C:91:THR:CG2	2.50	0.41
1:C:214:GLU:O	1:C:217:ALA:HB3	2.20	0.41
1:D:75:ASP:C	1:D:77:ARG:N	2.77	0.41
1:D:200:THR:O	1:D:200:THR:HG22	2.20	0.41
1:C:139:VAL:O	1:C:143:LEU:HG	2.20	0.41
1:C:113:TYR:O	1:C:114:ALA:C	2.64	0.41
1:C:23:VAL:HG12	1:C:24:ASP:O	2.20	0.41
1:C:101:VAL:HG22	1:C:112:LEU:HD12	2.02	0.41
1:D:22:TYR:HB2	1:D:54:LEU:HB3	2.01	0.41
1:A:170:GLN:HA	1:A:195:LEU:HD11	2.01	0.41
1:C:174:LEU:HD13	1:C:188:ILE:CG2	2.50	0.41
1:B:220:ILE:O	1:B:221:LYS:C	2.63	0.41
1:C:32:VAL:O	1:C:33:PRO:C	2.64	0.41
1:A:27:GLU:O	1:A:30:SER:N	2.45	0.41
1:A:132:ASP:HB2	1:A:133:PRO:HD2	2.02	0.41
1:A:209:VAL:HB	1:A:212:ILE:HD12	2.02	0.41
1:B:107:GLY:C	1:B:109:GLU:N	2.77	0.41
1:D:174:LEU:HD23	1:D:174:LEU:HA	1.92	0.41
1:D:195:LEU:O	1:D:196:GLU:C	2.64	0.41
1:A:30:SER:HB2	1:A:33:PRO:HD3	2.02	0.41
1:C:65:THR:O	1:C:67:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ALA:O	1:C:116:MET:C	2.64	0.41
1:D:182:ARG:O	1:D:185:ALA:HB3	2.20	0.41
1:B:109:GLU:HA	1:B:112:LEU:HD12	2.04	0.40
1:A:83:SER:HB3	1:A:123:TYR:CE2	2.55	0.40
1:B:92:VAL:HG11	1:B:125:ILE:HD13	2.03	0.40
1:D:61:VAL:HG11	1:D:95:ILE:HD12	2.01	0.40
1:C:174:LEU:HD13	1:C:188:ILE:HG21	2.04	0.40
1:A:27:GLU:O	1:A:29:ARG:N	2.54	0.40
1:A:142:SER:O	1:A:146:LEU:HD12	2.21	0.40
1:A:184:THR:O	1:A:185:ALA:C	2.64	0.40

There are no symmetry-related clashes.

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	209/214 (98%)	179 (86%)	25 (12%)	5 (2%)	4	28
1	B	193/214 (90%)	167 (86%)	22 (11%)	4 (2%)	5	31
1	C	190/214 (89%)	158 (83%)	23 (12%)	9 (5%)	2	14
1	D	209/214 (98%)	172 (82%)	32 (15%)	5 (2%)	4	28
All	All	801/856 (94%)	676 (84%)	102 (13%)	23 (3%)	3	24

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	ILE
1	B	215	LYS
1	C	77	ARG
1	C	78	LEU
1	A	28	GLU

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Mol	Chain	Res	Type
1	A	57	ASP
1	B	57	ASP
1	D	76	GLY
1	D	77	ARG
1	B	28	GLU
1	B	56	SER
1	A	163	LEU
1	C	203	LYS
1	D	107	GLY
1	D	146	LEU
1	C	25	VAL
1	C	66	SER
1	C	100	PRO
1	C	125	ILE
1	D	204	ALA
1	A	51	GLY
1	C	107	GLY
1	C	55	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	150/187 (80%)	130 (87%)	20 (13%)	4	19
1	B	139/187 (74%)	129 (93%)	10 (7%)	13	44
1	C	125/187 (67%)	107 (86%)	18 (14%)	3	16
1	D	148/187 (79%)	126 (85%)	22 (15%)	3	15
All	All	562/748 (75%)	492 (88%)	70 (12%)	4	21

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	35	ILE
1	A	43	VAL

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Mol	Chain	Res	Type
1	A	50	MET
1	A	52	ASP
1	A	58	SER
1	A	67	SER
1	A	81	GLN
1	A	83	SER
1	A	90	GLU
1	A	104	ARG
1	A	109	GLU
1	A	111	SER
1	A	121	LEU
1	A	125	ILE
1	A	132	ASP
1	A	141	GLU
1	A	180	ILE
1	A	184	THR
1	A	212	ILE
1	B	22	TYR
1	B	30	SER
1	B	58	SER
1	B	66	SER
1	B	67	SER
1	B	108	ARG
1	B	147	SER
1	B	166	VAL
1	B	184	THR
1	B	194	SER
1	C	25	VAL
1	C	48	LEU
1	C	55	VAL
1	C	75	ASP
1	C	83	SER
1	C	90	GLU
1	C	91	THR
1	C	109	GLU
1	C	111	SER
1	C	125	ILE
1	C	127	LEU
1	C	140	ILE
1	C	142	SER
1	C	145	ARG
1	C	146	LEU

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Mol	Chain	Res	Type
1	C	188	ILE
1	C	198	PHE
1	C	200	THR
1	D	25	VAL
1	D	30	SER
1	D	54	LEU
1	D	58	SER
1	D	63	ARG
1	D	65	THR
1	D	83	SER
1	D	90	GLU
1	D	91	THR
1	D	101	VAL
1	D	112	LEU
1	D	127	LEU
1	D	132	ASP
1	D	136	THR
1	D	142	SER
1	D	147	SER
1	D	148	THR
1	D	150	GLU
1	D	173	ILE
1	D	180	ILE
1	D	183	ARG
1	D	208	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	129	ASN
1	A	158	HIS
1	B	42	GLN
1	C	170	GLN
1	D	81	GLN
1	D	175	GLN

5.3.3 RNA ⓘ

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.