



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:29 PM EDT

PDB ID : 5KH0 / pdb_00005kh0
Title : Crystal Structure of HydF from thermosipho melanesiensis in complex with a [4Fe-4S] cluster
Authors : Caserta, G.; Pecqueur, L.; Fontecave, M.
Deposited on : 2016-06-14
Resolution : 2.80 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

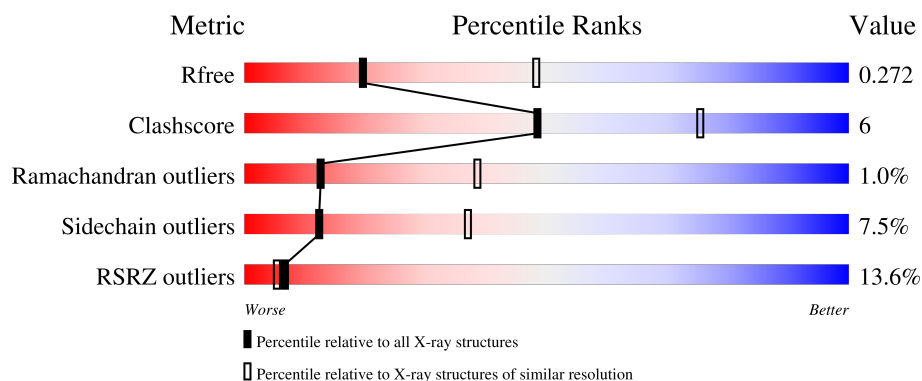
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	396	
1	B	396	
1	C	396	
1	D	396	

2 Entry composition [i](#)

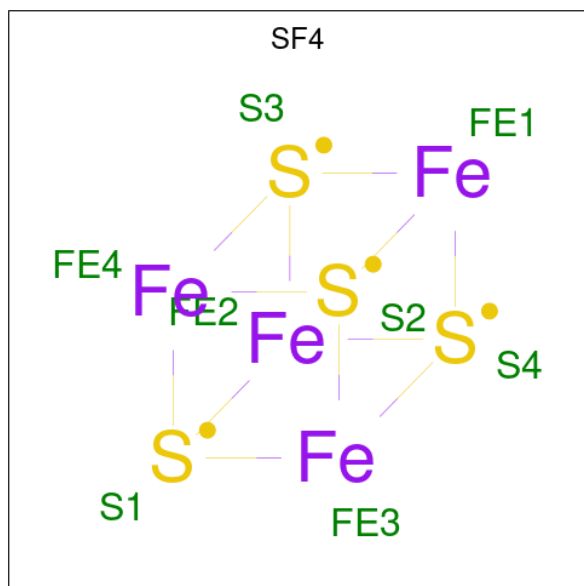
There are 2 unique types of molecules in this entry. The entry contains 11371 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Small GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2863	1833	489	525	16			
1	B	363	Total	C	N	O	S	0	0	0
			2854	1829	486	523	16			
1	C	356	Total	C	N	O	S	0	0	0
			2807	1798	482	511	16			
1	D	356	Total	C	N	O	S	0	0	0
			2815	1804	482	513	16			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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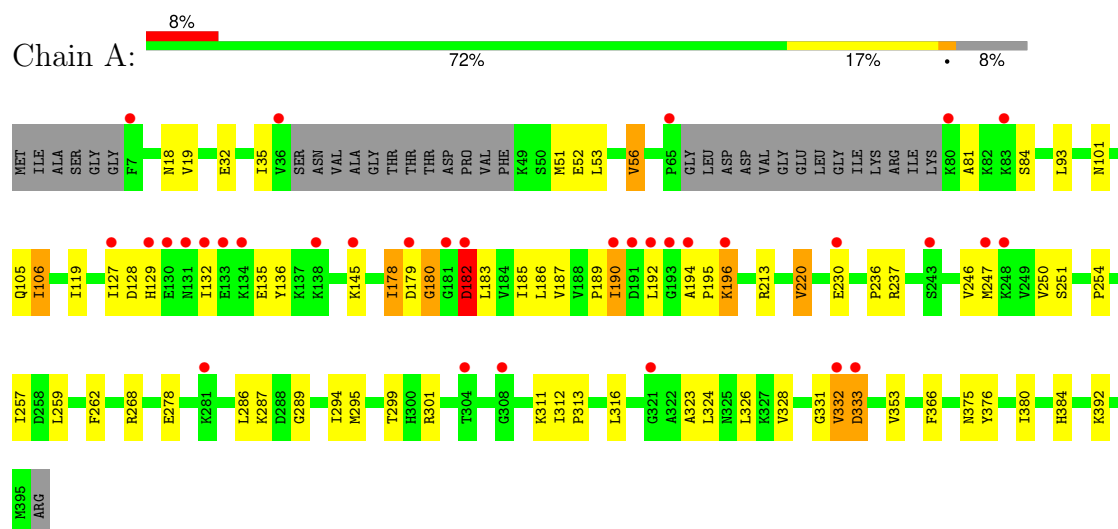
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

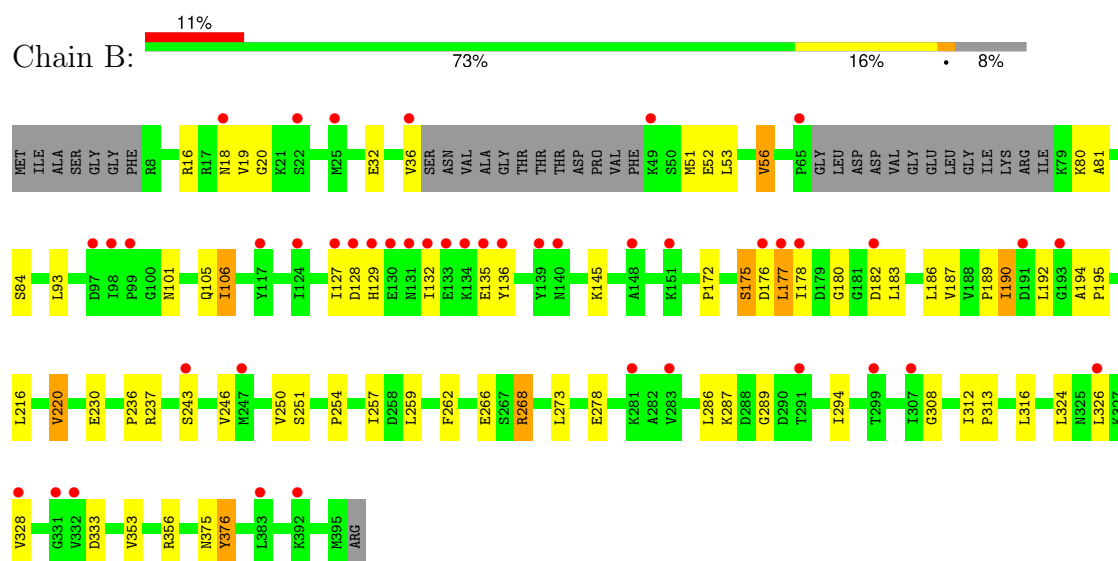
3 Residue-property plots [i](#)

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

• Molecule 1: Small GTP-binding protein

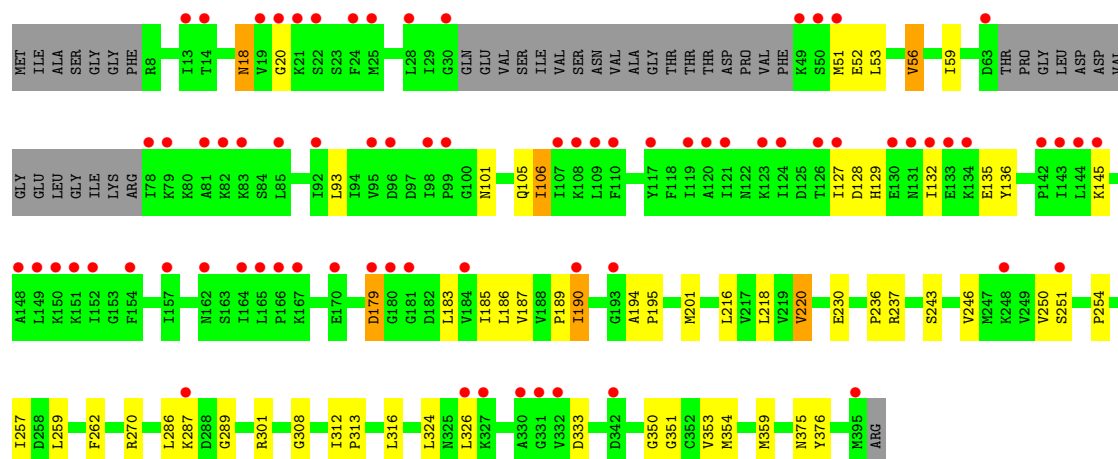


• Molecule 1: Small GTP-binding protein

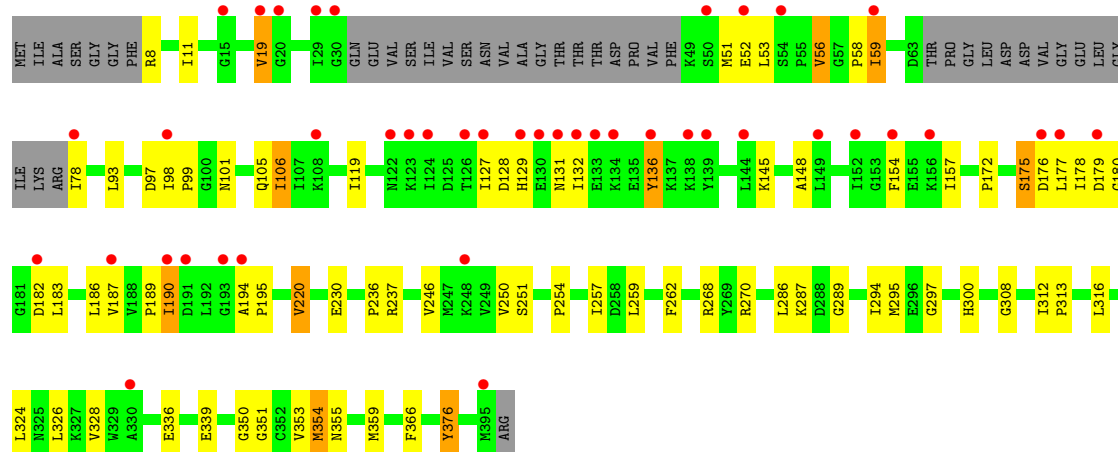


• Molecule 1: Small GTP-binding protein





• Molecule 1: Small GTP-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.01Å 173.48Å 89.32Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	47.62 – 2.80 47.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.62-2.80) 95.2 (47.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.233 , 0.262 0.245 , 0.272	Depositor DCC
R_{free} test set	1948 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11371	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	0.86	1/2907 (0.0%)	1.33	9/3924 (0.2%)
1	B	0.86	1/2898 (0.0%)	1.34	12/3913 (0.3%)
1	C	0.84	1/2850 (0.0%)	1.33	4/3843 (0.1%)
1	D	0.89	2/2858 (0.1%)	1.35	8/3854 (0.2%)
All	All	0.86	5/11513 (0.0%)	1.34	33/15534 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	354	MET	SD-CE	-6.80	1.62	1.79
1	A	312	ILE	CA-CB	5.61	1.57	1.54
1	C	312	ILE	CA-CB	5.57	1.57	1.54
1	B	312	ILE	CA-CB	5.38	1.57	1.54
1	D	312	ILE	CA-CB	5.09	1.57	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	CA-CB-CG	8.81	121.41	112.60
1	B	81	ALA	CA-C-N	7.09	129.78	120.28
1	B	81	ALA	C-N-CA	7.09	129.78	120.28
1	B	81	ALA	N-CA-C	-6.19	105.48	113.16
1	D	179	ASP	N-CA-C	6.11	118.70	109.23
1	B	20	GLY	CA-C-N	5.73	128.42	120.29
1	B	20	GLY	C-N-CA	5.73	128.42	120.29
1	C	20	GLY	CA-C-N	5.52	127.68	120.28
1	C	20	GLY	C-N-CA	5.52	127.68	120.28
1	B	376	TYR	N-CA-C	-5.33	105.55	111.36
1	A	81	ALA	N-CA-C	-5.32	106.74	113.18
1	A	311	LYS	CA-C-N	5.32	124.58	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	LYS	C-N-CA	5.32	124.58	120.33
1	B	268	ARG	CA-C-N	5.27	127.65	120.54
1	B	268	ARG	C-N-CA	5.27	127.65	120.54
1	B	266	GLU	CA-C-N	5.21	127.58	120.54
1	B	266	GLU	C-N-CA	5.21	127.58	120.54
1	D	182	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	18	ASN	CA-C-N	5.18	127.83	120.53
1	C	18	ASN	C-N-CA	5.18	127.83	120.53
1	D	376	TYR	CA-C-N	5.16	125.67	119.94
1	D	376	TYR	C-N-CA	5.16	125.67	119.94
1	A	376	TYR	N-CA-C	-5.13	105.77	111.36
1	D	355	ASN	CA-C-N	5.13	127.15	120.28
1	D	355	ASN	C-N-CA	5.13	127.15	120.28
1	B	376	TYR	CA-C-N	5.11	125.66	119.98
1	B	376	TYR	C-N-CA	5.11	125.66	119.98
1	A	268	ARG	CA-C-N	5.11	127.44	120.54
1	A	268	ARG	C-N-CA	5.11	127.44	120.54
1	D	179	ASP	CA-C-N	5.05	126.96	122.47
1	D	179	ASP	C-N-CA	5.05	126.96	122.47
1	A	323	ALA	CA-C-N	5.00	128.18	120.82
1	A	323	ALA	C-N-CA	5.00	128.18	120.82

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	2863	0	2987	29	0
1	B	2854	0	2974	33	0
1	C	2807	0	2929	25	0
1	D	2815	0	2947	42	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11371	0	11837	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (128) 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:189:PRO:HD2	1:D:220:VAL:O	1.69	0.92
1:A:189:PRO:HD2	1:A:220:VAL:O	1.70	0.92
1:C:189:PRO:HD2	1:C:220:VAL:O	1.71	0.90
1:B:189:PRO:HD2	1:B:220:VAL:O	1.73	0.89
1:D:11:ILE:CD1	1:D:59:ILE:HG13	2.03	0.88
1:D:351:GLY:HA3	1:D:354:MET:HE2	1.55	0.87
1:A:194:ALA:HB1	1:A:195:PRO:HD2	1.63	0.80
1:C:194:ALA:HB1	1:C:195:PRO:HD2	1.64	0.80
1:B:93:LEU:HD13	1:B:106:ILE:HD11	1.61	0.79
1:B:16:ARG:HE	1:B:18:ASN:HD21	1.31	0.79
1:C:351:GLY:HA3	1:C:354:MET:HE2	1.67	0.76
1:D:194:ALA:HB1	1:D:195:PRO:HD2	1.69	0.75
1:B:194:ALA:HB1	1:B:195:PRO:HD2	1.67	0.74
1:D:183:LEU:HD21	1:D:237:ARG:HH11	1.55	0.71
1:D:11:ILE:HD13	1:D:59:ILE:HG13	1.71	0.71
1:B:183:LEU:HD13	1:B:237:ARG:HG2	1.72	0.71
1:B:51:MET:HE2	1:B:53:LEU:HB2	1.74	0.69
1:A:129:HIS:HA	1:A:145:LYS:HE3	1.75	0.68
1:B:129:HIS:HA	1:B:145:LYS:HE3	1.75	0.68
1:C:129:HIS:HA	1:C:145:LYS:HE3	1.76	0.68
1:D:177:LEU:HD13	1:D:268:ARG:NH2	2.09	0.67
1:C:354:MET:HE1	1:C:359:MET:SD	2.36	0.66
1:D:129:HIS:HA	1:D:145:LYS:HE3	1.77	0.65
1:D:180:GLY:H	1:D:183:LEU:HD22	1.63	0.62
1:B:186:LEU:HD13	1:B:236:PRO:HB3	1.84	0.59
1:D:186:LEU:HD13	1:D:236:PRO:HB3	1.85	0.58
1:C:187:VAL:HG13	1:C:262:PHE:HZ	1.69	0.58
1:D:187:VAL:HG13	1:D:262:PHE:HZ	1.69	0.58
1:B:194:ALA:HB1	1:B:195:PRO:CD	2.34	0.58
1:D:194:ALA:HB1	1:D:195:PRO:CD	2.34	0.57
1:B:254:PRO:HD2	1:B:257:ILE:HD12	1.86	0.57
1:C:186:LEU:HD13	1:C:236:PRO:HB3	1.86	0.57
1:A:186:LEU:HD13	1:A:236:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:HG13	1:A:262:PHE:HZ	1.70	0.57
1:A:380:ILE:O	1:A:384:HIS:HD2	1.88	0.56
1:D:254:PRO:HD2	1:D:257:ILE:HD12	1.87	0.56
1:A:178:ILE:C	1:A:180:GLY:H	2.12	0.56
1:A:196:LYS:HE2	1:A:196:LYS:H	1.70	0.56
1:A:254:PRO:HD2	1:A:257:ILE:HD12	1.88	0.55
1:A:183:LEU:HD13	1:A:237:ARG:HG2	1.88	0.55
1:C:194:ALA:HB1	1:C:195:PRO:CD	2.35	0.55
1:C:179:ASP:HB2	1:C:237:ARG:HH12	1.72	0.54
1:B:132:ILE:HB	1:B:145:LYS:HE2	1.90	0.54
1:B:93:LEU:HD13	1:B:106:ILE:CD1	2.35	0.54
1:B:187:VAL:HG13	1:B:262:PHE:HZ	1.72	0.54
1:A:132:ILE:HB	1:A:145:LYS:HE2	1.90	0.53
1:C:132:ILE:HB	1:C:145:LYS:HE2	1.91	0.53
1:C:254:PRO:HD2	1:C:257:ILE:HD12	1.90	0.53
1:B:180:GLY:H	1:B:183:LEU:HD12	1.74	0.53
1:D:294:ILE:HB	1:D:328:VAL:HG22	1.91	0.52
1:B:183:LEU:HD13	1:B:237:ARG:CG	2.40	0.52
1:C:183:LEU:HD13	1:C:237:ARG:HG2	1.91	0.52
1:D:313:PRO:HB3	1:D:326:LEU:HG	1.90	0.52
1:D:148:ALA:HA	1:D:154:PHE:HE1	1.75	0.52
1:D:351:GLY:CA	1:D:354:MET:HE2	2.35	0.52
1:C:93:LEU:HD13	1:C:106:ILE:HG21	1.92	0.51
1:A:179:ASP:HA	1:A:213:ARG:NH2	2.26	0.51
1:C:313:PRO:HB3	1:C:326:LEU:HG	1.93	0.51
1:B:101:ASN:O	1:B:105:GLN:HB2	2.10	0.51
1:A:101:ASN:O	1:A:105:GLN:HB2	2.11	0.51
1:A:313:PRO:HB3	1:A:326:LEU:HG	1.92	0.51
1:D:8:ARG:HB3	1:D:58:PRO:HB2	1.91	0.50
1:A:194:ALA:HB1	1:A:195:PRO:CD	2.35	0.50
1:B:172:PRO:HB2	1:B:177:LEU:HG	1.93	0.50
1:B:313:PRO:HB3	1:B:326:LEU:HG	1.93	0.50
1:B:190:ILE:HD12	1:B:190:ILE:H	1.77	0.50
1:C:101:ASN:O	1:C:105:GLN:HB2	2.12	0.50
1:D:132:ILE:HB	1:D:145:LYS:HE2	1.93	0.50
1:D:101:ASN:O	1:D:105:GLN:HB2	2.12	0.49
1:D:177:LEU:HD13	1:D:268:ARG:CZ	2.43	0.48
1:A:332:VAL:O	1:A:333:ASP:HB2	2.13	0.48
1:B:268:ARG:HH21	1:B:356:ARG:HH12	1.61	0.48
1:D:295:MET:HE1	1:D:366:PHE:HZ	1.80	0.47
1:A:190:ILE:HD12	1:A:190:ILE:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD11	1:B:237:ARG:HH11	1.79	0.47
1:A:183:LEU:HD11	1:A:237:ARG:HH11	1.81	0.46
1:C:190:ILE:H	1:C:190:ILE:HD12	1.79	0.46
1:D:154:PHE:HD2	1:D:157:ILE:CD1	2.28	0.46
1:D:336:GLU:HB2	1:D:339:GLU:HG3	1.97	0.46
1:A:53:LEU:O	1:A:56:VAL:O	2.34	0.46
1:C:51:MET:HE2	1:C:53:LEU:HB2	1.98	0.46
1:D:190:ILE:H	1:D:190:ILE:HD12	1.80	0.46
1:B:182:ASP:CB	1:D:300:HIS:O	2.63	0.46
1:C:190:ILE:H	1:C:190:ILE:CD1	2.30	0.45
1:D:93:LEU:HD13	1:D:106:ILE:HG21	1.98	0.45
1:B:268:ARG:NH2	1:B:356:ARG:HH12	2.14	0.45
1:D:354:MET:HE1	1:D:359:MET:SD	2.56	0.45
1:A:93:LEU:HD13	1:A:106:ILE:HG21	1.98	0.45
1:A:295:MET:HE1	1:A:366:PHE:HZ	1.81	0.45
1:B:180:GLY:N	1:B:183:LEU:HD12	2.31	0.45
1:A:180:GLY:C	1:A:182:ASP:H	2.25	0.45
1:C:246:VAL:O	1:C:250:VAL:HG23	2.16	0.45
1:B:268:ARG:HD2	1:B:273:LEU:HB3	1.99	0.45
1:A:246:VAL:O	1:A:250:VAL:HG23	2.17	0.45
1:A:287:LYS:HD3	1:A:289:GLY:H	1.82	0.45
1:A:294:ILE:HB	1:A:328:VAL:HG22	1.99	0.44
1:B:246:VAL:O	1:B:250:VAL:HG23	2.17	0.44
1:D:190:ILE:H	1:D:190:ILE:CD1	2.30	0.44
1:C:270:ARG:HD2	1:C:350:GLY:O	2.17	0.44
1:C:53:LEU:O	1:C:56:VAL:O	2.36	0.44
1:D:119:ILE:HD13	1:D:136:TYR:CD1	2.53	0.44
1:D:286:LEU:HB3	1:D:324:LEU:HD21	2.00	0.44
1:A:380:ILE:O	1:A:384:HIS:CD2	2.68	0.43
1:B:172:PRO:HB3	1:B:175:SER:OG	2.17	0.43
1:C:287:LYS:HD3	1:C:289:GLY:H	1.83	0.43
1:D:287:LYS:HD3	1:D:289:GLY:H	1.83	0.43
1:B:53:LEU:O	1:B:56:VAL:O	2.35	0.43
1:B:286:LEU:HB3	1:B:324:LEU:HD21	2.00	0.43
1:A:286:LEU:HB3	1:A:324:LEU:HD21	2.01	0.43
1:D:246:VAL:O	1:D:250:VAL:HG23	2.18	0.43
1:B:287:LYS:HD3	1:B:289:GLY:H	1.82	0.43
1:D:98:ILE:HG13	1:D:99:PRO:HD2	2.01	0.43
1:C:286:LEU:HB3	1:C:324:LEU:HD21	2.00	0.43
1:D:308:GLY:HA3	1:D:376:TYR:CZ	2.54	0.42
1:D:175:SER:C	1:D:177:LEU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ARG:HD2	1:D:350:GLY:O	2.20	0.42
1:D:297:GLY:HA3	1:D:354:MET:SD	2.59	0.42
1:B:294:ILE:HB	1:B:328:VAL:HG22	2.01	0.42
1:D:53:LEU:O	1:D:56:VAL:O	2.37	0.42
1:C:308:GLY:HA3	1:C:376:TYR:CZ	2.55	0.41
1:A:299:THR:CG2	1:A:331:GLY:HA2	2.50	0.41
1:B:308:GLY:HA3	1:B:376:TYR:CZ	2.55	0.41
1:D:8:ARG:CB	1:D:58:PRO:HB2	2.51	0.41
1:A:51:MET:HE2	1:A:53:LEU:HB2	2.03	0.41
1:C:186:LEU:HG	1:C:218:LEU:HD23	2.03	0.40
1:B:175:SER:C	1:B:177:LEU:N	2.79	0.40
1:D:172:PRO:HB2	1:D:177:LEU:HD12	2.03	0.40
1:D:183:LEU:HD23	1:D:237:ARG:HG2	2.04	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	357/396 (90%)	335 (94%)	18 (5%)	4 (1%)	11	36
1	B	357/396 (90%)	338 (95%)	15 (4%)	4 (1%)	11	36
1	C	350/396 (88%)	330 (94%)	18 (5%)	2 (1%)	21	51
1	D	350/396 (88%)	327 (93%)	19 (5%)	4 (1%)	11	36
All	All	1414/1584 (89%)	1330 (94%)	70 (5%)	14 (1%)	12	38

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	SER
1	B	177	LEU

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Mol	Chain	Res	Type
1	C	179	ASP
1	D	19	VAL
1	D	175	SER
1	B	176	ASP
1	D	176	ASP
1	A	180	GLY
1	A	333	ASP
1	A	136	TYR
1	A	182	ASP
1	B	136	TYR
1	C	136	TYR
1	D	136	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/348 (92%)	292 (91%)	29 (9%)	9	28
1	B	319/348 (92%)	294 (92%)	25 (8%)	11	35
1	C	312/348 (90%)	290 (93%)	22 (7%)	13	39
1	D	315/348 (90%)	296 (94%)	19 (6%)	17	47
All	All	1267/1392 (91%)	1172 (92%)	95 (8%)	12	37

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	19	VAL
1	A	32	GLU
1	A	35	ILE
1	A	52	GLU
1	A	56	VAL
1	A	84	SER
1	A	106	ILE
1	A	119	ILE

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Mol	Chain	Res	Type
1	A	127	ILE
1	A	128	ASP
1	A	135	GLU
1	A	178	ILE
1	A	185	ILE
1	A	190	ILE
1	A	192	LEU
1	A	196	LYS
1	A	220	VAL
1	A	230	GLU
1	A	247	MET
1	A	251	SER
1	A	259	LEU
1	A	278	GLU
1	A	301	ARG
1	A	316	LEU
1	A	332	VAL
1	A	353	VAL
1	A	375	ASN
1	A	392	LYS
1	B	19	VAL
1	B	32	GLU
1	B	36	VAL
1	B	52	GLU
1	B	56	VAL
1	B	80	LYS
1	B	84	SER
1	B	106	ILE
1	B	127	ILE
1	B	128	ASP
1	B	135	GLU
1	B	178	ILE
1	B	190	ILE
1	B	192	LEU
1	B	216	LEU
1	B	220	VAL
1	B	230	GLU
1	B	243	SER
1	B	251	SER
1	B	259	LEU
1	B	278	GLU
1	B	316	LEU

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Mol	Chain	Res	Type
1	B	333	ASP
1	B	353	VAL
1	B	375	ASN
1	C	18	ASN
1	C	52	GLU
1	C	56	VAL
1	C	59	ILE
1	C	106	ILE
1	C	127	ILE
1	C	128	ASP
1	C	135	GLU
1	C	185	ILE
1	C	190	ILE
1	C	201	MET
1	C	216	LEU
1	C	220	VAL
1	C	230	GLU
1	C	243	SER
1	C	251	SER
1	C	259	LEU
1	C	301	ARG
1	C	316	LEU
1	C	333	ASP
1	C	353	VAL
1	C	375	ASN
1	D	19	VAL
1	D	51	MET
1	D	52	GLU
1	D	56	VAL
1	D	59	ILE
1	D	78	ILE
1	D	97	ASP
1	D	106	ILE
1	D	127	ILE
1	D	128	ASP
1	D	131	ASN
1	D	178	ILE
1	D	190	ILE
1	D	220	VAL
1	D	230	GLU
1	D	251	SER
1	D	259	LEU

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Mol	Chain	Res	Type
1	D	316	LEU
1	D	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	357	ASN
1	A	358	ASN
1	A	384	HIS
1	B	358	ASN
1	C	244	GLN
1	C	358	ASN
1	D	318	ASN
1	D	375	ASN

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](#)

4 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	SF4	A	401	1	0,12,12	-	-	-		
2	SF4	C	401	1	0,12,12	-	-	-		
2	SF4	D	401	1	0,12,12	-	-	-		
2	SF4	B	401	1	0,12,12	-	-	-		

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	SF4	A	401	1	-	-	0/6/5/5
2	SF4	C	401	1	-	-	0/6/5/5
2	SF4	D	401	1	-	-	0/6/5/5
2	SF4	B	401	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	363/396 (91%)	0.66	33 (9%) 15 11	50, 76, 108, 143	0
1	B	363/396 (91%)	0.92	44 (12%) 8 6	50, 81, 118, 152	0
1	C	356/396 (89%)	1.12	75 (21%) 2 2	48, 85, 161, 179	0
1	D	356/396 (89%)	0.79	43 (12%) 8 6	47, 74, 145, 167	0
All	All	1438/1584 (90%)	0.87	195 (13%) 7 5	47, 79, 146, 179	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	VAL	4.9
1	B	134	LYS	4.8
1	C	152	ILE	4.7
1	B	132	ILE	4.6
1	C	50	SER	4.5
1	C	127	ILE	4.4
1	D	176	ASP	4.3
1	B	177	LEU	4.3
1	C	180	GLY	4.3
1	A	191	ASP	4.2
1	A	134	LYS	4.1
1	B	131	ASN	4.1
1	C	149	LEU	4.1
1	A	332	VAL	4.1
1	C	132	ILE	4.1
1	C	25	MET	4.0
1	D	19	VAL	3.9
1	C	181	GLY	3.8
1	B	176	ASP	3.8
1	D	182	ASP	3.7
1	D	149	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	3.7
1	C	78	ILE	3.7
1	B	243	SER	3.7
1	D	190	ILE	3.6
1	D	134	LYS	3.5
1	B	182	ASP	3.5
1	A	182	ASP	3.5
1	B	99	PRO	3.5
1	D	144	LEU	3.4
1	C	63	ASP	3.4
1	B	128	ASP	3.4
1	C	98	ILE	3.4
1	C	21	LYS	3.4
1	C	131	ASN	3.3
1	C	166	PRO	3.3
1	B	281	LYS	3.3
1	C	49	LYS	3.3
1	A	190	ILE	3.3
1	A	127	ILE	3.3
1	C	332	VAL	3.3
1	D	177	LEU	3.3
1	D	131	ASN	3.2
1	D	122	ASN	3.2
1	B	178	ILE	3.2
1	B	98	ILE	3.2
1	C	179	ASP	3.1
1	A	281	LYS	3.1
1	B	124	ILE	3.1
1	C	148	ALA	3.1
1	B	36	VAL	3.1
1	C	134	LYS	3.0
1	C	330	ALA	3.0
1	C	14	THR	3.0
1	B	247	MET	3.0
1	B	22	SER	3.0
1	D	152	ILE	2.9
1	B	326	LEU	2.9
1	D	20	GLY	2.9
1	C	20	GLY	2.9
1	C	162	ASN	2.9
1	B	148	ALA	2.9
1	D	132	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	82	LYS	2.9
1	C	150	LYS	2.9
1	D	126	THR	2.9
1	A	131	ASN	2.8
1	C	28	LEU	2.8
1	C	193	GLY	2.8
1	D	124	ILE	2.8
1	C	120	ALA	2.8
1	A	181	GLY	2.8
1	A	36	VAL	2.7
1	B	383	LEU	2.7
1	C	108	LYS	2.7
1	C	92	ILE	2.7
1	C	164	ILE	2.7
1	B	392	LYS	2.7
1	C	151	LYS	2.7
1	C	126	THR	2.7
1	C	133	GLU	2.7
1	A	7	PHE	2.7
1	B	127	ILE	2.7
1	C	143	ILE	2.7
1	A	196	LYS	2.7
1	B	65	PRO	2.7
1	B	135	GLU	2.7
1	D	133	GLU	2.7
1	D	193	GLY	2.7
1	C	13	ILE	2.6
1	D	29	ILE	2.6
1	D	98	ILE	2.6
1	D	123	LYS	2.6
1	A	194	ALA	2.6
1	D	156	LYS	2.6
1	C	130	GLU	2.6
1	D	78	ILE	2.6
1	C	157	ILE	2.5
1	C	81	ALA	2.5
1	D	191	ASP	2.5
1	D	138	LYS	2.5
1	A	65	PRO	2.5
1	C	144	LEU	2.5
1	C	287	LYS	2.5
1	A	192	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	247	MET	2.5
1	B	130	GLU	2.5
1	C	24	PHE	2.5
1	C	342	ASP	2.5
1	C	51	MET	2.5
1	C	124	ILE	2.5
1	C	95	VAL	2.5
1	B	136	TYR	2.5
1	D	30	GLY	2.4
1	B	49	LYS	2.4
1	B	139	TYR	2.4
1	C	117	TYR	2.4
1	B	18	ASN	2.4
1	B	191	ASP	2.4
1	A	308	GLY	2.4
1	C	251	SER	2.4
1	C	165	LEU	2.4
1	D	330	ALA	2.4
1	C	331	GLY	2.4
1	C	85	LEU	2.4
1	C	119	ILE	2.4
1	D	127	ILE	2.4
1	D	108	LYS	2.3
1	D	187	VAL	2.3
1	A	333	ASP	2.3
1	B	133	GLU	2.3
1	D	50	SER	2.3
1	C	190	ILE	2.3
1	B	151	LYS	2.3
1	D	15	GLY	2.3
1	C	167	LYS	2.3
1	C	170	GLU	2.3
1	C	107	ILE	2.3
1	C	327	LYS	2.3
1	A	193	GLY	2.3
1	A	321	GLY	2.3
1	C	326	LEU	2.3
1	B	291	THR	2.3
1	B	328	VAL	2.3
1	C	142	PRO	2.3
1	C	184	VAL	2.3
1	C	121	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	243	SER	2.2
1	B	332	VAL	2.2
1	B	331	GLY	2.2
1	A	230	GLU	2.2
1	B	307	ILE	2.2
1	D	179	ASP	2.2
1	A	304	THR	2.2
1	C	395	MET	2.2
1	C	154	PHE	2.2
1	C	79	LYS	2.2
1	A	129	HIS	2.2
1	C	96	ASP	2.2
1	A	138	LYS	2.2
1	C	83	LYS	2.2
1	B	97	ASP	2.2
1	C	99	PRO	2.2
1	A	80	LYS	2.2
1	C	123	LYS	2.2
1	D	136	TYR	2.2
1	C	22	SER	2.2
1	A	133	GLU	2.2
1	D	59	ILE	2.1
1	C	248	LYS	2.1
1	C	110	PHE	2.1
1	D	194	ALA	2.1
1	D	139	TYR	2.1
1	D	54	SER	2.1
1	B	129	HIS	2.1
1	B	25	MET	2.1
1	B	140	ASN	2.1
1	B	299	THR	2.1
1	A	83	LYS	2.1
1	D	129	HIS	2.1
1	B	193	GLY	2.1
1	C	30	GLY	2.1
1	A	179	ASP	2.1
1	A	130	GLU	2.1
1	D	395	MET	2.0
1	D	130	GLU	2.0
1	A	145	LYS	2.0
1	A	248	LYS	2.0
1	C	145	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	283	VAL	2.0
1	C	109	LEU	2.0
1	D	154	PHE	2.0
1	D	52	GLU	2.0
1	D	248	LYS	2.0
1	B	117	TYR	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(Å ²)	Q<0.9
2	SF4	B	401	8/8	0.98	0.08	75,77,78,78	8
2	SF4	A	401	8/8	0.99	0.06	68,69,70,72	8
2	SF4	C	401	8/8	0.99	0.06	65,65,66,67	8
2	SF4	D	401	8/8	0.99	0.05	47,50,53,53	8

6.5 Other polymers [i](#)

There are no such residues in this entry.