



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2026 – 04:08 PM EDT

PDB ID : 10KU / pdb_000010ku
Title : Structure of hNSP4-S218A bound to MCP3 at 2.09 Å resolution
Authors : Tang, W.; Martinez, O.E.; Ultsch, M.H.; Sudhamsu, J.
Deposited on : 2026-01-25
Resolution : 2.09 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

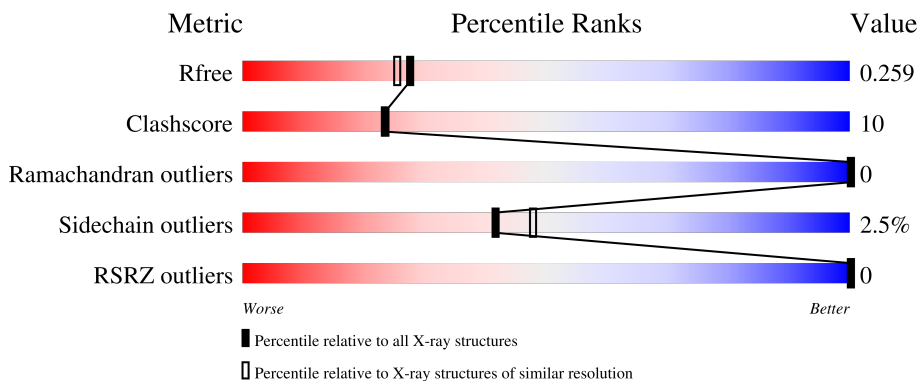
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	232	 79% 20%
1	B	232	 76% 22%
1	C	232	 82% 18%
1	D	232	 81% 18%
2	E	15	 67% 33%

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Mol	Chain	Length	Quality of chain	
2	F	15	 67%	33%
2	G	15	 53%	47%
2	I	15	 53%	47%

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
3	SO4	A	304	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7965 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 Serine protease 57.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1769	1114	335	307	13	0	0	0
1	B	232	1773	1116	339	304	14	0	1	0
1	C	232	1756	1107	332	305	12	0	0	0
1	D	232	1753	1106	327	306	14	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	LEU	PRO	variant	UNP Q6UWY2
A	195	ALA	SER	conflict	UNP Q6UWY2
B	123	LEU	PRO	variant	UNP Q6UWY2
B	195	ALA	SER	conflict	UNP Q6UWY2
C	123	LEU	PRO	variant	UNP Q6UWY2
C	195	ALA	SER	conflict	UNP Q6UWY2
D	123	LEU	PRO	variant	UNP Q6UWY2
D	195	ALA	SER	conflict	UNP Q6UWY2

- Molecule 2 is a protein called MCP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	15	113	69	26	17	1	0	0	1
2	I	15	113	69	26	17	1	0	0	1
2	F	15	113	69	26	17	1	0	0	1
2	E	15	113	69	26	17	1	0	0	1

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

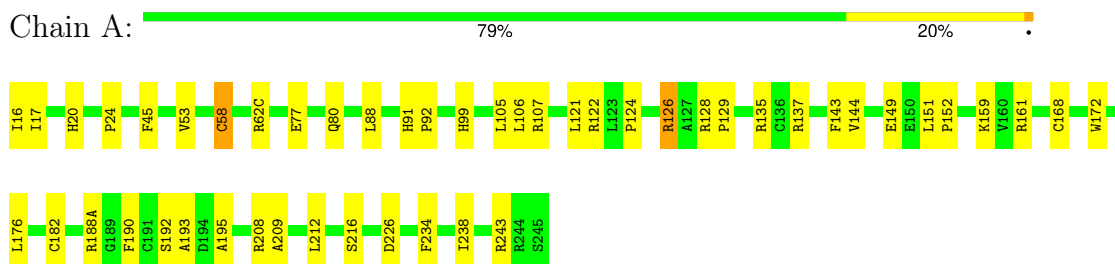
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	111	Total	O	0	0
			111	111		
4	C	55	Total	O	0	0
			55	55		
4	D	62	Total	O	0	0
			62	62		
4	F	4	Total	O	0	0
			4	4		
4	E	2	Total	O	0	0
			2	2		

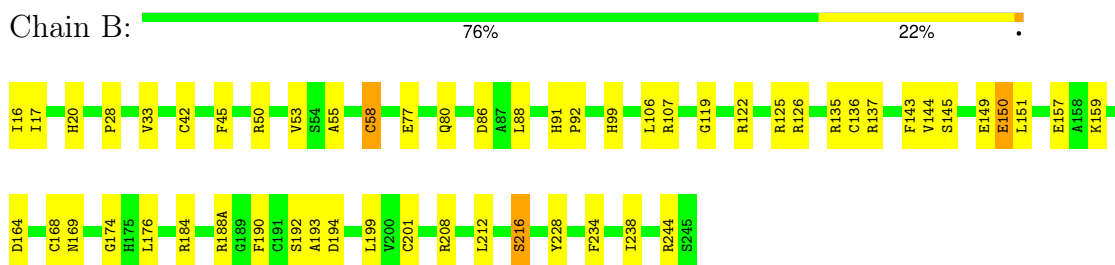
3 Residue-property plots [i](#)

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.

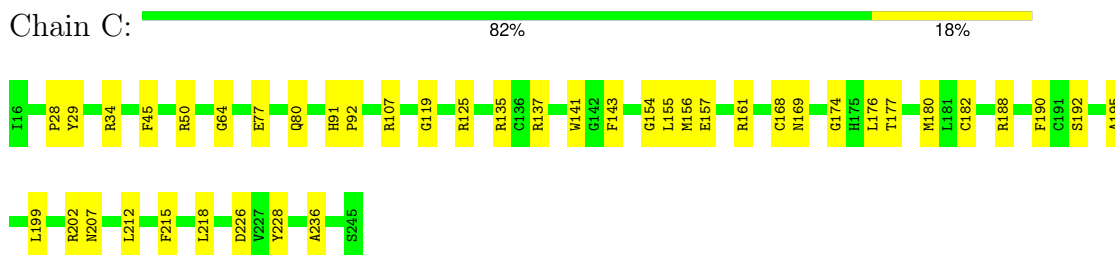
- Molecule 1: Serine protease 57



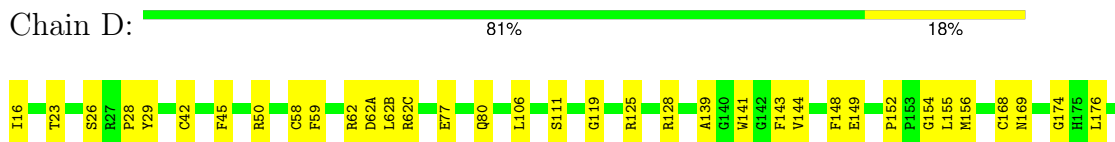
- Molecule 1: Serine protease 57



- Molecule 1: Serine protease 57

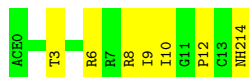


- Molecule 1: Serine protease 57

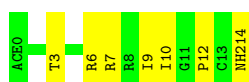




- Molecule 2: MCP3



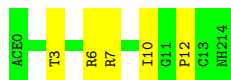
- Molecule 2: MCP3



- Molecule 2: MCP3



- Molecule 2: MCP3



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.04Å 43.67Å 124.03Å 90.00° 92.61° 90.00°	Depositor
Resolution (Å)	123.90 – 2.09 123.90 – 2.09	Depositor EDS
% Data completeness (in resolution range)	77.2 (123.90-2.09) 73.0 (123.90-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.08Å)	Xtrriage
Refinement program	PHENIX (1.20.1-4487_final: ???)	Depositor
R, R_{free}	0.228 , 0.262 0.232 , 0.259	Depositor DCC
R_{free} test set	2752 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 22.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.179 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7965	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: ACE, SO4, NH2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/1820	0.50	0/2479
1	B	0.35	0/1824	0.58	0/2484
1	C	0.18	0/1807	0.37	0/2464
1	D	0.14	0/1804	0.36	0/2461
2	E	0.58	0/111	0.90	0/148
2	F	0.55	0/111	0.88	0/148
2	G	0.15	0/111	0.39	0/148
2	I	0.13	0/111	0.29	0/148
All	All	0.28	0/7699	0.48	0/10480

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1769	0	1727	49	0
1	B	1773	0	1734	39	0
1	C	1756	0	1705	31	0
1	D	1753	0	1694	28	0
2	E	113	0	121	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	113	0	121	7	0
2	G	113	0	121	6	0
2	I	113	0	121	6	0
3	A	35	0	0	7	0
3	B	30	0	0	3	0
3	C	20	0	0	2	0
3	D	20	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	I	5	0	0	1	0
4	A	108	0	0	5	0
4	B	111	0	0	3	0
4	C	55	0	0	1	0
4	D	62	0	0	2	0
4	E	2	0	0	1	0
4	F	4	0	0	0	0
All	All	7965	0	7344	152	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 10.

All (152) 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:A:24:PRO:HB2	4:A:407:HOH:O	1.75	0.85
1:D:42:CYS:SG	1:D:58[A]:CYS:HB3	2.19	0.83
1:B:244:ARG:HD2	4:B:430:HOH:O	1.80	0.81
2:F:10:ILE:HG13	2:F:12:PRO:HD2	1.69	0.73
1:B:143:PHE:CD2	1:B:192:SER:HB2	2.26	0.70
2:I:10:ILE:HG13	2:I:12:PRO:HD2	1.73	0.69
1:B:136:CYS:SG	1:B:201[B]:CYS:HB2	2.32	0.68
2:G:10:ILE:HG13	2:G:12:PRO:HD2	1.75	0.67
1:D:190:PHE:CE2	1:D:226:ASP:HB3	2.30	0.67
1:C:50:ARG:HH11	1:C:107:ARG:NH2	1.93	0.66
1:A:137:ARG:NH2	1:A:159:LYS:HE2	2.11	0.65
1:D:208:ARG:NH1	3:D:303:SO4:O1	2.22	0.65
1:C:77:GLU:HB2	1:C:80:GLN:HG3	1.79	0.64
1:D:50:ARG:NH2	1:D:111:SER:OG	2.32	0.63
1:D:77:GLU:HB2	1:D:80:GLN:HG3	1.80	0.63
1:A:129:PRO:HA	4:A:472:HOH:O	1.99	0.63
1:A:135:ARG:NE	3:A:306:SO4:O2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:NH2	3:A:304:SO4:O2	2.33	0.62
1:B:164:ASP:HB2	4:B:493:HOH:O	1.99	0.62
1:A:161:ARG:NH1	1:B:184:ARG:NH1	2.47	0.62
1:A:137:ARG:HH21	1:A:159:LYS:HE2	1.65	0.62
1:B:50:ARG:NH1	3:B:305:SO4:O4	2.31	0.61
1:B:169:ASN:OD1	1:B:174:GLY:HA2	2.00	0.61
1:C:143:PHE:HD2	1:C:192:SER:HB3	1.66	0.60
2:E:10:ILE:HG13	2:E:12:PRO:HD2	1.82	0.60
1:D:59:PHE:CZ	1:D:106:LEU:HD11	2.37	0.59
3:A:302:SO4:O3	1:B:135:ARG:NH1	2.35	0.59
1:B:88:LEU:HD13	1:B:106:LEU:CD2	2.33	0.59
1:C:190:PHE:CE2	1:C:226:ASP:HB3	2.38	0.59
1:B:107:ARG:NH1	3:B:304:SO4:O4	2.36	0.59
1:A:168:CYS:SG	1:A:176:LEU:HD21	2.42	0.58
1:A:126:ARG:O	2:G:6:ARG:NH2	2.36	0.57
1:A:243:ARG:HB2	4:A:438:HOH:O	2.03	0.57
1:C:135:ARG:CZ	1:C:161:ARG:HH22	2.18	0.56
1:A:143:PHE:CG	1:A:149:GLU:HA	2.41	0.56
1:A:216:SER:HB3	2:F:7:ARG:HH22	1.71	0.55
1:A:122:ARG:HE	1:A:208:ARG:CZ	2.19	0.55
1:C:50:ARG:HD2	1:C:107:ARG:NH1	2.22	0.55
1:D:59:PHE:HZ	1:D:106:LEU:HD11	1.71	0.55
1:D:195:ALA:HB2	2:I:3:THR:OG1	2.06	0.55
1:C:135:ARG:NH2	1:C:161:ARG:HH22	2.05	0.55
1:A:190:PHE:CE2	1:A:226:ASP:HB3	2.43	0.54
1:B:16:ILE:HD13	1:B:190:PHE:HA	1.90	0.54
1:A:53:VAL:HG22	1:A:105:LEU:CD2	2.39	0.53
1:A:128:ARG:NH2	3:A:304:SO4:S	2.81	0.53
1:C:50:ARG:HH11	1:C:107:ARG:HH22	1.54	0.53
1:A:20:HIS:HB3	3:A:301:SO4:O4	2.08	0.53
1:A:121:LEU:CD2	1:A:209:ALA:HB2	2.40	0.52
1:A:234:PHE:O	1:A:238:ILE:HG13	2.10	0.51
1:A:16:ILE:HD13	1:A:190:PHE:HA	1.93	0.51
1:A:88:LEU:HD13	1:A:106:LEU:CD2	2.40	0.51
1:A:172:TRP:HB2	1:A:176:LEU:HD13	1.93	0.51
1:D:190:PHE:CE1	1:D:216:SER:HB2	2.46	0.51
1:B:168:CYS:SG	1:B:176:LEU:HD21	2.50	0.51
1:C:215:PHE:HA	2:G:3:THR:HG23	1.92	0.51
1:B:77:GLU:HB2	1:B:80:GLN:HG3	1.94	0.50
1:C:195:ALA:HB2	2:G:3:THR:OG1	2.11	0.50
1:D:128:ARG:N	4:D:406:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TRP:CE2	1:C:155:LEU:HD13	2.48	0.49
1:A:62(C):ARG:HG3	4:A:413:HOH:O	2.12	0.49
1:B:234:PHE:HA	4:B:411:HOH:O	2.11	0.49
1:A:58:CYS:SG	1:A:195:ALA:HB3	2.52	0.48
1:A:99:HIS:CE1	2:F:2:THR:HG22	2.49	0.48
1:D:216:SER:HB3	2:I:7:ARG:HH22	1.78	0.48
1:A:107:ARG:NH1	3:A:303:SO4:O2	2.46	0.48
1:C:141:TRP:CZ2	1:C:155:LEU:HD13	2.48	0.48
1:D:28:PRO:HB2	1:D:119:GLY:N	2.28	0.48
1:C:168:CYS:SG	1:C:176:LEU:HD21	2.53	0.48
1:D:144:VAL:CG1	1:D:152:PRO:HB3	2.44	0.48
1:C:29:TYR:HA	1:C:119:GLY:O	2.14	0.48
1:B:16:ILE:N	1:B:194:ASP:OD2	2.46	0.48
1:B:88:LEU:HD13	1:B:106:LEU:HD23	1.96	0.48
1:B:137:ARG:NH2	1:B:159:LYS:HE2	2.28	0.48
1:D:45:PHE:HE1	1:D:212:LEU:HD11	1.79	0.47
1:A:17:ILE:O	1:A:188(A):ARG:HA	2.13	0.47
1:C:202:ARG:NH2	3:C:302:SO4:O3	2.44	0.47
1:A:192:SER:OG	2:F:7:ARG:HD2	2.14	0.47
1:B:28:PRO:HB2	1:B:119:GLY:N	2.29	0.47
1:B:144:VAL:HG22	1:B:150:GLU:O	2.14	0.47
1:C:199:LEU:HB2	1:C:228:TYR:CE2	2.50	0.47
1:B:199:LEU:HB2	1:B:228:TYR:CE2	2.50	0.47
1:A:144:VAL:CG1	1:A:152:PRO:HB3	2.45	0.47
1:B:88:LEU:HD13	1:B:106:LEU:HD21	1.97	0.46
1:D:154:GLY:O	1:D:156:MET:HG2	2.15	0.46
1:D:23:THR:HB	1:D:26:SER:HB3	1.98	0.46
1:A:121:LEU:HD23	1:A:209:ALA:HB2	1.97	0.46
1:B:143:PHE:CG	1:B:149:GLU:HA	2.50	0.46
1:D:215:PHE:HA	2:I:3:THR:HG23	1.98	0.46
1:A:126:ARG:N	4:A:401:HOH:O	2.22	0.46
1:C:154:GLY:O	1:C:156:MET:HG2	2.16	0.46
1:A:190:PHE:CE1	2:F:3:THR:HG21	2.50	0.46
3:A:304:SO4:O2	2:G:8:ARG:NH2	2.36	0.46
1:C:29:TYR:O	1:C:45:PHE:HA	2.16	0.46
1:C:207:ASN:ND2	3:C:304:SO4:O1	2.41	0.46
1:B:137:ARG:HD3	1:B:157:GLU:OE1	2.16	0.46
1:B:122:ARG:HB2	1:B:208:ARG:HD3	1.97	0.45
1:A:176:LEU:HD21	1:A:182:CYS:SG	2.56	0.45
1:B:17:ILE:O	1:B:188(A):ARG:HA	2.17	0.45
1:D:143:PHE:CD2	1:D:192:SER:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:PRO:HB2	1:C:119:GLY:N	2.31	0.44
1:D:168:CYS:SG	1:D:176:LEU:HD21	2.57	0.44
1:D:139:ALA:HA	1:D:156:MET:O	2.16	0.44
1:A:77:GLU:HB2	1:A:80:GLN:HG3	1.99	0.44
1:A:182:CYS:HA	1:A:226:ASP:O	2.17	0.44
1:A:53:VAL:HG22	1:A:105:LEU:HD21	2.00	0.44
1:A:88:LEU:HD13	1:A:106:LEU:HD23	2.00	0.44
1:C:50:ARG:HD2	1:C:107:ARG:HH12	1.83	0.44
1:D:169:ASN:OD1	1:D:174:GLY:HA2	2.18	0.44
1:B:137:ARG:HH21	1:B:159:LYS:HE2	1.83	0.44
2:I:9:ILE:HD11	2:I:14:NH2:N	2.32	0.44
1:B:190:PHE:CE1	2:E:3:THR:HG21	2.53	0.44
1:A:53:VAL:HG22	1:A:105:LEU:HD23	2.00	0.43
1:B:91:HIS:CG	1:B:92:PRO:HD2	2.53	0.43
1:C:125:ARG:HH21	1:C:236:ALA:HA	1.83	0.43
1:B:20:HIS:HA	3:B:301:SO4:O2	2.19	0.43
1:C:188:ARG:NH1	4:C:406:HOH:O	2.45	0.43
1:C:50:ARG:NH1	1:C:107:ARG:HH22	2.17	0.43
2:E:6:ARG:HA	4:E:202:HOH:O	2.18	0.43
1:B:33:VAL:HB	1:B:42:CYS:HB2	2.00	0.43
1:A:124:PRO:HD3	1:A:209:ALA:O	2.19	0.43
1:D:125:ARG:H	1:D:125:ARG:HG3	1.48	0.43
1:B:234:PHE:O	1:B:238:ILE:HG13	2.18	0.42
1:C:137:ARG:HD2	1:C:157:GLU:OE2	2.19	0.42
1:C:143:PHE:CD2	1:C:192:SER:HB3	2.51	0.42
1:D:148:PHE:O	4:D:401:HOH:O	2.21	0.42
1:B:216:SER:OG	2:E:7:ARG:NH2	2.52	0.42
1:A:161:ARG:NH1	1:B:184:ARG:CZ	2.81	0.42
2:G:9:ILE:HD11	2:G:14:NH2:N	2.35	0.42
1:C:34:ARG:O	1:C:64:GLY:HA2	2.20	0.42
1:C:169:ASN:OD1	1:C:174:GLY:HA2	2.18	0.42
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.55	0.42
1:A:195:ALA:HB2	2:F:3:THR:OG1	2.19	0.42
1:A:192:SER:O	1:A:193:ALA:HB3	2.20	0.42
1:D:58[A]:CYS:SG	1:D:195:ALA:HB3	2.60	0.42
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.85	0.41
1:A:193:ALA:N	2:F:3:THR:O	2.50	0.41
1:B:55:ALA:O	1:B:58:CYS:HB2	2.21	0.41
1:D:190:PHE:HE1	1:D:216:SER:HB2	1.82	0.41
1:A:45:PHE:HE2	1:A:212:LEU:HD11	1.85	0.41
1:A:161:ARG:HH12	1:B:184:ARG:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:OG1	1:C:180:MET:HG3	2.20	0.41
2:I:6:ARG:HB2	3:I:101:SO4:O1	2.21	0.41
1:D:29:TYR:HA	1:D:119:GLY:O	2.21	0.41
1:B:45:PHE:CE1	1:B:53:VAL:HB	2.54	0.41
1:A:143:PHE:HD2	1:A:192:SER:HB2	1.86	0.41
1:B:88:LEU:CD1	1:B:106:LEU:HD23	2.51	0.41
1:C:91:HIS:CG	1:C:92:PRO:HD2	2.56	0.41
1:A:161:ARG:NH1	1:B:184:ARG:HD2	2.36	0.41
1:B:192:SER:O	1:B:193:ALA:HB3	2.21	0.40
1:C:176:LEU:HD21	1:C:182:CYS:SG	2.62	0.40
1:D:16:ILE:HD13	1:D:190:PHE:HA	2.04	0.40
1:D:141:TRP:CE2	1:D:155:LEU:HD13	2.57	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	230/232 (99%)	227 (99%)	3 (1%)	0	100	100
1	B	231/232 (100%)	226 (98%)	5 (2%)	0	100	100
1	C	230/232 (99%)	226 (98%)	4 (2%)	0	100	100
1	D	231/232 (100%)	228 (99%)	3 (1%)	0	100	100
2	E	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
2	F	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
2	G	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
2	I	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	974/988 (99%)	952 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	187/188 (100%)	185 (99%)	2 (1%)	65	74
1	B	187/188 (100%)	177 (95%)	10 (5%)	20	19
1	C	184/188 (98%)	182 (99%)	2 (1%)	65	74
1	D	184/188 (98%)	178 (97%)	6 (3%)	33	37
2	E	12/12 (100%)	12 (100%)	0	100	100
2	F	12/12 (100%)	12 (100%)	0	100	100
2	G	12/12 (100%)	12 (100%)	0	100	100
2	I	12/12 (100%)	12 (100%)	0	100	100
All	All	790/800 (99%)	770 (98%)	20 (2%)	42	48

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	CYS
1	A	126	ARG
1	B	58	CYS
1	B	86	ASP
1	B	99	HIS
1	B	125	ARG
1	B	126	ARG
1	B	145	SER
1	B	150	GLU
1	B	151	LEU
1	B	212	LEU
1	B	216	SER
1	C	212	LEU
1	C	218	LEU
1	D	62	ARG
1	D	62(A)	ASP
1	D	62(B)	LEU
1	D	62(C)	ARG
1	D	149	GLU

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Mol	Chain	Res	Type
1	D	212	LEU

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	99	HIS
1	A	230	GLN
1	B	101	ASN
1	B	230	GLN
1	C	41	HIS
1	C	230	GLN
1	D	230	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](#)

24 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	$\# Z > 2$
3	SO4	A	307	-	4,4,4	0.24	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	304	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	301	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	305	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	D	302	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	C	301	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	E	101	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	304	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	306	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	A	301	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	A	305	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	306	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	F	101	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	D	303	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	I	101	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	B	304	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.07	0

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.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	SO4	1	0
3	B	305	SO4	1	0
3	A	304	SO4	3	0
3	A	302	SO4	1	0
3	A	303	SO4	1	0
3	C	304	SO4	1	0
3	A	306	SO4	1	0
3	A	301	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	SO4	1	0
3	I	101	SO4	1	0
3	B	304	SO4	1	0
3	C	302	SO4	1	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 [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	232/232 (100%)	-1.28	0 100 100	11, 20, 38, 79	0
1	B	232/232 (100%)	-1.31	0 100 100	10, 19, 39, 63	1 (0%)
1	C	232/232 (100%)	-1.17	0 100 100	17, 31, 51, 62	0
1	D	232/232 (100%)	-1.17	0 100 100	16, 32, 49, 62	1 (0%)
2	E	13/15 (86%)	-1.44	0 100 100	15, 19, 29, 36	0
2	F	13/15 (86%)	-1.37	0 100 100	15, 19, 28, 38	0
2	G	13/15 (86%)	-1.36	0 100 100	20, 23, 33, 39	0
2	I	13/15 (86%)	-1.29	0 100 100	23, 26, 39, 40	0
All	All	980/988 (99%)	-1.24	0 100 100	10, 26, 46, 79	2 (0%)

There are no RSRZ outliers to report.

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(\AA^2)	Q<0.9
3	SO4	A	305	5/5	0.98	0.08	31,40,43,58	0
3	SO4	A	307	5/5	0.98	0.05	41,50,55,61	0
3	SO4	B	305	5/5	0.98	0.04	57,58,67,68	0
3	SO4	B	306	5/5	0.98	0.06	44,46,54,54	0
3	SO4	C	303	5/5	0.98	0.04	57,61,75,75	0
3	SO4	D	303	5/5	0.98	0.03	52,55,62,63	0
3	SO4	I	101	5/5	0.98	0.05	36,41,52,55	0
3	SO4	B	302	5/5	0.99	0.05	47,47,60,60	0
3	SO4	B	303	5/5	0.99	0.08	27,36,38,43	0
3	SO4	B	304	5/5	0.99	0.05	35,39,47,50	0
3	SO4	A	304	5/5	0.99	0.06	41,46,49,53	0
3	SO4	A	301	5/5	0.99	0.05	31,38,40,41	0
3	SO4	C	301	5/5	0.99	0.05	41,48,53,58	0
3	SO4	C	302	5/5	0.99	0.03	46,55,58,63	0
3	SO4	A	306	5/5	0.99	0.05	35,42,44,53	0
3	SO4	C	304	5/5	0.99	0.03	53,54,60,70	0
3	SO4	D	301	5/5	0.99	0.02	50,54,58,62	0
3	SO4	D	302	5/5	0.99	0.03	54,59,67,69	0
3	SO4	A	303	5/5	0.99	0.04	31,39,40,44	0
3	SO4	D	304	5/5	0.99	0.04	50,56,62,72	0
3	SO4	B	301	5/5	0.99	0.05	33,33,45,52	0
3	SO4	F	101	5/5	0.99	0.07	31,34,37,42	0
3	SO4	E	101	5/5	0.99	0.04	42,48,55,58	0
3	SO4	A	302	5/5	1.00	0.04	30,31,42,46	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.