



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 AM UTC

PDB ID : 3FVI / pdb_00003fvi
Title : Crystal Structure of Complex of Phospholipase A2 with Octyl Sulfates
Authors : Pan, Y.H.
Deposited on : 2009-01-15
Resolution : 2.70 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

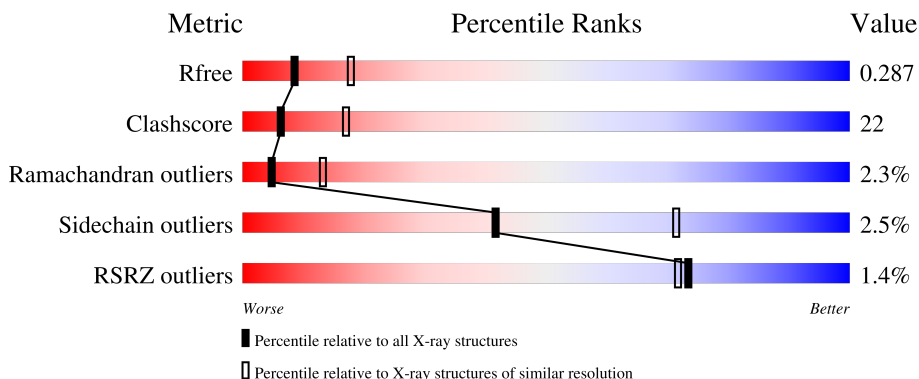
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	124	69% 26% 5%
1	B	124	56% 43% .
1	C	124	60% 37% .
1	D	124	3% 55% 44% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4112 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 Phospholipase A2, major isoenzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			971	596	166	193	16			
1	B	124	Total	C	N	O	S	0	0	0
			971	596	166	193	16			
1	C	124	Total	C	N	O	S	0	0	0
			971	596	166	193	16			
1	D	124	Total	C	N	O	S	0	0	0
			971	596	166	193	16			

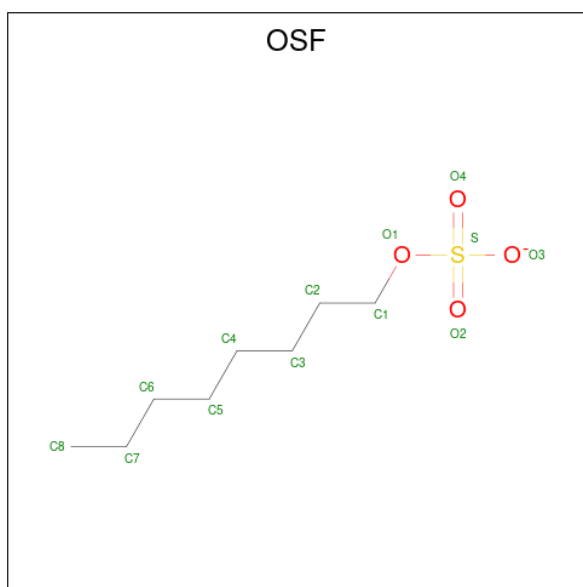
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is octyl sulfate (CCD ID: OSF) (formula: C₈H₁₇O₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			13	8	4	1		
4	B	1	Total	C	O	S	0	0
			13	8	4	1		
4	B	1	Total	C	O	S	0	0
			13	8	4	1		
4	B	1	Total	C	O	S	0	0
			13	8	4	1		
4	C	1	Total	C	O	S	0	0
			13	8	4	1		
4	C	1	Total	C	O	S	0	0
			13	8	4	1		
4	C	1	Total	C	O	S	0	0
			13	8	4	1		
4	D	1	Total	C	O	S	0	0
			13	8	4	1		
4	D	1	Total	C	O	S	0	0
			13	8	4	1		
4	D	1	Total	C	O	S	0	0
			13	8	4	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

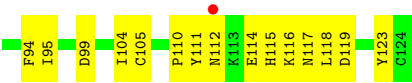
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Na 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total 30	O 30	0	0
6	B	12	Total 12	O 12	0	0
6	C	15	Total 15	O 15	0	0
6	D	8	Total 8	O 8	0	0

- Molecule 1: Phospholipase A2, major isoenzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.99Å 82.06Å 123.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.70 33.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	83.7 (33.54-2.70) 94.2 (33.54-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.275 0.225 , 0.287	Depositor DCC
R_{free} test set	866 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4112	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: CA, CL, NA, OSF

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	0.46	0/993	0.97	5/1340 (0.4%)
1	B	0.44	0/993	1.06	9/1340 (0.7%)
1	C	0.44	0/993	1.04	8/1340 (0.6%)
1	D	0.40	0/993	0.92	3/1340 (0.2%)
All	All	0.44	0/3972	1.00	25/5360 (0.5%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ALA	N-CA-C	-8.03	102.48	111.07
1	B	17	HIS	CA-C-N	7.24	128.89	119.84
1	B	17	HIS	C-N-CA	7.24	128.89	119.84
1	B	13	ILE	CA-C-N	7.22	128.87	119.84
1	B	13	ILE	C-N-CA	7.22	128.87	119.84
1	B	22	PHE	N-CA-C	6.90	121.86	113.17
1	B	21	ASP	N-CA-C	6.78	118.46	111.14
1	C	62	LYS	N-CA-C	6.77	118.35	110.97
1	B	98	CYS	N-CA-C	-6.61	104.00	111.07
1	A	22	PHE	N-CA-C	6.58	120.61	112.59
1	C	13	ILE	CA-C-N	6.28	127.69	119.84
1	C	13	ILE	C-N-CA	6.28	127.69	119.84
1	A	13	ILE	CA-C-N	6.17	127.55	119.84
1	A	13	ILE	C-N-CA	6.17	127.55	119.84
1	B	2	LEU	N-CA-C	6.05	118.37	111.11
1	B	17	HIS	N-CA-C	-5.98	98.95	108.82
1	D	22	PHE	N-CA-C	5.73	120.34	113.23
1	C	123	TYR	N-CA-C	5.60	120.10	113.16
1	C	17	HIS	CA-C-N	5.54	126.76	119.84
1	C	17	HIS	C-N-CA	5.54	126.76	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	ASP	N-CA-C	5.26	116.87	111.03
1	D	123	TYR	N-CA-C	5.16	119.54	112.88
1	A	17	HIS	CA-C-N	5.16	126.29	119.84
1	A	17	HIS	C-N-CA	5.16	126.29	119.84
1	C	63	PHE	N-CA-C	5.09	117.99	110.46

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	971	0	886	32	0
1	B	971	0	888	46	0
1	C	971	0	886	39	0
1	D	971	0	886	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	13	0	17	2	0
4	B	39	0	51	13	0
4	C	52	0	68	13	0
4	D	52	0	68	12	0
5	D	1	0	0	0	0
6	A	30	0	0	1	0
6	B	12	0	0	0	0
6	C	15	0	0	2	0
6	D	8	0	0	0	0
All	All	4112	0	3750	172	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 22.

All (172) 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:8:MET:HG2	1:A:82:ILE:HD13	1.50	0.91
1:C:7:SER:HB3	1:C:75:TYR:OH	1.73	0.89
1:B:44:CYS:HG	1:B:105:CYS:HG	0.92	0.88
1:A:112:ASN:HB3	1:A:114:GLU:CD	2.01	0.86
1:A:2:LEU:HD23	4:A:127:OSF:H1A	1.58	0.84
1:A:71:GLU:HG2	1:A:95:ILE:HD12	1.62	0.81
1:C:116:LYS:HD2	1:C:117:ASN:OD1	1.81	0.81
1:D:112:ASN:HB3	1:D:114:GLU:OE1	1.79	0.81
1:D:6:ARG:HG3	4:D:129:OSF:H8B	1.63	0.80
1:D:68:PRO:HA	1:D:95:ILE:HD13	1.64	0.79
1:D:63:PHE:HB3	4:D:130:OSF:O2	1.83	0.79
1:C:33:GLY:H	1:D:57:ASN:ND2	1.82	0.76
1:C:3:TRP:CD1	4:D:130:OSF:H8	2.22	0.75
1:D:19:LEU:HB2	4:D:129:OSF:H8A	1.70	0.73
4:B:127:OSF:H4A	4:D:128:OSF:H8B	1.70	0.72
1:B:44:CYS:HG	1:B:105:CYS:CB	2.02	0.72
1:B:19:LEU:HG	1:C:65:VAL:HG11	1.72	0.72
4:B:126:OSF:H4A	1:C:70:THR:HG21	1.72	0.72
4:B:126:OSF:H8	1:C:64:LEU:HB3	1.72	0.71
1:B:52:TYR:CE2	1:B:68:PRO:HB2	2.26	0.71
1:C:120:THR:HG21	4:C:129:OSF:H1	1.74	0.70
4:C:129:OSF:H4A	1:D:59:ASP:HB2	1.75	0.69
1:C:6:ARG:HD2	4:C:128:OSF:H8B	1.76	0.67
1:B:52:TYR:CD2	1:B:68:PRO:HB2	2.29	0.67
1:A:90:ALA:HB3	6:A:152:HOH:O	1.95	0.64
6:C:141:HOH:O	1:D:53:ARG:HD2	1.96	0.64
1:D:74:SER:C	1:D:85:ASN:HD22	2.06	0.64
4:C:126:OSF:H6A	1:D:3:TRP:HE3	1.63	0.64
1:D:6:ARG:CG	4:D:129:OSF:H8B	2.28	0.63
1:A:112:ASN:HB3	1:A:114:GLU:OE2	1.98	0.62
1:A:78:SER:O	1:A:81:GLU:HB3	2.00	0.62
1:A:3:TRP:H	1:A:3:TRP:CD1	2.18	0.61
1:B:29:CYS:HA	4:B:127:OSF:O4	2.00	0.61
1:D:2:LEU:O	1:D:2:LEU:HD13	2.00	0.61
1:B:34:SER:O	1:B:124:CYS:HB3	2.02	0.60
1:B:74:SER:H	1:B:88:ASN:HD21	1.49	0.60
1:D:2:LEU:HD23	1:D:69:TYR:CD1	2.37	0.60
1:B:6:ARG:NH1	4:B:128:OSF:H3	2.17	0.59
1:B:3:TRP:CE2	1:B:4:GLN:HG3	2.38	0.58
1:D:114:GLU:OE2	1:D:114:GLU:N	2.30	0.58
1:B:4:GLN:NE2	1:B:73:TYR:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:O	1:D:44:CYS:HB2	2.04	0.57
1:B:6:ARG:NH2	1:B:10:LYS:HE3	2.19	0.57
1:C:25:TYR:CZ	1:C:41:LEU:HD23	2.39	0.57
4:A:127:OSF:H6	4:D:130:OSF:H2	1.86	0.56
1:C:41:LEU:O	1:C:44:CYS:HB2	2.04	0.56
1:D:13:ILE:CG2	1:D:16:SER:HB3	2.35	0.56
1:A:11:CYS:O	1:A:80:THR:HG22	2.06	0.56
1:B:67:ASN:HD21	1:B:69:TYR:HB2	1.71	0.56
1:B:67:ASN:ND2	1:B:69:TYR:HB2	2.21	0.56
1:A:55:ALA:O	1:A:58:LEU:HB2	2.05	0.56
1:D:12:ALA:C	1:D:14:PRO:HD3	2.31	0.55
1:A:55:ALA:HA	1:A:58:LEU:HD12	1.87	0.55
1:C:56:LYS:HG2	1:D:31:LEU:HD11	1.88	0.55
1:B:3:TRP:NE1	1:B:4:GLN:HG3	2.22	0.54
1:B:58:LEU:HD22	1:B:60:SER:H	1.71	0.54
1:C:64:LEU:HD23	4:C:126:OSF:O4	2.07	0.54
1:D:1:ALA:N	1:D:4:GLN:OE1	2.40	0.54
1:C:120:THR:CG2	4:C:129:OSF:H1	2.38	0.54
1:B:4:GLN:HE22	1:B:73:TYR:H	1.56	0.54
1:B:89:ASN:HB2	1:B:92:GLU:OE2	2.08	0.54
1:C:25:TYR:O	1:C:29:CYS:HB2	2.08	0.53
1:D:1:ALA:HB1	1:D:69:TYR:O	2.09	0.53
1:D:27:CYS:O	1:D:33:GLY:HA2	2.09	0.53
1:B:6:ARG:HH12	4:B:128:OSF:H1A	1.74	0.53
1:B:78:SER:O	1:B:81:GLU:HB3	2.09	0.52
1:A:25:TYR:CZ	1:A:41:LEU:HD23	2.44	0.52
1:D:2:LEU:HD23	1:D:69:TYR:HD1	1.74	0.52
1:A:6:ARG:HH21	1:A:19:LEU:HD12	1.75	0.51
1:D:6:ARG:HG2	1:D:18:PRO:HB2	1.92	0.51
1:D:26:GLY:HA2	1:D:118:LEU:HD22	1.93	0.51
1:B:19:LEU:HD21	4:C:126:OSF:H3	1.91	0.51
1:C:61:CYS:O	1:D:31:LEU:HD23	2.11	0.51
1:D:112:ASN:HD22	1:D:115:HIS:HD2	1.59	0.51
1:C:58:LEU:HD11	1:C:94:PHE:CD2	2.46	0.51
1:C:57:ASN:HD22	1:D:32:GLY:HA2	1.75	0.50
1:C:68:PRO:HA	1:C:95:ILE:HD13	1.94	0.50
1:D:78:SER:O	1:D:79:ASN:HB3	2.11	0.50
1:B:19:LEU:HD13	4:B:127:OSF:H6	1.94	0.50
1:A:52:TYR:CE2	1:A:68:PRO:HB2	2.46	0.50
1:B:37:PRO:HA	1:B:42:ASP:OD2	2.12	0.50
1:D:8:MET:SD	1:D:99:ASP:HB3	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HD11	1:A:107:SER:HA	1.95	0.49
1:A:116:LYS:O	1:A:117:ASN:C	2.55	0.49
1:D:71:GLU:HG2	1:D:95:ILE:HD12	1.95	0.49
1:D:58:LEU:HD11	1:D:94:PHE:CD2	2.48	0.49
1:B:19:LEU:HD23	4:B:126:OSF:H3	1.94	0.48
1:B:67:ASN:ND2	1:B:69:TYR:HD2	2.12	0.48
1:C:66:ASP:HA	1:C:71:GLU:OE2	2.14	0.48
1:C:88:ASN:HB2	6:C:142:HOH:O	2.13	0.48
1:C:55:ALA:O	1:C:58:LEU:HB2	2.13	0.48
1:A:8:MET:HG2	1:A:82:ILE:CD1	2.34	0.48
1:B:74:SER:CB	1:B:87:LYS:HE2	2.43	0.48
1:C:2:LEU:HD13	1:C:69:TYR:CD1	2.48	0.48
1:A:58:LEU:HD11	1:A:94:PHE:CD2	2.49	0.48
1:D:79:ASN:O	1:D:80:THR:HB	2.14	0.48
1:B:25:TYR:C	1:B:25:TYR:CD1	2.91	0.48
1:A:28:TYR:CE2	1:A:37:PRO:HG3	2.49	0.47
1:C:27:CYS:O	1:C:33:GLY:HA2	2.14	0.47
1:D:112:ASN:HB2	1:D:115:HIS:CD2	2.49	0.47
1:B:6:ARG:HH22	1:B:10:LYS:HE3	1.77	0.47
1:B:122:LYS:O	1:B:122:LYS:HD3	2.14	0.47
1:D:25:TYR:CE1	1:D:41:LEU:HD23	2.49	0.47
4:D:130:OSF:H2A	4:D:130:OSF:H5	1.63	0.47
1:C:6:ARG:HB2	4:C:128:OSF:C8	2.44	0.47
1:A:3:TRP:CE3	1:A:4:GLN:HG3	2.50	0.47
1:B:39:ASP:OD2	1:B:115:HIS:HD2	1.98	0.47
1:C:89:ASN:HB2	1:C:92:GLU:H	1.80	0.47
1:A:20:MET:O	1:A:116:LYS:HE2	2.14	0.46
1:B:45:CYS:HB3	4:B:127:OSF:O4	2.16	0.46
1:D:19:LEU:HA	4:D:129:OSF:H6	1.96	0.46
1:B:19:LEU:HD23	4:B:126:OSF:C3	2.45	0.46
1:B:8:MET:O	1:B:11:CYS:HB3	2.15	0.46
1:D:8:MET:HG2	1:D:82:ILE:HD13	1.98	0.46
1:A:17:HIS:O	1:A:21:ASP:HB2	2.16	0.46
4:C:126:OSF:H5	1:D:2:LEU:HD12	1.97	0.46
1:C:71:GLU:HG2	1:C:95:ILE:HD12	1.98	0.46
1:C:6:ARG:HB2	4:C:128:OSF:H8B	1.98	0.45
1:C:28:TYR:CE2	1:C:37:PRO:HG3	2.51	0.45
1:D:2:LEU:HD13	1:D:2:LEU:C	2.41	0.45
1:D:31:LEU:O	4:D:131:OSF:S	2.75	0.45
1:B:20:MET:O	1:B:116:LYS:HE2	2.16	0.45
1:C:25:TYR:CE1	1:C:41:LEU:HD23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:CYS:SG	1:B:105:CYS:CB	3.05	0.44
1:D:25:TYR:CZ	1:D:115:HIS:HB2	2.51	0.44
1:D:58:LEU:HD11	1:D:94:PHE:CG	2.52	0.44
1:D:112:ASN:HB2	1:D:115:HIS:HD2	1.81	0.44
1:B:66:ASP:HB3	1:B:70:THR:OG1	2.18	0.44
1:B:48:HIS:HE1	1:B:99:ASP:OD1	1.99	0.44
1:B:65:VAL:HG23	1:B:66:ASP:N	2.32	0.44
1:D:58:LEU:C	1:D:60:SER:N	2.74	0.44
1:A:6:ARG:HH22	4:B:128:OSF:H1	1.82	0.44
1:C:13:ILE:O	1:C:16:SER:HB2	2.17	0.44
1:A:58:LEU:HD11	1:A:94:PHE:CE2	2.53	0.44
1:D:5:PHE:O	1:D:9:ILE:HG13	2.17	0.44
1:A:6:ARG:HH21	1:A:19:LEU:CD1	2.31	0.44
1:D:25:TYR:CD1	1:D:25:TYR:C	2.95	0.44
1:B:48:HIS:CE1	1:B:99:ASP:OD1	2.71	0.43
1:A:13:ILE:HD11	1:A:107:SER:CA	2.48	0.43
1:A:25:TYR:CE1	1:A:41:LEU:HD23	2.53	0.43
1:B:23:ASN:O	1:B:24:ASN:HB3	2.18	0.43
1:B:27:CYS:H	1:B:42:ASP:CG	2.26	0.43
1:C:16:SER:C	1:C:18:PRO:HD3	2.43	0.43
1:D:31:LEU:O	4:D:131:OSF:O4	2.37	0.43
1:D:6:ARG:HG2	1:D:18:PRO:CB	2.48	0.42
4:C:126:OSF:H6A	1:D:3:TRP:CE3	2.47	0.42
1:D:116:LYS:HD3	1:D:117:ASN:H	1.84	0.42
1:B:58:LEU:CD2	1:B:60:SER:H	2.32	0.42
1:D:2:LEU:HD23	1:D:69:TYR:CE1	2.54	0.42
4:D:129:OSF:H4	4:D:129:OSF:H7A	1.74	0.42
1:C:33:GLY:H	1:D:57:ASN:HD21	1.60	0.42
1:C:8:MET:O	1:C:11:CYS:HB3	2.20	0.42
1:D:16:SER:O	1:D:18:PRO:HD3	2.19	0.41
1:C:63:PHE:O	1:C:66:ASP:HB2	2.20	0.41
1:D:58:LEU:C	1:D:60:SER:H	2.28	0.41
1:C:57:ASN:HD22	1:D:32:GLY:CA	2.33	0.41
4:C:128:OSF:H4	4:C:128:OSF:H7A	1.80	0.41
1:D:119:ASP:OD2	1:D:119:ASP:C	2.62	0.41
1:A:1:ALA:HB1	1:A:3:TRP:CE2	2.56	0.41
1:B:6:ARG:HD2	4:B:126:OSF:O3	2.19	0.41
1:A:71:GLU:CG	1:A:95:ILE:HD12	2.43	0.41
1:A:116:LYS:HG3	1:A:117:ASN:N	2.36	0.41
1:C:58:LEU:HD11	1:C:94:PHE:CG	2.55	0.41
1:B:119:ASP:OD2	1:B:119:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ASP:OD2	1:C:115:HIS:HD2	2.04	0.41
1:D:104:ILE:O	1:D:105:CYS:C	2.62	0.41
1:A:69:TYR:HB2	4:C:127:OSF:H5A	2.03	0.40
1:B:71:GLU:HG2	1:B:95:ILE:HD12	2.02	0.40
1:D:73:TYR:CD1	1:D:73:TYR:C	2.99	0.40
1:A:111:TYR:OH	1:A:116:LYS:HD3	2.20	0.40
1:C:5:PHE:O	1:C:9:ILE:HG13	2.21	0.40
1:B:69:TYR:OH	4:B:127:OSF:O2	2.40	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	122/124 (98%)	114 (93%)	5 (4%)	3 (2%)	4	11
1	B	122/124 (98%)	110 (90%)	11 (9%)	1 (1%)	16	37
1	C	122/124 (98%)	111 (91%)	9 (7%)	2 (2%)	7	20
1	D	122/124 (98%)	105 (86%)	12 (10%)	5 (4%)	2	5
All	All	488/496 (98%)	440 (90%)	37 (8%)	11 (2%)	5	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	PRO
1	A	14	PRO
1	B	14	PRO
1	D	110	PRO
1	A	90	ALA
1	D	18	PRO
1	D	111	TYR

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Mol	Chain	Res	Type
1	A	18	PRO
1	D	14	PRO
1	C	18	PRO
1	D	86	SER

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	110/110 (100%)	107 (97%)	3 (3%)	39	69
1	B	110/110 (100%)	106 (96%)	4 (4%)	31	60
1	C	110/110 (100%)	107 (97%)	3 (3%)	39	69
1	D	110/110 (100%)	109 (99%)	1 (1%)	70	87
All	All	440/440 (100%)	429 (98%)	11 (2%)	42	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TRP
1	A	14	PRO
1	A	19	LEU
1	B	14	PRO
1	B	75	TYR
1	B	87	LYS
1	B	114	GLU
1	C	14	PRO
1	C	60	SER
1	C	113	LYS
1	D	18	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN

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Mol	Chain	Res	Type
1	A	57	ASN
1	A	85	ASN
1	A	117	ASN
1	B	23	ASN
1	B	67	ASN
1	B	85	ASN
1	B	89	ASN
1	B	115	HIS
1	B	117	ASN
1	C	57	ASN
1	C	89	ASN
1	C	115	HIS
1	D	23	ASN
1	D	24	ASN
1	D	48	HIS
1	D	57	ASN
1	D	85	ASN
1	D	115	HIS
1	D	117	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
4	OSF	B	128	-	12,12,12	3.01	4 (33%)	13,14,14	0.79	0
4	OSF	D	130	-	12,12,12	2.72	4 (33%)	13,14,14	1.12	2 (15%)
4	OSF	D	131	-	12,12,12	2.77	4 (33%)	13,14,14	0.64	0
4	OSF	D	128	-	12,12,12	2.70	4 (33%)	13,14,14	0.84	0
4	OSF	D	129	2	12,12,12	2.74	4 (33%)	13,14,14	1.06	1 (7%)
4	OSF	C	126	-	12,12,12	2.72	4 (33%)	13,14,14	0.74	0
4	OSF	C	128	2	12,12,12	2.57	4 (33%)	13,14,14	1.05	1 (7%)
4	OSF	B	126	-	12,12,12	2.65	4 (33%)	13,14,14	0.87	0
4	OSF	A	127	-	12,12,12	2.91	4 (33%)	13,14,14	0.78	0
4	OSF	C	129	-	12,12,12	2.85	4 (33%)	13,14,14	0.70	0
4	OSF	B	127	2	12,12,12	2.58	4 (33%)	13,14,14	0.97	0
4	OSF	C	127	-	12,12,12	2.71	4 (33%)	13,14,14	0.97	1 (7%)

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
4	OSF	B	128	-	-	0/10/10/10	-
4	OSF	D	130	-	-	0/10/10/10	-
4	OSF	D	131	-	-	0/10/10/10	-
4	OSF	D	128	-	-	0/10/10/10	-
4	OSF	D	129	2	-	0/10/10/10	-
4	OSF	C	126	-	-	0/10/10/10	-
4	OSF	C	128	2	-	0/10/10/10	-
4	OSF	B	126	-	-	0/10/10/10	-
4	OSF	A	127	-	-	0/10/10/10	-
4	OSF	C	129	-	-	0/10/10/10	-
4	OSF	B	127	2	-	0/10/10/10	-
4	OSF	C	127	-	-	0/10/10/10	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	128	OSF	O1-S	5.82	1.72	1.56
4	A	127	OSF	O2-S	5.76	1.70	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	131	OSF	O4-S	5.65	1.69	1.45
4	D	130	OSF	O4-S	5.63	1.69	1.45
4	B	128	OSF	O2-S	5.61	1.69	1.45
4	D	129	OSF	O4-S	5.60	1.69	1.45
4	A	127	OSF	O4-S	5.59	1.69	1.45
4	B	128	OSF	O4-S	5.58	1.69	1.45
4	C	129	OSF	O4-S	5.52	1.69	1.45
4	C	126	OSF	O2-S	5.52	1.69	1.45
4	D	128	OSF	O4-S	5.50	1.69	1.45
4	B	126	OSF	O4-S	5.47	1.69	1.45
4	D	129	OSF	O2-S	5.45	1.69	1.45
4	D	131	OSF	O2-S	5.44	1.68	1.45
4	C	129	OSF	O2-S	5.42	1.68	1.45
4	C	127	OSF	O2-S	5.39	1.68	1.45
4	C	128	OSF	O2-S	5.37	1.68	1.45
4	D	128	OSF	O2-S	5.37	1.68	1.45
4	C	127	OSF	O4-S	5.28	1.68	1.45
4	B	127	OSF	O2-S	5.25	1.68	1.45
4	B	127	OSF	O4-S	5.25	1.68	1.45
4	C	128	OSF	O4-S	5.24	1.68	1.45
4	B	126	OSF	O2-S	5.21	1.67	1.45
4	D	130	OSF	O2-S	5.19	1.67	1.45
4	C	126	OSF	O4-S	5.13	1.67	1.45
4	C	129	OSF	O1-S	5.05	1.70	1.56
4	A	127	OSF	O1-S	5.03	1.70	1.56
4	C	127	OSF	O1-S	4.59	1.69	1.56
4	C	126	OSF	O1-S	4.54	1.69	1.56
4	D	131	OSF	O1-S	4.36	1.68	1.56
4	D	128	OSF	O1-S	4.31	1.68	1.56
4	D	129	OSF	O1-S	4.26	1.68	1.56
4	B	126	OSF	O1-S	4.07	1.67	1.56
4	D	130	OSF	O1-S	4.04	1.67	1.56
4	B	127	OSF	O1-S	3.97	1.67	1.56
4	C	128	OSF	O1-S	3.80	1.67	1.56
4	B	128	OSF	O3-S	3.10	1.69	1.50
4	D	130	OSF	O3-S	3.10	1.69	1.50
4	D	131	OSF	O3-S	3.08	1.69	1.50
4	C	129	OSF	O3-S	3.06	1.69	1.50
4	A	127	OSF	O3-S	3.06	1.69	1.50
4	D	129	OSF	O3-S	3.00	1.69	1.50
4	C	127	OSF	O3-S	2.99	1.69	1.50
4	D	128	OSF	O3-S	2.96	1.68	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	126	OSF	O3-S	2.95	1.68	1.50
4	B	126	OSF	O3-S	2.95	1.68	1.50
4	B	127	OSF	O3-S	2.84	1.68	1.50
4	C	128	OSF	O3-S	2.70	1.67	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	129	OSF	C3-C2-C1	-2.61	102.11	113.47
4	C	128	OSF	C3-C2-C1	-2.47	102.74	113.47
4	C	127	OSF	C3-C2-C1	-2.39	103.07	113.47
4	D	130	OSF	C4-C3-C2	-2.37	102.40	114.37
4	D	130	OSF	O3-S-O1	2.08	111.15	106.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	128	OSF	3	0
4	D	130	OSF	4	0
4	D	131	OSF	2	0
4	D	128	OSF	1	0
4	D	129	OSF	5	0
4	C	126	OSF	5	0
4	C	128	OSF	4	0
4	B	126	OSF	5	0
4	A	127	OSF	2	0
4	C	129	OSF	3	0
4	B	127	OSF	5	0
4	C	127	OSF	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	124/124 (100%)	-0.17	1 (0%) 82 81	6, 17, 27, 34	1 (0%)
1	B	124/124 (100%)	-0.13	1 (0%) 82 81	10, 19, 34, 45	1 (0%)
1	C	124/124 (100%)	-0.01	1 (0%) 82 81	13, 23, 34, 40	0
1	D	124/124 (100%)	0.43	4 (3%) 50 46	16, 31, 48, 54	1 (0%)
All	All	496/496 (100%)	0.03	7 (1%) 73 72	6, 22, 41, 54	3 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	TRP	3.6
1	A	121	LYS	2.1
1	D	112	ASN	2.1
1	D	83	THR	2.1
1	D	14	PRO	2.1
1	B	3	TRP	2.1
1	C	89	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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
4	OSF	B	128	13/13	0.64	0.25	55,56,58,60	0
4	OSF	D	131	13/13	0.81	0.28	43,50,60,60	0
4	OSF	C	129	13/13	0.83	0.23	49,55,61,61	0
5	NA	D	126	1/1	0.83	0.15	20,20,20,20	0
4	OSF	D	129	13/13	0.85	0.21	40,44,49,49	0
4	OSF	A	127	13/13	0.89	0.18	49,50,51,51	0
4	OSF	C	128	13/13	0.91	0.20	25,29,39,41	0
4	OSF	D	128	13/13	0.93	0.15	30,34,36,36	0
4	OSF	C	126	13/13	0.93	0.14	21,25,33,34	0
4	OSF	B	127	13/13	0.94	0.14	24,28,31,31	0
3	CL	D	127	1/1	0.94	0.10	30,30,30,30	0
4	OSF	B	126	13/13	0.94	0.14	18,25,32,33	0
2	CA	A	125	1/1	0.95	0.05	33,33,33,33	0
4	OSF	D	130	13/13	0.95	0.14	21,29,46,47	0
4	OSF	C	127	13/13	0.96	0.13	16,20,30,30	0
2	CA	C	125	1/1	0.97	0.04	19,19,19,19	0
3	CL	A	126	1/1	0.97	0.05	29,29,29,29	0
2	CA	D	125	1/1	0.99	0.02	18,18,18,18	0
2	CA	B	125	1/1	0.99	0.03	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.