



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:52 PM UTC

PDB ID : 3WLA / pdb_00003wla
Title : Crystal Structure of sOPH Native
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Deposited on : 2013-11-08
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

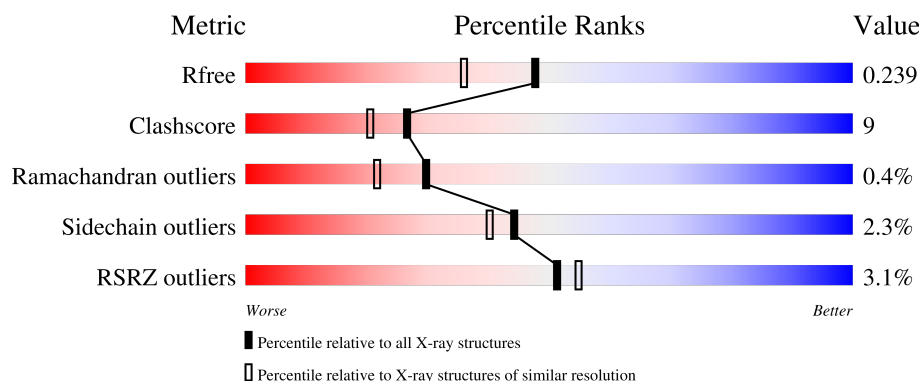
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

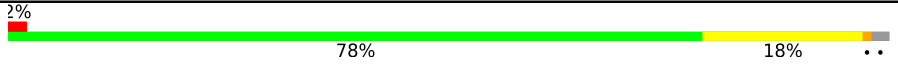
The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	
1	C	336	

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
2	SO4	A	901	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8396 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.

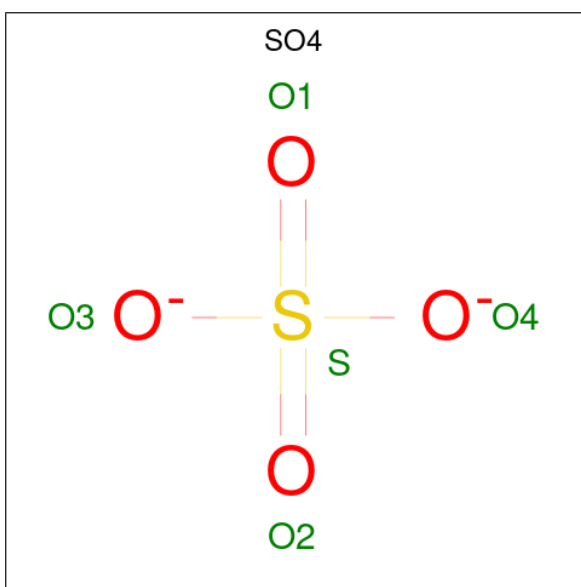
- Molecule 1 is a protein called Oxidized polyvinyl alcohol hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2514	1591	437	469	17			
1	B	329	Total	C	N	O	S	0	0	0
			2514	1591	437	469	17			
1	C	329	Total	C	N	O	S	0	0	0
			2514	1591	437	469	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLU	-	expression tag	UNP Q588Z2
A	-4	ALA	-	expression tag	UNP Q588Z2
A	-3	GLU	-	expression tag	UNP Q588Z2
A	-2	ALA	-	expression tag	UNP Q588Z2
A	-1	TYR	-	expression tag	UNP Q588Z2
A	0	VAL	-	expression tag	UNP Q588Z2
B	-5	GLU	-	expression tag	UNP Q588Z2
B	-4	ALA	-	expression tag	UNP Q588Z2
B	-3	GLU	-	expression tag	UNP Q588Z2
B	-2	ALA	-	expression tag	UNP Q588Z2
B	-1	TYR	-	expression tag	UNP Q588Z2
B	0	VAL	-	expression tag	UNP Q588Z2
C	-5	GLU	-	expression tag	UNP Q588Z2
C	-4	ALA	-	expression tag	UNP Q588Z2
C	-3	GLU	-	expression tag	UNP Q588Z2
C	-2	ALA	-	expression tag	UNP Q588Z2
C	-1	TYR	-	expression tag	UNP Q588Z2
C	0	VAL	-	expression tag	UNP Q588Z2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

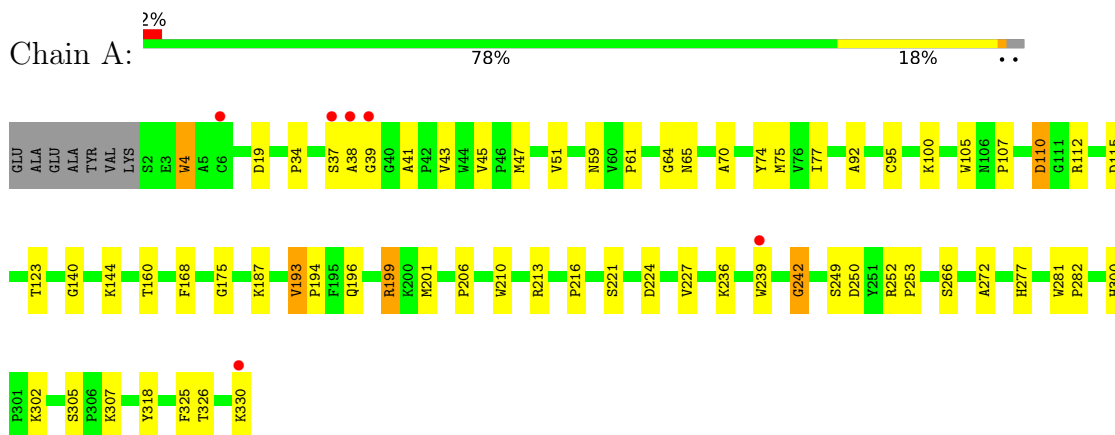
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	312	Total	O	0	0
			312	312		
3	B	263	Total	O	0	0
			263	263		
3	C	259	Total	O	0	0
			259	259		

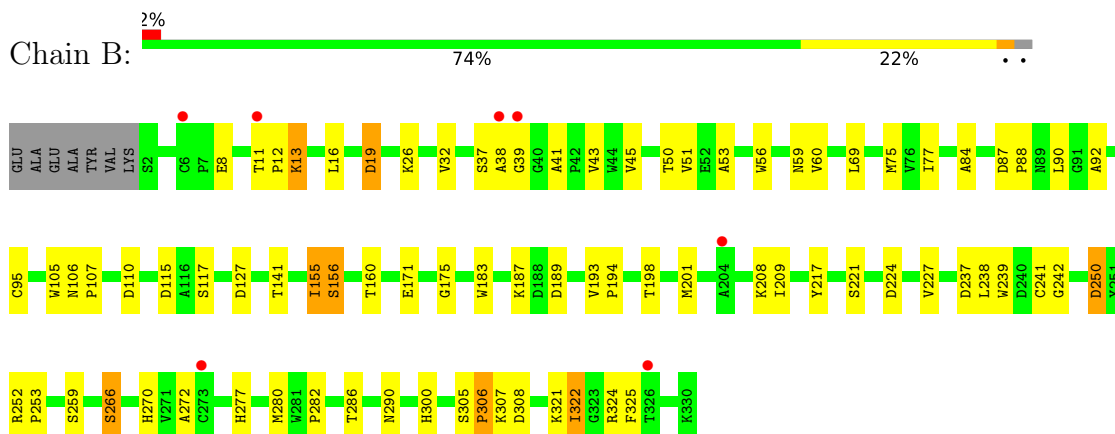
3 Residue-property plots [i](#)

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.

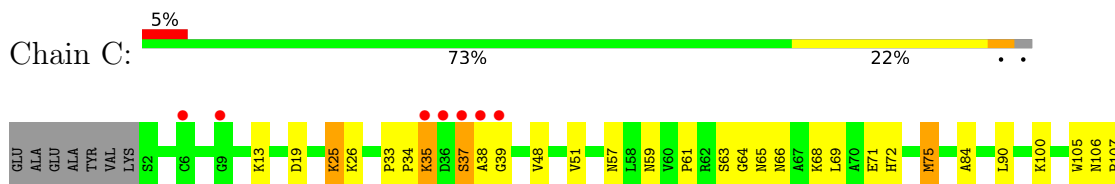
- Molecule 1: Oxidized polyvinyl alcohol hydrolase

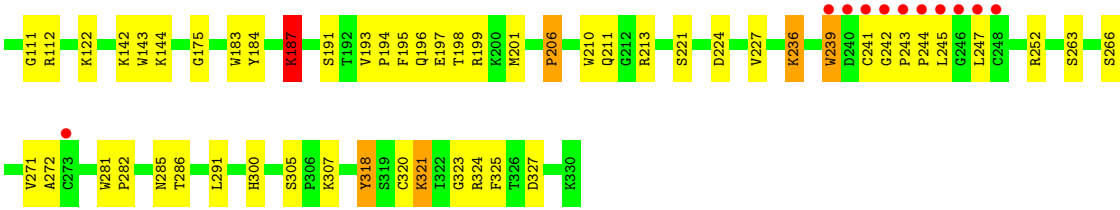


- Molecule 1: Oxidized polyvinyl alcohol hydrolase



- Molecule 1: Oxidized polyvinyl alcohol hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.34Å 75.74Å 75.98Å 74.04° 88.67° 74.01°	Depositor
Resolution (Å)	25.00 – 1.90 25.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-1.90) 93.7 (25.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.89Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.193 , 0.239 0.193 , 0.239	Depositor DCC
R_{free} test set	4490 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.00	1/2594 (0.0%)	1.18	15/3535 (0.4%)
1	B	1.04	1/2594 (0.0%)	1.21	22/3535 (0.6%)
1	C	1.05	1/2594 (0.0%)	1.25	23/3535 (0.7%)
All	All	1.03	3/7782 (0.0%)	1.22	60/10605 (0.6%)

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	A	0	1
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	MET	SD-CE	6.76	1.96	1.79
1	B	156	SER	CA-C	5.41	1.57	1.52
1	C	271	VAL	CA-CB	-5.30	1.47	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	GLY	CA-C-N	11.11	127.77	119.66
1	A	242	GLY	C-N-CA	11.11	127.77	119.66
1	B	183	TRP	N-CA-C	-8.28	104.04	114.56
1	C	106	ASN	N-CA-C	8.12	124.77	113.57
1	C	286	THR	N-CA-C	7.63	119.29	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	VAL	N-CA-C	7.45	120.05	112.90
1	B	266	SER	N-CA-C	7.25	120.05	111.71
1	C	266	SER	N-CA-C	6.90	120.80	112.38
1	C	59	ASN	N-CA-C	6.79	122.39	113.30
1	C	75	MET	N-CA-C	-6.76	98.22	108.96
1	A	51	VAL	N-CA-C	6.75	119.65	113.10
1	A	266	SER	N-CA-C	6.74	119.48	111.33
1	B	221	SER	N-CA-C	-6.74	105.09	113.38
1	C	122	LYS	N-CA-C	-6.73	104.55	112.89
1	B	32	VAL	CA-C-N	6.66	124.45	119.66
1	B	32	VAL	C-N-CA	6.66	124.45	119.66
1	C	187	LYS	N-CA-C	-6.58	102.31	110.41
1	C	206	PRO	N-CA-C	6.46	121.97	114.03
1	C	252	ARG	CA-C-N	-6.36	112.44	119.19
1	C	252	ARG	C-N-CA	-6.36	112.44	119.19
1	C	318	TYR	N-CA-C	6.36	119.55	109.50
1	B	250	ASP	N-CA-C	-6.29	98.16	108.41
1	B	106	ASN	N-CA-C	6.12	123.34	109.81
1	C	197	GLU	N-CA-C	-6.09	104.55	111.07
1	C	37	SER	N-CA-C	6.07	121.70	113.21
1	A	193	VAL	N-CA-C	-6.04	101.13	107.84
1	B	59	ASN	N-CA-C	6.01	121.53	113.72
1	A	41	ALA	N-CA-C	5.95	117.31	109.93
1	A	110	ASP	N-CA-C	5.88	120.58	113.17
1	A	221	SER	N-CA-C	-5.75	106.27	113.28
1	B	41	ALA	N-CA-C	5.68	116.98	109.93
1	C	66	ASN	N-CA-C	5.64	118.20	111.71
1	B	43	VAL	N-CA-C	5.63	116.69	108.53
1	C	51	VAL	N-CA-C	5.60	118.53	113.10
1	A	277	HIS	N-CA-C	5.47	119.82	113.20
1	C	183	TRP	N-CA-C	-5.39	107.36	114.31
1	C	211	GLN	N-CA-C	-5.33	103.49	110.53
1	A	59	ASN	N-CA-C	5.33	121.52	114.12
1	A	326	THR	N-CA-C	-5.30	106.75	114.12
1	B	127	ASP	N-CA-C	5.30	117.05	111.28
1	A	43	VAL	N-CA-C	5.29	116.20	108.53
1	A	19	ASP	N-CA-C	5.27	118.98	112.24
1	C	239	TRP	CA-CB-CG	-5.26	103.60	113.60
1	B	286	THR	N-CA-C	5.26	117.43	111.02
1	B	242	GLY	CA-C-N	5.25	125.79	120.38
1	B	242	GLY	C-N-CA	5.25	125.79	120.38
1	C	33	PRO	N-CA-C	5.23	115.49	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	CYS	N-CA-C	5.16	117.66	109.50
1	B	224	ASP	CA-C-N	5.13	125.42	119.93
1	B	224	ASP	C-N-CA	5.13	125.42	119.93
1	A	206	PRO	N-CA-C	5.13	120.59	113.98
1	B	50	THR	N-CA-C	5.10	117.97	111.69
1	B	141	THR	N-CA-C	-5.10	106.91	113.23
1	C	63	SER	CA-C-N	-5.09	117.91	123.30
1	C	63	SER	C-N-CA	-5.09	117.91	123.30
1	B	322	ILE	N-CA-C	-5.04	102.35	109.21
1	B	75	MET	N-CA-C	-5.04	100.95	108.96
1	B	19	ASP	N-CA-C	5.03	118.54	111.90
1	A	4	TRP	N-CA-C	5.03	117.16	109.07
1	C	221	SER	N-CA-C	-5.03	106.66	112.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	TYR	Sidechain
1	C	318	TYR	Sidechain

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	2514	0	2401	40	0
1	B	2514	0	2401	42	0
1	C	2514	0	2401	56	0
2	A	5	0	0	3	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
3	A	312	0	0	8	0
3	B	263	0	0	4	0
3	C	259	0	0	10	0
All	All	8396	0	7203	137	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 9.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:VAL:HG21	1:C:201:MET:HE1	1.31	1.06
1:A:239:TRP:HZ3	2:A:901:SO4:O3	1.41	1.01
1:C:198:THR:HA	1:C:201:MET:HE3	1.46	0.97
1:A:330:LYS:HA	3:A:1257:HOH:O	1.70	0.92
1:A:239:TRP:CZ3	2:A:901:SO4:O3	2.26	0.89
1:B:13:LYS:HB2	1:B:13:LYS:NZ	1.93	0.83
1:A:37:SER:O	1:A:39:GLY:N	2.22	0.72
1:C:236:LYS:HE3	1:C:236:LYS:HA	1.70	0.72
1:A:236:LYS:HE2	3:A:1108:HOH:O	1.88	0.71
1:A:224:ASP:OD2	1:A:302:LYS:HE3	1.90	0.70
1:C:195:PHE:O	1:C:199:ARG:HG3	1.92	0.68
1:B:187:LYS:HE2	3:B:544:HOH:O	1.93	0.68
1:A:305:SER:OG	1:A:307:LYS:HG2	1.93	0.68
1:C:187:LYS:HG3	1:C:191:SER:OG	1.94	0.67
1:C:199:ARG:NH2	3:C:759:HOH:O	2.28	0.67
1:C:19:ASP:OD1	1:C:26:LYS:HD3	1.95	0.67
1:C:68:LYS:HE3	3:C:611:HOH:O	1.93	0.66
1:B:84:ALA:HA	1:B:90:LEU:HD23	1.77	0.66
1:C:195:PHE:CZ	1:C:199:ARG:HD2	2.32	0.65
1:C:236:LYS:HA	1:C:236:LYS:CE	2.28	0.63
1:C:193:VAL:CG2	1:C:201:MET:HE1	2.20	0.63
1:C:198:THR:CA	1:C:201:MET:HE3	2.27	0.62
1:B:13:LYS:HB2	1:B:13:LYS:HZ2	1.64	0.62
1:C:84:ALA:HA	1:C:90:LEU:HD23	1.82	0.61
1:C:206:PRO:O	1:C:324:ARG:NH2	2.32	0.61
1:C:305:SER:OG	1:C:307:LYS:HE3	2.00	0.61
1:A:307:LYS:HE2	3:A:1240:HOH:O	2.01	0.60
1:C:201:MET:HG3	1:C:210:TRP:CH2	2.37	0.59
1:B:189:ASP:HA	1:B:217:TYR:OH	2.02	0.59
1:B:300:HIS:HE1	3:B:513:HOH:O	1.85	0.59
1:A:105:TRP:CD1	1:A:107:PRO:HD2	2.39	0.58
1:B:305:SER:OG	1:B:307:LYS:HE2	2.04	0.58
1:C:193:VAL:HB	1:C:194:PRO:HD2	1.85	0.58
1:C:285:ASN:OD1	3:C:668:HOH:O	2.17	0.57
1:B:37:SER:O	1:B:39:GLY:N	2.37	0.56
1:B:277:HIS:O	1:B:280:MET:HE3	2.06	0.56
1:C:105:TRP:CD1	1:C:107:PRO:HD2	2.41	0.56
1:C:193:VAL:HG21	1:C:201:MET:CE	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LYS:HB2	1:B:13:LYS:HZ3	1.70	0.56
1:C:100:LYS:HE3	3:C:720:HOH:O	2.06	0.55
1:A:110:ASP:HB2	1:A:160:THR:HG22	1.88	0.54
1:A:193:VAL:HB	1:A:194:PRO:HD2	1.90	0.54
1:A:239:TRP:CD1	1:A:239:TRP:C	2.86	0.54
1:B:105:TRP:CD1	1:B:107:PRO:HD2	2.43	0.53
1:B:19:ASP:OD1	1:B:26:LYS:HD3	2.08	0.53
1:C:239:TRP:O	1:C:247:LEU:HD12	2.08	0.53
1:A:239:TRP:HZ3	2:A:901:SO4:S	2.30	0.53
1:C:272:ALA:HB1	1:C:325:PHE:CD1	2.45	0.52
1:C:236:LYS:HD2	1:C:236:LYS:N	2.24	0.52
1:A:4:TRP:CE3	1:A:140:GLY:HA3	2.45	0.51
1:B:16:LEU:HD13	1:B:88:PRO:HG3	1.92	0.51
1:B:266:SER:O	1:B:306:PRO:HG2	2.12	0.50
1:B:115:ASP:OD1	1:B:117:SER:OG	2.25	0.50
1:C:239:TRP:CE3	1:C:239:TRP:HA	2.47	0.50
1:A:168:PHE:CE1	1:A:216:PRO:HG3	2.47	0.50
1:A:242:GLY:HA2	3:A:1262:HOH:O	2.12	0.49
1:B:239:TRP:CZ3	1:B:241:CYS:HB3	2.48	0.49
1:A:201:MET:HE3	1:A:210:TRP:CZ3	2.47	0.49
1:A:175:GLY:HA3	1:A:227:VAL:O	2.13	0.49
1:B:238:LEU:HD23	1:B:250:ASP:HA	1.93	0.49
1:C:48:VAL:HG12	1:C:57:ASN:HB2	1.95	0.48
1:B:193:VAL:HB	1:B:194:PRO:HD2	1.94	0.48
1:A:252:ARG:HB3	1:A:253:PRO:CD	2.43	0.48
1:C:142:LYS:HD3	1:C:143:TRP:CH2	2.48	0.48
1:B:321:LYS:HE2	1:B:322:ILE:O	2.13	0.48
1:A:168:PHE:CZ	1:A:216:PRO:HG3	2.49	0.48
1:B:12:PRO:C	1:B:13:LYS:HG3	2.38	0.48
1:B:45:VAL:HA	1:B:77:ILE:O	2.14	0.48
1:C:144:LYS:HD3	1:C:144:LYS:HA	1.60	0.48
1:C:300:HIS:HD2	3:C:550:HOH:O	1.95	0.48
1:A:199:ARG:HD3	1:A:250:ASP:OD2	2.14	0.47
1:C:64:GLY:HA2	1:C:281:TRP:CD1	2.49	0.47
1:C:37:SER:O	1:C:39:GLY:N	2.46	0.47
1:B:305:SER:HB3	1:B:308:ASP:OD2	2.14	0.47
1:B:155:ILE:HG13	1:B:156:SER:N	2.28	0.47
1:C:327:ASP:OD1	1:C:327:ASP:C	2.58	0.47
1:B:175:GLY:HA3	1:B:227:VAL:O	2.15	0.47
1:C:112:ARG:HG2	1:C:213:ARG:HB3	1.96	0.47
1:C:300:HIS:HE1	3:C:554:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TRP:N	3:C:537:HOH:O	2.46	0.47
1:C:34:PRO:HD3	1:C:75:MET:HA	1.97	0.46
1:A:34:PRO:HD3	1:A:75:MET:HA	1.98	0.46
1:A:272:ALA:HB1	1:A:325:PHE:CD1	2.51	0.46
1:C:321:LYS:HD2	1:C:324:ARG:O	2.15	0.46
1:B:237:ASP:C	1:B:238:LEU:HG	2.40	0.46
1:A:239:TRP:HB3	1:A:249:SER:HB2	1.98	0.46
1:B:324:ARG:HD2	3:B:695:HOH:O	2.15	0.46
1:A:123:THR:HG22	3:A:1248:HOH:O	2.16	0.45
1:A:187:LYS:HE2	1:A:193:VAL:CG1	2.46	0.45
1:A:194:PRO:HG2	3:B:657:HOH:O	2.16	0.45
1:C:175:GLY:HA3	1:C:227:VAL:O	2.15	0.45
1:A:115:ASP:OD1	1:B:194:PRO:HD3	2.16	0.45
1:A:300:HIS:HE1	3:A:1086:HOH:O	1.99	0.45
1:C:72:HIS:CE1	1:C:291:LEU:HD22	2.51	0.45
1:C:281:TRP:CD1	1:C:282:PRO:HD2	2.52	0.45
1:C:111:GLY:HA3	1:C:184:TYR:CE2	2.52	0.45
1:B:198:THR:O	1:B:201:MET:HG2	2.17	0.45
1:C:142:LYS:HD3	1:C:143:TRP:CZ3	2.51	0.45
1:A:61:PRO:HA	1:A:65:ASN:HB2	1.98	0.44
1:B:56:TRP:HA	1:B:60:VAL:HG23	1.99	0.44
1:C:37:SER:HA	3:C:749:HOH:O	2.17	0.44
1:A:236:LYS:HD3	3:C:678:HOH:O	2.18	0.44
1:A:307:LYS:CE	3:A:1240:HOH:O	2.62	0.44
1:A:272:ALA:HB1	1:A:325:PHE:CE1	2.52	0.44
1:C:242:GLY:O	1:C:243:PRO:C	2.61	0.44
1:B:87:ASP:OD1	1:B:87:ASP:C	2.60	0.43
1:C:61:PRO:HA	1:C:65:ASN:HB2	2.00	0.43
1:C:263:SER:OG	1:C:323:GLY:HA2	2.18	0.43
1:B:69:LEU:HD21	1:B:290:ASN:HB3	2.01	0.43
1:C:25:LYS:HD3	3:C:593:HOH:O	2.19	0.43
1:B:272:ALA:HB1	1:B:325:PHE:CE1	2.54	0.43
1:B:259:SER:HB2	1:B:270:HIS:CE1	2.53	0.42
1:A:92:ALA:O	1:A:95:CYS:HB2	2.19	0.42
1:A:187:LYS:HE2	1:A:193:VAL:HG11	2.00	0.42
1:C:187:LYS:HD2	1:C:193:VAL:CG1	2.49	0.42
1:C:241:CYS:SG	1:C:245:LEU:HB2	2.60	0.42
1:B:53:ALA:HB3	1:B:56:TRP:CD1	2.55	0.42
1:B:92:ALA:O	1:B:95:CYS:HB2	2.19	0.42
1:C:35:LYS:HD2	1:C:71:GLU:HA	2.02	0.42
1:A:144:LYS:NZ	3:A:1233:HOH:O	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:MET:HE2	1:C:201:MET:HB3	1.77	0.42
1:C:236:LYS:CE	1:C:236:LYS:CA	2.97	0.42
1:B:12:PRO:C	1:B:13:LYS:CG	2.93	0.42
1:C:142:LYS:HB3	1:C:143:TRP:CE3	2.55	0.42
1:A:112:ARG:HG2	1:A:213:ARG:HB3	2.02	0.41
1:B:11:THR:O	1:B:11:THR:HG23	2.18	0.41
1:C:247:LEU:HD12	1:C:247:LEU:HA	1.91	0.41
1:B:171:GLU:H	1:B:171:GLU:CD	2.28	0.41
1:B:110:ASP:HB2	1:B:160:THR:HG22	2.03	0.41
1:A:64:GLY:HA2	1:A:281:TRP:CD1	2.56	0.41
1:B:87:ASP:HA	1:B:88:PRO:HD2	2.00	0.41
1:B:208:LYS:HG2	1:B:209:ILE:N	2.32	0.41
1:A:70:ALA:HA	1:A:74:TYR:O	2.21	0.40
1:A:45:VAL:HA	1:A:77:ILE:O	2.21	0.40
1:B:252:ARG:HB3	1:B:253:PRO:CD	2.52	0.40
1:C:281:TRP:O	1:C:282:PRO:C	2.64	0.40
1:C:305:SER:OG	1:C:307:LYS:HG2	2.21	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	327/336 (97%)	315 (96%)	11 (3%)	1 (0%)	36	29
1	B	327/336 (97%)	315 (96%)	11 (3%)	1 (0%)	36	29
1	C	327/336 (97%)	311 (95%)	14 (4%)	2 (1%)	21	13
All	All	981/1008 (97%)	941 (96%)	36 (4%)	4 (0%)	30	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	B	38	ALA
1	C	38	ALA
1	C	35	LYS

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	265/270 (98%)	261 (98%)	4 (2%)	57	56
1	B	265/270 (98%)	260 (98%)	5 (2%)	50	47
1	C	265/270 (98%)	256 (97%)	9 (3%)	32	25
All	All	795/810 (98%)	777 (98%)	18 (2%)	44	40

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LYS
1	A	196	GLN
1	A	199	ARG
1	A	282	PRO
1	B	8	GLU
1	B	13	LYS
1	B	155	ILE
1	B	282	PRO
1	B	306	PRO
1	C	13	LYS
1	C	25	LYS
1	C	69	LEU
1	C	187	LYS
1	C	196	GLN
1	C	224	ASP
1	C	236	LYS
1	C	244	PRO
1	C	321	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	300	HIS
1	B	82	GLN
1	B	109	ASN
1	B	300	HIS
1	C	72	HIS
1	C	82	GLN
1	C	109	ASN
1	C	283	GLN
1	C	285	ASN
1	C	300	HIS

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	SO4	C	401	-	4,4,4	0.62	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	402	-	4,4,4	0.50	0	6,6,6	0.20	0
2	SO4	B	401	-	4,4,4	0.53	0	6,6,6	0.36	0
2	SO4	A	901	-	4,4,4	0.49	0	6,6,6	0.34	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	SO4	3	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

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	329/336 (97%)	-0.14	6 (1%) 67 71	18, 28, 42, 51	0
1	B	329/336 (97%)	0.10	7 (2%) 63 67	17, 30, 45, 62	0
1	C	329/336 (97%)	0.24	18 (5%) 30 32	17, 30, 54, 90	0
All	All	987/1008 (97%)	0.07	31 (3%) 51 55	17, 30, 45, 90	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	PRO	6.0
1	C	245	LEU	5.9
1	C	246	GLY	5.2
1	C	242	GLY	4.8
1	C	247	LEU	4.4
1	C	239	TRP	4.3
1	C	38	ALA	4.2
1	C	36	ASP	4.2
1	C	243	PRO	4.0
1	C	241	CYS	3.8
1	C	6	CYS	3.6
1	B	39	GLY	3.4
1	A	6	CYS	3.1
1	B	6	CYS	3.1
1	B	38	ALA	2.7
1	B	11	THR	2.7
1	A	39	GLY	2.7
1	C	9	GLY	2.6
1	C	240	ASP	2.6
1	B	204	ALA	2.5
1	A	330	LYS	2.4
1	A	239	TRP	2.4
1	C	273	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	248	CYS	2.4
1	B	273	CYS	2.3
1	C	37	SER	2.2
1	C	35	LYS	2.2
1	C	39	GLY	2.1
1	B	326	THR	2.1
1	A	38	ALA	2.0
1	A	37	SER	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	401	5/5	0.96	0.11	40,41,42,43	0
2	SO4	C	402	5/5	0.97	0.07	36,38,39,41	0
2	SO4	C	401	5/5	0.99	0.04	20,20,22,22	0
2	SO4	A	901	5/5	0.99	0.03	22,22,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.