



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 01:40 PM EDT

PDB ID : 1ZI7
Title : Structure of truncated yeast oxysterol binding protein Osh4
Authors : Im, Y.J.; Raychaudhuri, S.; Prinz, W.A.; Hurley, J.H.
Deposited on : 2005-04-27
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

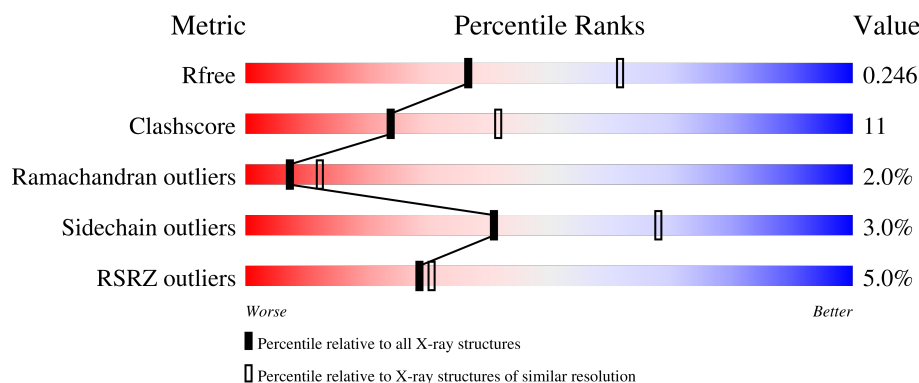
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	406	<div> <div>4%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
1	B	406	<div> <div>4%</div> <div>69%</div> <div>25%</div> <div>..</div> </div>
1	C	406	<div> <div>6%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9873 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 KES1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3256	2088	537	625	6			
1	B	398	Total	C	N	O	S	0	0	0
			3223	2063	533	621	6			
1	C	398	Total	C	N	O	S	0	0	0
			3223	2063	533	621	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	cloning artifact	UNP P35844
A	27	ALA	-	cloning artifact	UNP P35844
A	28	MET	-	cloning artifact	UNP P35844
A	29	ASP	-	cloning artifact	UNP P35844
A	?	-	ARG	deletion	UNP P35844
A	?	-	GLY	deletion	UNP P35844
A	?	-	TYR	deletion	UNP P35844
A	239	VAL	PHE	engineered mutation	UNP P35844
A	240	ASP	SER	engineered mutation	UNP P35844
B	26	GLY	-	cloning artifact	UNP P35844
B	27	ALA	-	cloning artifact	UNP P35844
B	28	MET	-	cloning artifact	UNP P35844
B	29	ASP	-	cloning artifact	UNP P35844
B	?	-	ARG	deletion	UNP P35844
B	?	-	GLY	deletion	UNP P35844
B	?	-	TYR	deletion	UNP P35844
B	239	VAL	PHE	engineered mutation	UNP P35844
B	240	ASP	SER	engineered mutation	UNP P35844
C	26	GLY	-	cloning artifact	UNP P35844
C	27	ALA	-	cloning artifact	UNP P35844
C	28	MET	-	cloning artifact	UNP P35844
C	29	ASP	-	cloning artifact	UNP P35844
C	?	-	ARG	deletion	UNP P35844

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P35844
C	?	-	TYR	deletion	UNP P35844
C	239	VAL	PHE	engineered mutation	UNP P35844
C	240	ASP	SER	engineered mutation	UNP P35844

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	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	46	Total	O	0	0
			46	46		

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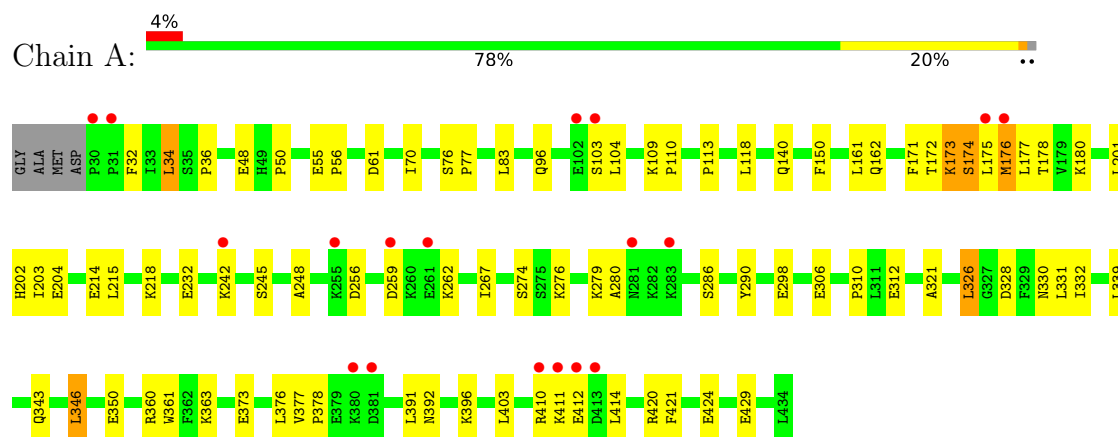
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	47	Total	O	0	0
			47	47		
3	C	48	Total	O	0	0
			48	48		

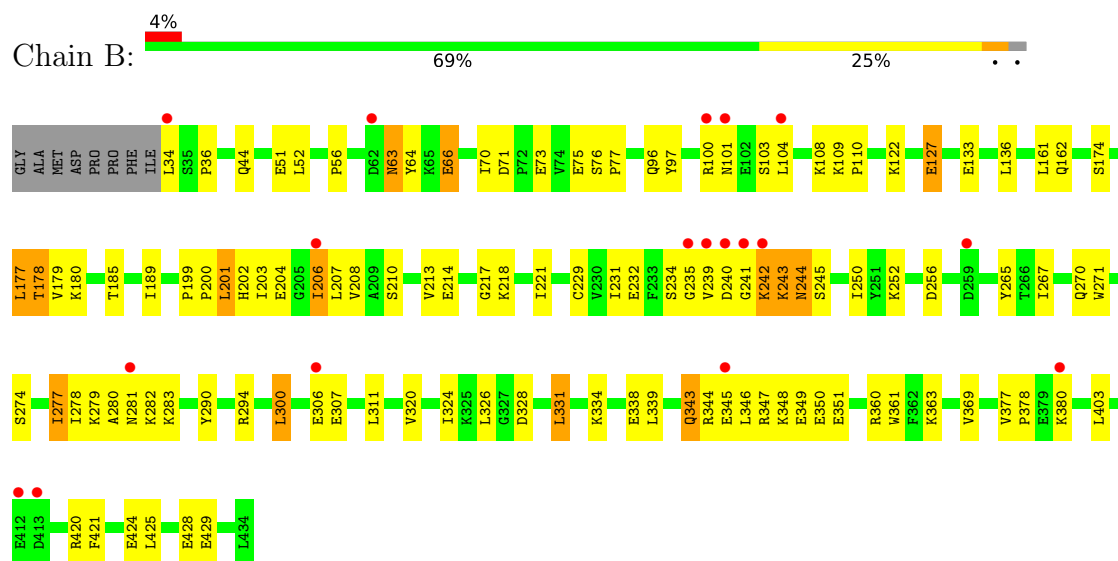
3 Residue-property plots

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

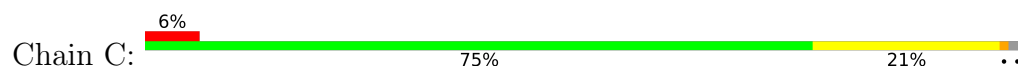
• Molecule 1: KES1 protein

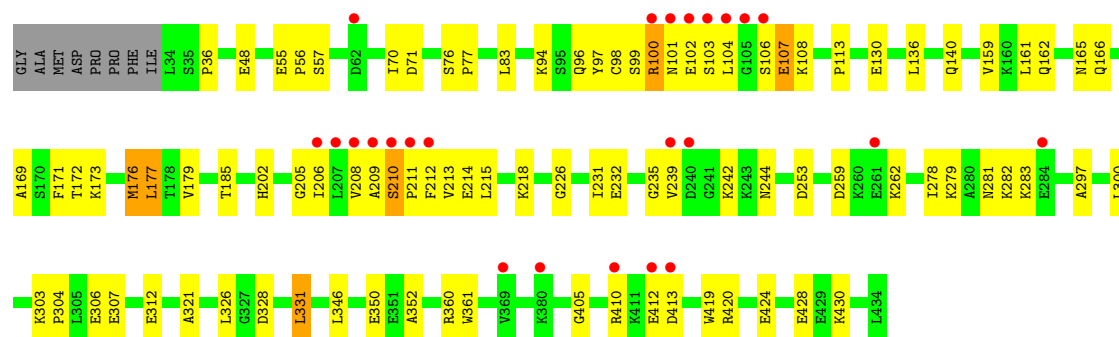


• Molecule 1: KES1 protein



• Molecule 1: KES1 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.90Å 100.85Å 117.62Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	45.11 – 2.50 45.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.11-2.50) 99.2 (45.11-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.246 0.210 , 0.246	Depositor DCC
R_{free} test set	3818 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9873	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.36	0/3337	0.58	0/4507
1	B	0.38	0/3301	0.59	0/4457
1	C	0.38	0/3301	0.60	0/4457
All	All	0.37	0/9939	0.59	0/13421

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

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	3256	0	3222	67	0
1	B	3223	0	3187	95	0
1	C	3223	0	3187	59	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
3	A	46	0	0	0	0
3	B	47	0	0	1	0
3	C	48	0	0	0	0
All	All	9873	0	9596	214	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 11.

All (214) 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:174:SER:HB3	1:A:176:MET:HG2	1.52	0.91
1:B:347:ARG:O	1:B:351:GLU:HG3	1.74	0.86
1:B:344:ARG:O	1:B:348:LYS:HD3	1.77	0.84
1:A:177:LEU:HD12	1:A:204:GLU:HB2	1.60	0.84
1:B:214:GLU:HG3	1:B:235:GLY:HA2	1.58	0.83
1:B:103:SER:HB2	1:B:213:VAL:HG23	1.61	0.81
1:A:175:LEU:HD12	1:B:180:LYS:HD2	1.63	0.80
1:B:127:GLU:CD	1:B:127:GLU:H	1.87	0.78
1:B:214:GLU:HG2	1:B:239:VAL:H	1.49	0.78
1:A:175:LEU:HD21	1:B:178:THR:HG21	1.66	0.75
1:A:70:ILE:HD11	1:A:83:LEU:HD13	1.70	0.74
1:B:204:GLU:HG2	1:B:213:VAL:HG22	1.69	0.73
1:A:242:LYS:HB2	1:A:245:SER:HB3	1.70	0.73
1:C:424:GLU:H	1:C:424:GLU:CD	1.93	0.71
1:A:218:LYS:HG2	1:A:232:GLU:HG2	1.73	0.70
1:B:162:GLN:NE2	1:B:421:PHE:H	1.88	0.70
1:B:214:GLU:CG	1:B:235:GLY:HA2	2.21	0.70
1:C:177:LEU:HB2	1:C:206:ILE:HD11	1.75	0.69
1:A:173:LYS:O	1:A:174:SER:HB2	1.95	0.67
1:A:175:LEU:O	1:A:175:LEU:HD23	1.95	0.66
1:A:172:THR:HG22	1:A:173:LYS:N	2.10	0.66
1:C:101:ASN:C	1:C:103:SER:H	1.97	0.66
1:C:169:ALA:HB1	1:C:177:LEU:HD21	1.76	0.66
1:A:377:VAL:HG13	1:A:378:PRO:HD2	1.78	0.64
1:A:76:SER:HB2	1:A:77:PRO:HD2	1.80	0.63
1:A:172:THR:HG22	1:A:173:LYS:H	1.63	0.63
1:C:76:SER:HB2	1:C:77:PRO:HD2	1.80	0.63
1:B:369:VAL:HG22	3:B:1308:HOH:O	1.99	0.63
1:A:162:GLN:NE2	1:A:421:PHE:H	1.98	0.62
1:B:307:GLU:HG2	1:C:352:ALA:HB1	1.81	0.61
1:C:171:PHE:HE2	1:C:206:ILE:HD13	1.65	0.61
1:B:267:ILE:HG12	1:B:277:ILE:HG12	1.82	0.61
1:A:178:THR:CG2	1:A:201:LEU:HD22	2.30	0.61
1:B:161:LEU:HD11	1:B:185:THR:CG2	2.30	0.60
1:C:218:LYS:HG2	1:C:232:GLU:HG2	1.83	0.60
1:A:203:ILE:N	1:A:203:ILE:HD12	2.17	0.60
1:C:278:ILE:HD13	1:C:283:LYS:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ASN:HB3	1:B:271:TRP:CE2	2.38	0.59
1:B:97:TYR:OH	1:B:199:PRO:HG2	2.04	0.58
1:A:48:GLU:O	1:A:50:PRO:HD3	2.05	0.57
1:B:177:LEU:HD22	1:B:179:VAL:HG23	1.87	0.57
1:C:231:ILE:N	1:C:231:ILE:HD12	2.20	0.57
1:A:202:HIS:HB3	1:A:215:LEU:HD23	1.86	0.57
1:B:311:LEU:HD23	1:B:343:GLN:NE2	2.20	0.57
1:C:172:THR:HG22	1:C:173:LYS:N	2.20	0.57
1:A:350:GLU:OE1	1:A:360:ARG:NH2	2.38	0.56
1:B:162:GLN:NE2	1:B:420:ARG:HA	2.19	0.56
1:B:424:GLU:O	1:B:428:GLU:HG2	2.06	0.56
1:A:360:ARG:HD3	1:A:429:GLU:OE1	2.05	0.56
1:C:100:ARG:N	1:C:108:LYS:HE3	2.20	0.56
1:C:350:GLU:OE1	1:C:360:ARG:NH2	2.39	0.55
1:C:100:ARG:HG3	1:C:108:LYS:HE3	1.89	0.55
1:C:419:TRP:O	1:C:420:ARG:HD3	2.06	0.55
1:A:172:THR:O	1:A:174:SER:N	2.40	0.55
1:B:311:LEU:HD23	1:B:343:GLN:HE22	1.72	0.55
1:C:136:LEU:HD23	1:C:300:LEU:HD13	1.89	0.54
1:C:70:ILE:HD11	1:C:83:LEU:HD13	1.88	0.54
1:B:127:GLU:CD	1:B:127:GLU:N	2.60	0.54
1:B:162:GLN:HE22	1:B:421:PHE:H	1.54	0.54
1:B:234:SER:HB2	1:B:240:ASP:HB3	1.90	0.54
1:B:243:LYS:O	1:B:245:SER:N	2.41	0.54
1:B:100:ARG:O	1:B:101:ASN:HB2	2.07	0.54
1:B:208:VAL:HG12	1:B:210:SER:H	1.73	0.54
1:C:100:ARG:H	1:C:108:LYS:HE3	1.73	0.53
1:C:306:GLU:CD	1:C:306:GLU:H	2.12	0.53
1:B:360:ARG:HG2	1:B:361:TRP:CD1	2.42	0.53
1:C:239:VAL:HG12	1:C:239:VAL:O	2.09	0.53
1:B:203:ILE:N	1:B:203:ILE:HD12	2.24	0.53
1:A:36:PRO:HG2	1:A:321:ALA:HB1	1.91	0.53
1:C:205:GLY:O	1:C:206:ILE:HB	2.09	0.53
1:B:320:VAL:O	1:B:324:ILE:HG12	2.08	0.53
1:C:281:ASN:O	1:C:283:LYS:N	2.42	0.52
1:B:56:PRO:HB2	1:B:189:ILE:HD12	1.91	0.52
1:B:265:TYR:HD2	1:B:277:ILE:HD11	1.74	0.52
1:C:97:TYR:HB3	1:C:213:VAL:HG11	1.91	0.52
1:B:265:TYR:CD2	1:B:277:ILE:HD11	2.44	0.52
1:B:277:ILE:HD13	1:B:278:ILE:N	2.24	0.52
1:B:350:GLU:OE1	1:B:360:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLY:O	1:C:253:ASP:HA	2.10	0.52
1:B:348:LYS:HD2	1:B:348:LYS:N	2.23	0.52
1:C:161:LEU:HD11	1:C:185:THR:CG2	2.40	0.52
1:B:377:VAL:HG13	1:B:378:PRO:HD2	1.91	0.52
1:B:363:LYS:HE2	1:B:425:LEU:HD11	1.92	0.51
1:A:161:LEU:HD23	1:A:162:GLN:N	2.25	0.51
1:B:122:LYS:HD2	1:B:133:GLU:OE2	2.10	0.51
1:A:162:GLN:HE22	1:A:421:PHE:H	1.58	0.51
1:A:175:LEU:HB2	1:B:180:LYS:CE	2.41	0.51
1:B:281:ASN:O	1:B:283:LYS:N	2.42	0.51
1:B:63:ASN:O	1:B:66:GLU:HG2	2.11	0.50
1:B:70:ILE:HB	1:B:277:ILE:HG21	1.94	0.50
1:B:76:SER:HB2	1:B:77:PRO:HD2	1.94	0.50
1:B:201:LEU:HD23	1:B:202:HIS:N	2.26	0.50
1:B:250:ILE:N	1:B:250:ILE:HD12	2.26	0.50
1:A:360:ARG:HG2	1:A:361:TRP:CD1	2.47	0.50
1:B:265:TYR:HB3	1:B:277:ILE:HD11	1.93	0.50
1:C:101:ASN:C	1:C:103:SER:N	2.65	0.50
1:B:177:LEU:HB2	1:B:206:ILE:HD11	1.94	0.50
1:B:306:GLU:CD	1:B:306:GLU:H	2.15	0.49
1:A:173:LYS:O	1:A:174:SER:CB	2.60	0.49
1:C:304:PRO:HG2	1:C:307:GLU:HG2	1.93	0.49
1:B:200:PRO:HG2	1:B:217:GLY:HA3	1.94	0.49
1:B:34:LEU:HD13	1:B:109:LYS:HB2	1.93	0.49
1:A:175:LEU:HB2	1:B:180:LYS:HE3	1.94	0.49
1:B:44:GLN:HA	1:B:136:LEU:CD1	2.42	0.49
1:C:172:THR:HB	1:C:176:MET:HG3	1.94	0.49
1:C:424:GLU:O	1:C:428:GLU:HG3	2.13	0.49
1:B:279:LYS:O	1:B:280:ALA:C	2.52	0.48
1:C:162:GLN:NE2	1:C:420:ARG:HA	2.28	0.48
1:B:234:SER:OG	1:B:245:SER:HB2	2.13	0.48
1:B:334:LYS:O	1:B:338:GLU:HG3	2.14	0.48
1:C:405:GLY:O	1:C:410:ARG:HD3	2.13	0.48
1:A:162:GLN:HE22	1:A:420:ARG:HA	1.79	0.47
1:C:360:ARG:HG2	1:C:361:TRP:CD1	2.49	0.47
1:B:103:SER:CB	1:B:213:VAL:HG23	2.40	0.47
1:B:136:LEU:HD13	1:B:300:LEU:HD13	1.97	0.47
1:B:162:GLN:HE22	1:B:420:ARG:HA	1.79	0.47
1:B:345:GLU:O	1:B:349:GLU:HG3	2.14	0.47
1:B:339:LEU:O	1:B:343:GLN:HB2	2.15	0.47
1:A:162:GLN:NE2	1:A:420:ARG:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LYS:HG2	1:B:232:GLU:HG2	1.95	0.47
1:B:243:LYS:HD2	1:B:243:LYS:N	2.29	0.47
1:A:150:PHE:HE2	1:A:161:LEU:HD21	1.78	0.47
1:C:36:PRO:HG2	1:C:321:ALA:HB1	1.97	0.47
1:C:103:SER:O	1:C:104:LEU:HB2	2.14	0.47
1:A:61:ASP:OD1	1:A:77:PRO:HG3	2.15	0.47
1:A:70:ILE:HD12	1:A:70:ILE:C	2.35	0.47
1:A:328:ASP:O	1:A:332:ILE:HG13	2.15	0.47
1:B:424:GLU:CD	1:B:424:GLU:H	2.19	0.46
1:C:55:GLU:HB3	1:C:56:PRO:HD3	1.97	0.46
1:B:108:LYS:O	1:B:110:PRO:HD3	2.16	0.46
1:A:339:LEU:C	1:A:339:LEU:HD23	2.35	0.46
1:B:103:SER:HB2	1:B:213:VAL:CG2	2.39	0.46
1:B:339:LEU:HD23	1:B:339:LEU:C	2.36	0.46
1:A:103:SER:O	1:A:104:LEU:HD23	2.16	0.46
1:A:391:LEU:O	1:A:392:ASN:HB3	2.15	0.46
1:A:172:THR:CG2	1:A:173:LYS:N	2.78	0.46
1:C:209:ALA:O	1:C:210:SER:HB3	2.16	0.46
1:C:48:GLU:HB3	1:C:297:ALA:HB1	1.97	0.45
1:C:94:LYS:O	1:C:98:CYS:HB2	2.16	0.45
1:C:101:ASN:O	1:C:102:GLU:HB2	2.16	0.45
1:C:136:LEU:HD23	1:C:300:LEU:CD1	2.46	0.45
1:C:281:ASN:O	1:C:283:LYS:HG3	2.16	0.45
1:A:161:LEU:HD23	1:A:161:LEU:C	2.37	0.45
1:C:71:ASP:OD2	1:C:279:LYS:HD2	2.17	0.45
1:C:106:SER:C	1:C:107:GLU:HG2	2.37	0.45
1:A:424:GLU:CD	1:A:424:GLU:H	2.19	0.45
1:C:100:ARG:HG3	1:C:108:LYS:CE	2.46	0.45
1:B:177:LEU:HD23	1:B:178:THR:N	2.32	0.45
1:B:201:LEU:HD22	1:B:203:ILE:HD12	1.98	0.45
1:A:34:LEU:CD1	1:A:109:LYS:HB2	2.47	0.45
1:A:118:LEU:O	1:A:312:GLU:HA	2.17	0.45
1:B:44:GLN:HA	1:B:136:LEU:HD11	1.99	0.45
1:A:276:LYS:HD2	1:A:286:SER:HB3	1.98	0.45
1:A:34:LEU:HD11	1:A:109:LYS:HB2	1.99	0.45
1:A:172:THR:CG2	1:A:173:LYS:H	2.29	0.45
1:C:430:LYS:HA	1:C:430:LYS:HD3	1.66	0.45
1:A:55:GLU:HB3	1:A:56:PRO:HD3	1.99	0.44
1:A:175:LEU:O	1:A:176:MET:C	2.55	0.44
1:A:176:MET:O	1:A:177:LEU:HB3	2.18	0.44
1:A:326:LEU:HD12	1:A:326:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:GLU:OE2	1:C:244:ASN:HA	2.17	0.44
1:C:161:LEU:HD11	1:C:185:THR:HG21	1.99	0.44
1:A:174:SER:C	1:A:176:MET:N	2.68	0.43
1:B:36:PRO:HA	1:B:109:LYS:O	2.17	0.43
1:A:248:ALA:HB3	1:A:267:ILE:HB	2.00	0.43
1:A:306:GLU:H	1:A:306:GLU:CD	2.20	0.43
1:B:239:VAL:HG12	1:B:239:VAL:O	2.18	0.43
1:B:331:LEU:HD23	1:B:331:LEU:HA	1.83	0.43
1:B:201:LEU:HD22	1:B:203:ILE:CD1	2.49	0.43
1:B:208:VAL:HG12	1:B:210:SER:N	2.34	0.43
1:B:241:GLY:O	1:B:242:LYS:C	2.57	0.43
1:B:348:LYS:N	1:B:348:LYS:CD	2.81	0.43
1:A:202:HIS:HA	1:A:214:GLU:O	2.18	0.43
1:A:259:ASP:HB3	1:A:262:LYS:HE2	2.01	0.43
1:A:396:LYS:HD3	1:A:414:LEU:HB3	2.00	0.43
1:B:360:ARG:HD3	1:B:429:GLU:OE1	2.19	0.43
1:C:113:PRO:HB2	1:C:140:GLN:HG2	2.01	0.42
1:A:113:PRO:HB2	1:A:140:GLN:CD	2.39	0.42
1:B:136:LEU:C	1:B:136:LEU:HD23	2.40	0.42
1:A:50:PRO:HG2	1:A:298:GLU:HB2	2.00	0.42
1:C:259:ASP:HB3	1:C:262:LYS:HE2	2.00	0.42
1:A:171:PHE:CZ	1:A:177:LEU:HD23	2.55	0.42
1:C:57:SER:HB3	1:C:159:VAL:CG2	2.50	0.42
1:B:328:ASP:HB3	1:B:331:LEU:HB2	2.02	0.41
1:B:363:LYS:HE2	1:B:425:LEU:CD1	2.50	0.41
1:B:51:GLU:HG2	1:B:52:LEU:N	2.35	0.41
1:C:103:SER:O	1:C:104:LEU:CB	2.69	0.41
1:C:202:HIS:HB2	1:C:215:LEU:HD23	2.03	0.41
1:A:180:LYS:HA	1:A:201:LEU:HD23	2.01	0.41
1:B:208:VAL:HG13	2:B:1102:SO4:S	2.61	0.41
1:B:221:ILE:HB	1:B:229:CYS:HB3	2.02	0.41
1:A:310:PRO:HG2	1:A:346:LEU:HD21	2.03	0.41
1:A:363:LYS:HB3	1:A:376:LEU:CD1	2.51	0.41
1:A:410:ARG:O	1:A:411:LYS:C	2.59	0.41
1:B:206:ILE:HG22	1:B:207:LEU:HG	2.03	0.41
1:A:274:SER:HA	1:A:290:TYR:O	2.19	0.41
1:A:279:LYS:O	1:A:280:ALA:C	2.58	0.41
1:B:64:TYR:CD2	1:B:77:PRO:HB3	2.56	0.41
1:B:71:ASP:C	1:B:73:GLU:H	2.23	0.41
1:B:218:LYS:HA	1:B:231:ILE:O	2.21	0.41
1:C:165:ASN:HD22	1:C:166:GLN:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LYS:HE2	1:C:312:GLU:OE2	2.21	0.41
1:A:175:LEU:HB2	1:B:180:LYS:HD2	2.03	0.41
1:A:110:PRO:HD2	1:B:174:SER:HA	2.04	0.40
1:C:172:THR:CG2	1:C:173:LYS:N	2.84	0.40
1:C:210:SER:O	1:C:212:PHE:N	2.54	0.40
1:C:328:ASP:CG	1:C:331:LEU:HB2	2.42	0.40
1:A:328:ASP:OD1	1:A:330:ASN:HB2	2.21	0.40
1:B:104:LEU:HD23	1:B:104:LEU:O	2.21	0.40
1:C:179:VAL:HB	1:C:202:HIS:CD2	2.56	0.40
1:B:71:ASP:OD2	1:B:279:LYS:HD2	2.21	0.40
1:B:274:SER:HA	1:B:290:TYR:O	2.21	0.40
1:B:343:GLN:O	1:B:347:ARG:HG3	2.22	0.40
1:C:130:GLU:OE1	1:C:130:GLU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	400/406 (98%)	367 (92%)	27 (7%)	6 (2%)	10	18
1	B	396/406 (98%)	371 (94%)	17 (4%)	8 (2%)	7	12
1	C	396/406 (98%)	363 (92%)	23 (6%)	10 (2%)	5	8
All	All	1192/1218 (98%)	1101 (92%)	67 (6%)	24 (2%)	7	12

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	A	176	MET
1	A	412	GLU
1	B	243	LYS

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Mol	Chain	Res	Type
1	B	244	ASN
1	B	282	LYS
1	C	99	SER
1	C	210	SER
1	A	173	LYS
1	A	373	GLU
1	B	75	GLU
1	C	100	ARG
1	C	211	PRO
1	C	235	GLY
1	C	282	LYS
1	A	32	PHE
1	B	63	ASN
1	B	206	ILE
1	C	208	VAL
1	C	242	LYS
1	C	412	GLU
1	B	242	LYS
1	B	294	ARG
1	C	107	GLU

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	362/364 (100%)	354 (98%)	8 (2%)	52	77
1	B	358/364 (98%)	341 (95%)	17 (5%)	26	49
1	C	358/364 (98%)	351 (98%)	7 (2%)	55	79
All	All	1078/1092 (99%)	1046 (97%)	32 (3%)	41	68

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	96	GLN

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	326	LEU
1	A	331	LEU
1	A	343	GLN
1	A	346	LEU
1	A	403	LEU
1	B	66	GLU
1	B	96	GLN
1	B	127	GLU
1	B	177	LEU
1	B	178	THR
1	B	201	LEU
1	B	252	LYS
1	B	256	ASP
1	B	270	GLN
1	B	277	ILE
1	B	300	LEU
1	B	326	LEU
1	B	331	LEU
1	B	343	GLN
1	B	346	LEU
1	B	380	LYS
1	B	403	LEU
1	C	96	GLN
1	C	176	MET
1	C	177	LEU
1	C	326	LEU
1	C	331	LEU
1	C	346	LEU
1	C	413	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	96	GLN
1	A	144	HIS
1	A	157	ASN
1	A	162	GLN
1	A	166	GLN
1	A	181	GLN
1	A	343	GLN

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Mol	Chain	Res	Type
1	B	96	GLN
1	B	162	GLN
1	B	166	GLN
1	B	343	GLN
1	B	358	GLN
1	C	44	GLN
1	C	67	HIS
1	C	96	GLN
1	C	101	ASN
1	C	157	ASN
1	C	162	GLN
1	C	165	ASN
1	C	166	GLN
1	C	181	GLN
1	C	343	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	1201	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	A	1101	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	B	1102	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	C	1202	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	A	1103	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	1301	-	4,4,4	0.26	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1102	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

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	402/406 (99%)	0.24	18 (4%) 33 36	29, 47, 77, 97	0
1	B	398/406 (98%)	0.18	18 (4%) 33 36	25, 44, 81, 98	0
1	C	398/406 (98%)	0.28	24 (6%) 21 22	26, 42, 81, 115	0
All	All	1198/1218 (98%)	0.24	60 (5%) 28 30	25, 45, 79, 115	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	VAL	9.8
1	C	210	SER	7.6
1	C	209	ALA	6.7
1	C	207	LEU	6.5
1	C	101	ASN	6.4
1	C	104	LEU	5.6
1	B	34	LEU	5.2
1	C	211	PRO	5.0
1	C	100	ARG	4.5
1	C	206	ILE	4.4
1	C	106	SER	4.1
1	B	412	GLU	4.0
1	A	410	ARG	3.9
1	C	103	SER	3.8
1	A	103	SER	3.8
1	A	30	PRO	3.7
1	A	281	ASN	3.7
1	A	31	PRO	3.6
1	B	235	GLY	3.6
1	C	102	GLU	3.5
1	B	239	VAL	3.5
1	A	412	GLU	3.4
1	A	176	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	175	LEU	3.4
1	B	101	ASN	3.3
1	A	411	LYS	3.3
1	A	381	ASP	3.3
1	A	413	ASP	3.2
1	B	62	ASP	3.0
1	B	259	ASP	3.0
1	B	380	LYS	2.9
1	B	240	ASP	2.9
1	C	62	ASP	2.9
1	A	380	LYS	2.8
1	B	241	GLY	2.8
1	B	100	ARG	2.7
1	C	410	ARG	2.7
1	C	412	GLU	2.6
1	C	380	LYS	2.6
1	C	212	PHE	2.6
1	B	242	LYS	2.6
1	A	242	LYS	2.4
1	A	259	ASP	2.4
1	C	261	GLU	2.3
1	A	255	LYS	2.3
1	C	240	ASP	2.3
1	B	206	ILE	2.2
1	C	105	GLY	2.2
1	C	369	VAL	2.1
1	B	306	GLU	2.1
1	B	281	ASN	2.1
1	C	413	ASP	2.1
1	A	102	GLU	2.1
1	A	261	GLU	2.1
1	B	104	LEU	2.1
1	B	345	GLU	2.1
1	C	239	VAL	2.0
1	C	284	GLU	2.0
1	A	283	LYS	2.0
1	B	413	ASP	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 [i](#)

There are no monosaccharides 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
2	SO4	A	1101	5/5	0.81	0.22	134,134,135,135	0
2	SO4	C	1201	5/5	0.85	0.19	104,104,105,106	0
2	SO4	B	1102	5/5	0.91	0.12	115,115,116,116	0
2	SO4	B	1301	5/5	0.96	0.09	100,101,101,101	0
2	SO4	C	1202	5/5	0.96	0.13	103,104,104,104	0
2	SO4	A	1103	5/5	0.97	0.13	89,90,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.