



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:31 AM UTC

PDB ID : 6YSV / pdb_00006ysv
Title : E. coli anaerobic trifunctional enzyme subunit-alpha
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Deposited on : 2020-04-23
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

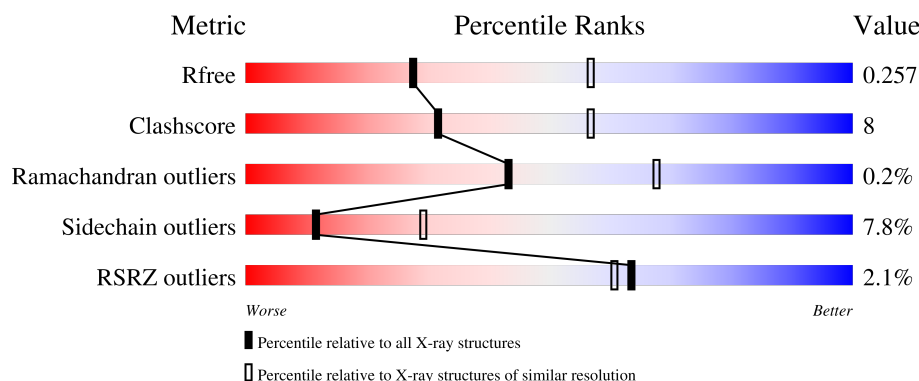
1 Overall quality at a glance

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	728	78% 19% .
1	B	728	3% 70% 23% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10549 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 Fatty acid oxidation complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	1	0
			5303	3353	947	980	23			
1	B	699	Total	C	N	O	S	0	0	0
			5167	3273	912	959	23			

There are 28 discrepancies between the modelled and reference sequences:

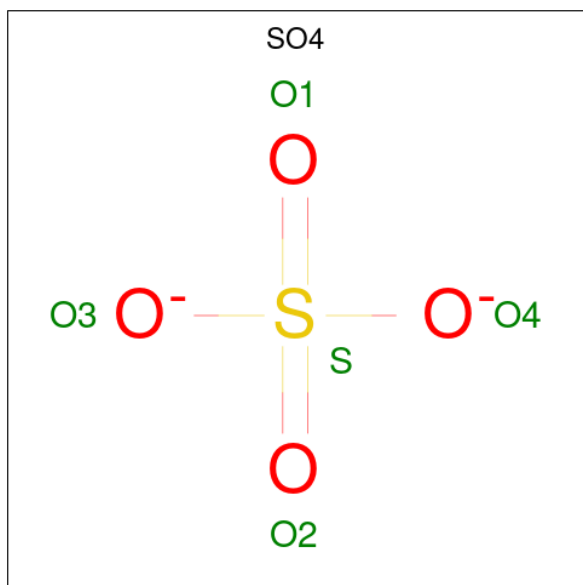
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P77399
A	-12	GLY	-	expression tag	UNP P77399
A	-11	SER	-	expression tag	UNP P77399
A	-10	SER	-	expression tag	UNP P77399
A	-9	HIS	-	expression tag	UNP P77399
A	-8	HIS	-	expression tag	UNP P77399
A	-7	HIS	-	expression tag	UNP P77399
A	-6	HIS	-	expression tag	UNP P77399
A	-5	HIS	-	expression tag	UNP P77399
A	-4	HIS	-	expression tag	UNP P77399
A	-3	SER	-	expression tag	UNP P77399
A	-2	GLN	-	expression tag	UNP P77399
A	-1	ASP	-	expression tag	UNP P77399
A	0	PRO	-	expression tag	UNP P77399
B	-13	MET	-	initiating methionine	UNP P77399
B	-12	GLY	-	expression tag	UNP P77399
B	-11	SER	-	expression tag	UNP P77399
B	-10	SER	-	expression tag	UNP P77399
B	-9	HIS	-	expression tag	UNP P77399
B	-8	HIS	-	expression tag	UNP P77399
B	-7	HIS	-	expression tag	UNP P77399
B	-6	HIS	-	expression tag	UNP P77399
B	-5	HIS	-	expression tag	UNP P77399
B	-4	HIS	-	expression tag	UNP P77399
B	-3	SER	-	expression tag	UNP P77399

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP P77399
B	-1	ASP	-	expression tag	UNP P77399
B	0	PRO	-	expression tag	UNP P77399

- 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	A	1	Total	O	S	0	0
			5	4	1		
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		

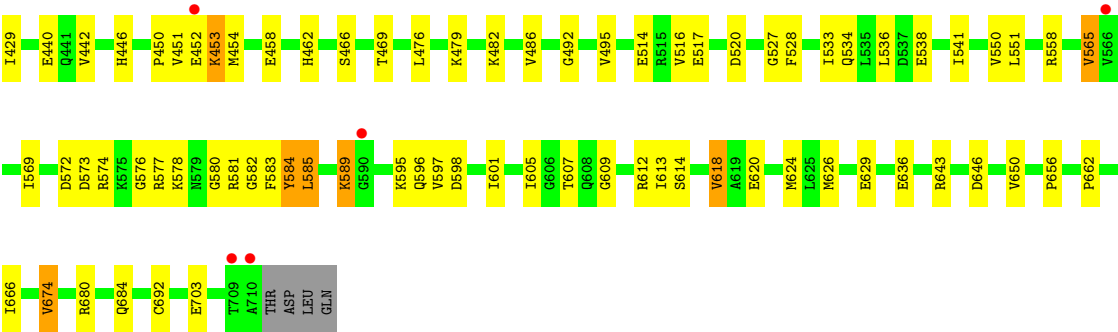
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	10	Total	O	0	0
			10	10		



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.58Å 90.75Å 172.91Å 90.00° 96.11° 90.00°	Depositor
Resolution (Å)	54.51 – 2.70 54.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (54.51-2.70) 97.6 (54.51-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.16 3549	Depositor
R, R_{free}	0.224 , 0.255 0.228 , 0.257	Depositor DCC
R_{free} test set	2800 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	85.7	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10549	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: 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	0.10	0/5397	0.27	0/7314
1	B	0.11	0/5252	0.31	0/7121
All	All	0.10	0/10649	0.29	0/14435

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	5303	0	5389	71	0
1	B	5167	0	5207	100	0
2	A	25	0	0	1	0
2	B	10	0	0	0	0
3	A	34	0	0	2	0
3	B	10	0	0	0	0
All	All	10549	0	10596	170	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 8.

All (170) 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:110:GLY:H	1:A:134:THR:HG22	1.43	0.83
1:B:584:TYR:HB3	1:B:597:VAL:HA	1.61	0.82
1:B:577:ARG:HA	1:B:585:LEU:HD11	1.62	0.81
1:A:558:ARG:NH1	1:A:629:GLU:OE2	2.15	0.80
1:B:175:ARG:HE	1:B:362:ARG:HH22	1.29	0.78
1:B:572:ASP:O	1:B:581:ARG:NH2	2.16	0.78
1:A:313:ILE:HG22	1:A:393:ILE:HB	1.68	0.76
1:B:23:VAL:O	1:B:61:LYS:NZ	2.22	0.72
1:A:537:ASP:OD1	1:A:541:ILE:HD11	1.91	0.71
1:B:117:LEU:HD23	1:B:138:LEU:HG	1.74	0.69
1:B:240:THR:HG23	1:B:242:GLY:H	1.57	0.69
1:A:450:PRO:HG2	1:A:453:LYS:HB2	1.74	0.69
1:A:17:ALA:HB3	1:A:55:VAL:HG12	1.73	0.69
1:B:451:VAL:O	1:B:482:LYS:NZ	2.27	0.68
1:B:386:PHE:HA	1:B:389:ARG:HG2	1.76	0.67
1:B:589:LYS:HE3	1:B:589:LYS:H	1.59	0.66
1:A:9:LEU:HD22	1:A:42:ILE:HG23	1.77	0.66
1:B:23:VAL:HG13	1:B:25:GLY:H	1.61	0.65
1:A:584:TYR:HA	1:A:597:VAL:HA	1.78	0.65
1:A:394:GLU:OE2	1:A:403:LYS:NZ	2.19	0.63
1:B:29:ASN:N	1:B:29:ASN:OD1	2.30	0.63
1:A:527:GLY:HA3	1:A:656:PRO:HB3	1.80	0.63
1:A:308:LEU:HD21	1:A:476:LEU:HB2	1.80	0.62
1:B:516:VAL:HG12	1:B:533:ILE:HD13	1.82	0.62
1:B:527:GLY:HA3	1:B:656:PRO:HB3	1.79	0.62
1:B:450:PRO:HG2	1:B:453:LYS:HB2	1.80	0.62
1:B:17:ALA:HB3	1:B:55:VAL:HG12	1.81	0.62
1:B:7:PHE:HD2	1:B:19:ILE:HD11	1.64	0.61
1:A:572:ASP:OD2	1:A:581:ARG:NH1	2.34	0.60
1:B:308:LEU:HD21	1:B:476:LEU:HB2	1.83	0.60
1:B:220:ALA:HB3	1:B:224:GLY:H	1.66	0.60
1:A:450:PRO:HD2	1:A:454:MET:HE2	1.84	0.60
1:B:528:PHE:HZ	1:B:626:MET:HE1	1.65	0.59
1:A:129:THR:HB	1:A:134:THR:HG21	1.84	0.59
1:A:451:VAL:O	1:A:482:LYS:NZ	2.29	0.59
1:B:558:ARG:NH1	1:B:629:GLU:OE2	2.36	0.59
1:A:414:CYS:HB3	1:A:418:THR:HG21	1.85	0.59
1:B:127:VAL:HG12	1:B:187:ASP:HB3	1.86	0.58
1:B:601:ILE:O	1:B:605:ILE:HG13	2.04	0.57
1:A:9:LEU:HD11	1:A:17:ALA:HB1	1.86	0.57
1:B:168:ILE:HG22	1:B:250:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:MET:HB3	1:B:67:ALA:HB2	1.87	0.56
1:A:440:GLU:HB2	1:A:466:SER:HB3	1.87	0.56
1:B:175:ARG:NE	1:B:362:ARG:HH22	2.01	0.56
1:A:219:LEU:HD13	1:A:228:LEU:HB2	1.88	0.56
1:B:165:LEU:HD21	1:B:254:VAL:HG21	1.86	0.56
1:A:214:VAL:HG12	1:A:217:ARG:HH22	1.69	0.56
1:A:537:ASP:OD2	1:A:586:TYR:OH	2.21	0.55
1:A:360:VAL:HA	1:A:365:LEU:HA	1.87	0.55
1:B:193:ILE:O	1:B:197:ALA:N	2.39	0.55
1:A:84:GLU:OE2	1:A:271:ARG:NE	2.39	0.54
1:A:673:GLU:OE1	1:A:673:GLU:N	2.40	0.54
1:A:537:ASP:OD1	1:A:583:PHE:HD1	1.91	0.54
1:A:79:THR:HG22	1:A:82:GLU:HG3	1.91	0.53
1:A:679:GLN:HG3	1:A:691:PRO:HG2	1.90	0.53
1:B:336:ARG:HG3	1:B:389:ARG:HH12	1.74	0.53
1:B:419:ILE:HG12	1:B:469:THR:HG23	1.91	0.53
1:B:10:ASN:O	1:B:18:VAL:N	2.41	0.53
1:B:123:CYS:O	1:B:126:ARG:NH1	2.40	0.53
1:A:446:HIS:HB3	1:A:458:GLU:HB2	1.91	0.53
1:A:680[A]:ARG:NH2	3:A:902:HOH:O	2.41	0.52
1:B:282:SER:OG	1:B:286:ARG:NH1	2.43	0.52
1:A:327:THR:HB	1:A:480:GLN:HE21	1.74	0.52
1:B:100:LEU:HD13	1:B:124:HIS:CE1	2.45	0.52
1:A:310:SER:HB2	1:A:389:ARG:HH11	1.75	0.52
1:B:414:CYS:HB3	1:B:418:THR:HG21	1.92	0.52
1:B:569:ILE:HG12	1:B:574:ARG:HB2	1.92	0.52
1:A:91:GLN:NE2	1:A:269:GLU:OE1	2.40	0.51
1:B:311:VAL:HG21	1:B:327:THR:HG21	1.91	0.51
1:B:107:ALA:HA	1:B:127:VAL:HG23	1.94	0.50
1:B:225:ARG:HH22	1:B:259:ALA:HB2	1.76	0.50
1:A:396:VAL:HG22	1:A:397:PHE:H	1.77	0.50
1:A:319:MET:HE2	1:A:423:ASN:HD21	1.76	0.49
1:A:505:GLU:HB2	1:A:625:LEU:HD12	1.94	0.49
1:B:336:ARG:HH11	1:B:385:GLY:H	1.60	0.49
1:B:88:ARG:HA	1:B:91:GLN:HG2	1.94	0.49
1:B:440:GLU:HB3	1:B:466:SER:HB3	1.93	0.49
1:A:624:MET:HE3	1:A:677:ILE:HG21	1.94	0.49
1:A:656:PRO:HG2	1:A:659:LEU:HD12	1.94	0.49
1:B:21:ILE:HG22	1:B:29:ASN:HD22	1.78	0.48
1:B:175:ARG:HD2	1:B:362:ARG:HH12	1.78	0.48
1:A:46:LEU:HD13	1:A:55:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:VAL:O	1:A:203:LYS:HG2	2.14	0.48
1:B:78:LYS:N	1:B:82:GLU:OE1	2.46	0.48
1:B:516:VAL:HG21	1:B:597:VAL:HG11	1.96	0.48
1:A:351:TYR:OH	1:A:452:GLU:OE2	2.28	0.47
1:B:335:VAL:HG22	1:B:377:ILE:HG12	1.96	0.47
1:B:446:HIS:HB3	1:B:458:GLU:HB2	1.97	0.47
1:A:59:SER:HB2	1:A:65:PHE:HA	1.96	0.47
1:B:169:LEU:HD23	1:B:236:THR:HG21	1.97	0.47
1:B:318:LEU:HD11	1:B:347:HIS:ND1	2.30	0.47
1:A:542:ASP:N	1:A:542:ASP:OD1	2.47	0.46
1:B:79:THR:HG23	1:B:82:GLU:H	1.80	0.46
1:B:229:PHE:HE2	1:B:254:VAL:HG23	1.79	0.46
1:B:237:GLU:HA	1:B:240:THR:HG22	1.97	0.46
1:A:319:MET:O	1:A:323:ILE:HG12	2.14	0.46
1:A:313:ILE:HD11	1:A:337:ILE:HG12	1.96	0.46
1:B:565:VAL:HG23	1:B:605:ILE:HG22	1.98	0.46
1:B:46:LEU:HD13	1:B:52:LEU:HD23	1.98	0.45
1:A:504:ASN:ND2	1:A:559:PHE:O	2.50	0.45
1:A:520:ASP:OD2	1:A:584:TYR:OH	2.26	0.45
1:B:73:MET:HB3	1:B:86:LEU:HD21	1.98	0.45
1:B:538:GLU:OE1	1:B:577:ARG:NH1	2.50	0.45
1:B:163:THR:HG21	1:B:182:LEU:HD13	1.98	0.45
1:A:37:SER:HB3	1:B:703:GLU:HG2	1.98	0.45
1:B:164:ALA:O	1:B:168:ILE:HG12	2.16	0.45
1:B:294:ASP:OD2	1:B:643:ARG:NH1	2.40	0.45
1:A:357:GLU:HG2	1:A:370:ARG:HH11	1.81	0.45
1:B:520:ASP:OD2	1:B:584:TYR:OH	2.34	0.45
1:B:609:GLY:HA3	1:B:612:ARG:HH12	1.81	0.45
1:B:614:SER:O	1:B:618:VAL:HG12	2.17	0.45
1:A:323:ILE:HD13	1:A:451:VAL:HG11	1.99	0.44
1:B:279:THR:HG23	1:B:282:SER:H	1.82	0.44
1:B:356:LEU:H	1:B:356:LEU:HG	1.62	0.44
1:B:339:ASP:HB3	1:B:345:ILE:HG13	1.99	0.44
1:A:678:MET:HB3	1:A:689:PHE:O	2.18	0.44
1:B:584:TYR:CD1	1:B:584:TYR:N	2.86	0.44
1:A:117:LEU:HD23	1:A:138:LEU:HG	2.00	0.44
1:A:419:ILE:HD12	1:A:469:THR:HG23	1.99	0.44
1:B:585:LEU:HD23	1:B:585:LEU:HA	1.77	0.44
1:B:233:GLY:O	1:B:237:GLU:HB2	2.17	0.44
1:A:391:LEU:HG	1:A:419:ILE:HB	1.99	0.43
1:A:64:ASN:HA	1:A:111:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:LYS:HE3	1:B:589:LYS:N	2.31	0.43
1:A:505:GLU:OE2	1:A:621:ARG:NH2	2.40	0.43
1:B:91:GLN:HB3	1:B:149:SER:HA	2.00	0.43
1:A:537:ASP:OD2	1:A:583:PHE:HB2	2.19	0.43
1:B:146:LEU:HD22	1:B:276:LEU:HD12	2.00	0.43
1:B:49:ASN:C	1:B:51:GLU:H	2.27	0.43
1:B:64:ASN:HA	1:B:111:ALA:H	1.84	0.43
1:B:426:SER:HB2	1:B:550:VAL:HG21	2.01	0.43
1:A:488:ARG:HH21	1:A:490:LYS:HD2	1.83	0.43
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.79	0.42
1:B:16:ILE:HG22	1:B:54:GLY:HA3	2.01	0.42
1:A:519:ILE:HA	1:A:618:VAL:HG11	2.00	0.42
1:A:121:LEU:HD11	1:A:155:LEU:HD13	2.01	0.42
1:A:385:GLY:N	2:A:804:SO4:O3	2.38	0.42
1:A:646:ASP:HA	1:A:662:PRO:HD2	2.01	0.42
1:B:534:GLN:HB2	1:B:584:TYR:OH	2.20	0.42
1:B:666:ILE:HG23	1:B:674:VAL:HG11	2.02	0.42
1:A:557:GLU:N	3:A:903:HOH:O	2.42	0.42
1:A:695:LEU:HD12	1:A:695:LEU:HA	1.91	0.42
1:B:12:ARG:HB2	1:B:16:ILE:HD12	2.01	0.42
1:B:23:VAL:HG13	1:B:25:GLY:N	2.32	0.42
1:B:580:GLY:HA2	1:B:585:LEU:HD12	2.01	0.42
1:B:605:ILE:HG13	1:B:605:ILE:H	1.73	0.42
1:B:50:LYS:HA	1:B:50:LYS:HD2	1.69	0.42
1:B:55:VAL:HG22	1:B:102:ILE:HG22	2.02	0.42
1:B:646:ASP:HA	1:B:662:PRO:HD2	2.02	0.42
1:A:693:GLU:H	1:A:693:GLU:CD	2.27	0.41
1:B:219:LEU:HD13	1:B:219:LEU:HA	1.81	0.41
1:B:620:GLU:OE2	1:B:680:ARG:NH2	2.53	0.41
1:A:54:GLY:HA3	1:A:202:ALA:HB1	2.02	0.41
1:B:450:PRO:O	1:B:454:MET:HG2	2.20	0.41
1:A:363:ARG:HB3	1:A:364:HIS:H	1.65	0.41
1:A:501:PRO:HB2	1:A:625:LEU:HB3	2.01	0.41
1:A:246:ALA:HA	1:A:276:LEU:HD21	2.03	0.41
1:B:514:GLU:OE2	1:B:613:ILE:HG22	2.20	0.41
1:A:523:LEU:HD21	1:A:622:CYS:HB2	2.03	0.41
1:B:155:LEU:HB3	1:B:156:PRO:HD3	2.02	0.41
1:B:429:ILE:HB	1:B:462:HIS:HB3	2.03	0.41
1:B:620:GLU:O	1:B:624:MET:HG2	2.21	0.41
1:A:600:ALA:C	1:A:603:PRO:HD2	2.46	0.41
1:B:288:ILE:HD13	1:B:650:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:VAL:HG12	1:B:420:PHE:CE1	2.56	0.41
1:B:8:THR:HG1	1:B:20:THR:HB	1.86	0.40
1:B:99:ALA:C	1:B:101:PRO:HD3	2.47	0.40
1:B:492:GLY:HA3	1:B:551:LEU:HD21	2.03	0.40
1:B:576:GLY:HA2	1:B:582:GLY:HA3	2.04	0.40
1:B:541:ILE:HD12	1:B:583:PHE:HE1	1.87	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	707/728 (97%)	677 (96%)	29 (4%)	1 (0%)	48 73
1	B	695/728 (96%)	660 (95%)	33 (5%)	2 (0%)	36 60
All	All	1402/1456 (96%)	1337 (95%)	62 (4%)	3 (0%)	43 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	PRO
1	A	363	ARG
1	B	573	ASP

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	548/583 (94%)	520 (95%)	28 (5%)	21	48
1	B	524/583 (90%)	468 (89%)	56 (11%)	6	16
All	All	1072/1166 (92%)	988 (92%)	84 (8%)	11	29

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	16	ILE
1	A	93	LEU
1	A	105	ILE
1	A	127	VAL
1	A	141	VAL
1	A	158	LEU
1	A	159	ILE
1	A	188	VAL
1	A	189	VAL
1	A	208	SER
1	A	212	LEU
1	A	262	THR
1	A	267	ASP
1	A	292	SER
1	A	366	LYS
1	A	369	GLU
1	A	510	LEU
1	A	565	VAL
1	A	585	LEU
1	A	588	GLN
1	A	589	LYS
1	A	591	ARG
1	A	593	SER
1	A	594	LYS
1	A	597	VAL
1	A	610	GLN
1	A	612	ARG
1	B	16	ILE
1	B	19	ILE
1	B	23	VAL
1	B	26	GLU
1	B	29	ASN
1	B	46	LEU
1	B	48	GLU

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Mol	Chain	Res	Type
1	B	64	ASN
1	B	97	ILE
1	B	127	VAL
1	B	161	VAL
1	B	169	LEU
1	B	185	VAL
1	B	189	VAL
1	B	218	ILE
1	B	219	LEU
1	B	227	LEU
1	B	228	LEU
1	B	308	LEU
1	B	311	VAL
1	B	318	LEU
1	B	326	VAL
1	B	335	VAL
1	B	336	ARG
1	B	350	LYS
1	B	356	LEU
1	B	359	LYS
1	B	369	GLU
1	B	373	GLN
1	B	388	HIS
1	B	389	ARG
1	B	396	VAL
1	B	407	VAL
1	B	418	THR
1	B	442	VAL
1	B	452	GLU
1	B	453	LYS
1	B	479	LYS
1	B	486	VAL
1	B	495	VAL
1	B	517	GLU
1	B	536	LEU
1	B	565	VAL
1	B	578	LYS
1	B	584	TYR
1	B	585	LEU
1	B	589	LYS
1	B	595	LYS
1	B	596	GLN

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Mol	Chain	Res	Type
1	B	598	ASP
1	B	607	THR
1	B	618	VAL
1	B	636	GLU
1	B	674	VAL
1	B	684	GLN
1	B	692	CYS

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	29	ASN
1	A	72	ASN
1	A	588	GLN
1	B	91	GLN
1	B	417	HIS
1	B	441	GLN
1	B	446	HIS

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 ⓘ

7 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	B	802	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	805	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	804	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	801	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.08	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	A	804	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	708/728 (97%)	0.13	5 (0%) 84 83	44, 90, 158, 218	1 (0%)
1	B	699/728 (96%)	0.29	24 (3%) 48 44	64, 110, 177, 220	0
All	All	1407/1456 (96%)	0.21	29 (2%) 63 61	44, 100, 171, 220	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	THR	3.6
1	B	318	LEU	3.4
1	B	709	THR	3.2
1	B	218	ILE	3.1
1	B	217	ARG	3.0
1	B	219	LEU	3.0
1	B	100	LEU	2.9
1	B	410	VAL	2.8
1	A	13	LEU	2.8
1	B	452	GLU	2.8
1	B	31	LEU	2.6
1	B	710	ALA	2.6
1	A	566	VAL	2.5
1	A	252	GLU	2.4
1	B	215	ARG	2.4
1	B	69	ALA	2.4
1	B	375	ALA	2.4
1	B	195	LEU	2.3
1	B	71	ILE	2.3
1	B	99	ALA	2.2
1	B	220	ALA	2.2
1	A	673	GLU	2.2
1	B	566	VAL	2.2
1	B	247	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	590	GLY	2.2
1	B	101	PRO	2.1
1	B	175	ARG	2.0
1	B	205	GLU	2.0
1	B	104	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	802	5/5	0.64	0.08	178,179,179,180	0
2	SO4	A	805	5/5	0.75	0.16	216,218,219,219	5
2	SO4	B	802	5/5	0.82	0.11	164,164,165,165	0
2	SO4	A	803	5/5	0.86	0.16	149,150,151,152	0
2	SO4	B	801	5/5	0.91	0.15	164,166,166,167	0
2	SO4	A	801	5/5	0.92	0.21	147,147,149,151	0
2	SO4	A	804	5/5	0.93	0.16	124,128,128,128	5

6.5 Other polymers [i](#)

There are no such residues in this entry.