Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2021 – 03:06 pm BST

PDB ID	:	6YSV
Title	:	E. coli anaerobic trifunctional enzyme subunit-alpha
Authors	:	Sah-Teli, S.K.; Hynonen, M.J.; Wierenga, R.K.; Venkatesan, R.
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 following versions of software and data (see references ⓘ) were used in the production of this report:

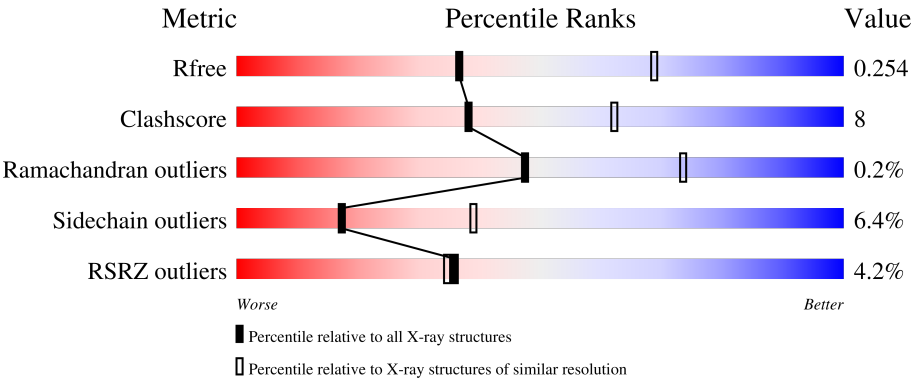
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	3% 80% 17%
1	B	728	5% 71% 22%

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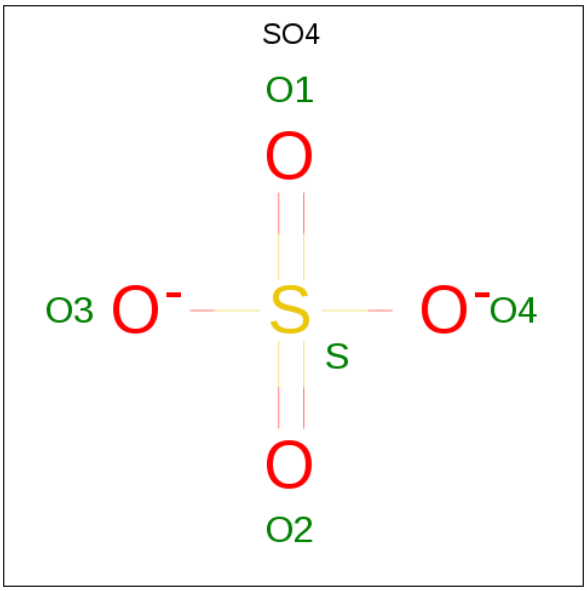
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP P77399
B	-1	ASP	-	expression tag	UNP P77399
B	0	PRO	-	expression tag	UNP P77399

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

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

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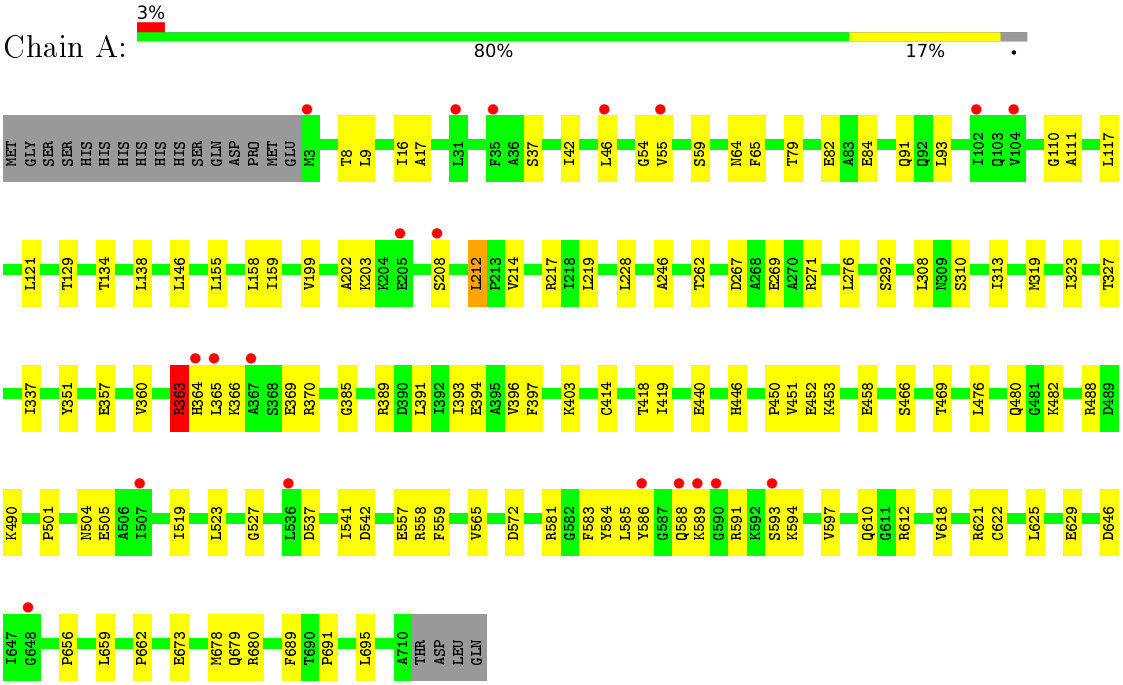
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	10	Total	O	0	0
			10	10		

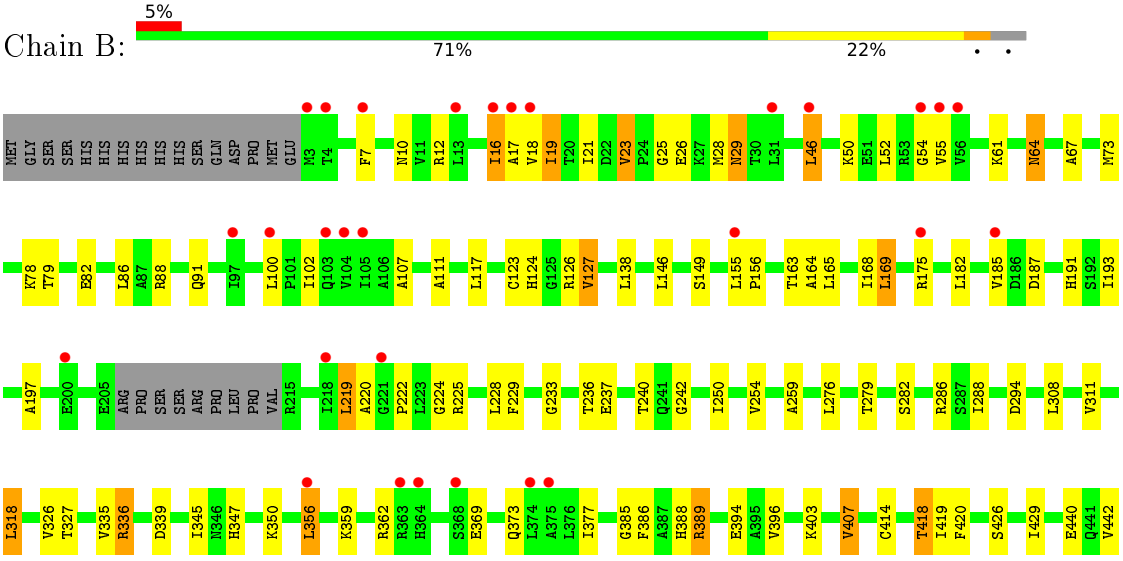
3 Residue-property plots (i)

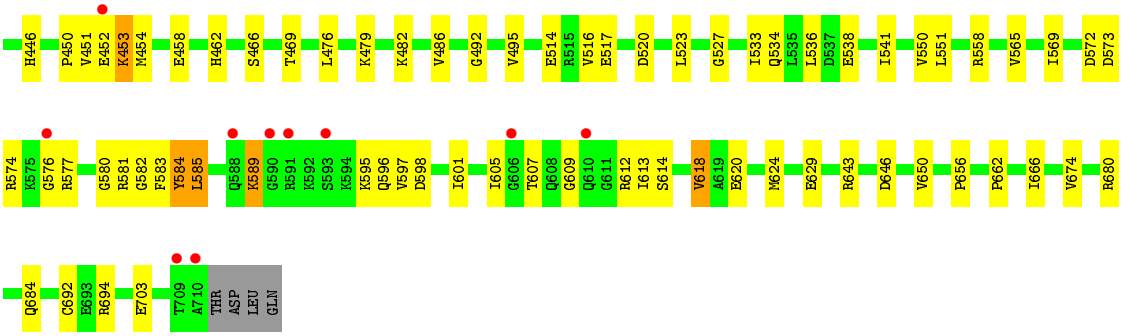
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Fatty acid oxidation complex subunit alpha




H446
P450
V451
E452
K453
M454
E458
H462
S466
T469
L476
K479
K482
V486
G492
V495
E514
R515
V516
E517
D520
L523
G527
I533
Q534
L535
L536
D537
E538
I541
V550
L551
R558
V565
I569
D572
D573
R574
K575
G576
R577
G580
R581
G582
F583
Y584
L585
Q588
K589
G590
R591
K592
S593
K594
K595
Q596
V597
D598
I601
I605
G606
T607
Q608
G609
Q610
G611
R612
I613
S614
V618
A619
E620
M624
E629
R643
D646
V650
P656
P662
I666
V674
R680
Q684
C692
E693
R694
E703
T709
A710
THR
ASP
LEU
GLN

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.16 3549	Depositor
R, R_{free}	0.224 , 0.255 0.224 , 0.254	Depositor DCC
R_{free} test set	2749 reflections (5.16%)	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 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/5397	0.41	0/7314
1	B	0.24	0/5252	0.42	0/7121
All	All	0.24	0/10649	0.42	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

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	65	0
1	B	5167	0	5207	97	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	161	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 (161) 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:A:394:GLU:OE2	1:A:403:LYS:NZ	2.19	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:394:GLU:OE2	1:B:403:LYS:NZ	2.39	0.48
1:A:46:LEU:HD13	1:A:55:VAL:HG11	1.95	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD22	1:B:276:LEU:HD12	2.00	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: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:B:288:ILE:HD13	1:B:650:VAL:HG11	2.03	0.41
1:B:407:VAL:HG12	1:B:420:PHE:CE1	2.56	0.41
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

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	707/728 (97%)	677 (96%)	29 (4%)	1 (0%)	51 78
1	B	695/728 (96%)	660 (95%)	33 (5%)	2 (0%)	41 66
All	All	1402/1456 (96%)	1337 (95%)	62 (4%)	3 (0%)	47 73

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

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%)	525 (96%)	23 (4%)	30 58
1	B	524/583 (90%)	478 (91%)	46 (9%)	10 23
All	All	1072/1166 (92%)	1003 (94%)	69 (6%)	17 39

All (69) 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

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Mol	Chain	Res	Type
1	A	146	LEU
1	A	158	LEU
1	A	159	ILE
1	A	208	SER
1	A	212	LEU
1	A	262	THR
1	A	267	ASP
1	A	292	SER
1	A	363	ARG
1	A	366	LYS
1	A	369	GLU
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	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	64	ASN
1	B	127	VAL
1	B	169	LEU
1	B	185	VAL
1	B	191	HIS
1	B	219	LEU
1	B	228	LEU
1	B	318	LEU
1	B	326	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

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Mol	Chain	Res	Type
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	523	LEU
1	B	536	LEU
1	B	584	TYR
1	B	585	LEU
1	B	589	LYS
1	B	595	LYS
1	B	596	GLN
1	B	598	ASP
1	B	607	THR
1	B	618	VAL
1	B	684	GLN
1	B	692	CYS
1	B	694	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	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)

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	0.14	0	6,6,6	0.05	0
2	SO4	B	801	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	805	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	802	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.05	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

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, 95^{th} 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%)	0.23	20 (2%)	53	54	60, 90, 158, 218	0
1	B	699/728 (96%)	0.38	39 (5%)	24	23	64, 110, 177, 220	0
All	All	1407/1456 (96%)	0.31	59 (4%)	36	35	60, 100, 171, 220	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	MET	10.4
1	B	709	THR	7.8
1	B	710	ALA	7.3
1	B	105	ILE	6.2
1	B	104	VAL	5.3
1	B	54	GLY	5.0
1	A	46	LEU	4.7
1	A	365	LEU	4.6
1	A	590	GLY	4.5
1	B	375	ALA	4.3
1	A	104	VAL	3.8
1	A	102	ILE	3.8
1	B	17	ALA	3.7
1	B	18	VAL	3.5
1	B	218	ILE	3.3
1	A	593	SER	3.3
1	B	175	ARG	3.3
1	B	221	GLY	3.3
1	B	4	THR	3.2
1	B	97	ILE	3.1
1	A	208	SER	3.0
1	A	205	GLU	3.0
1	B	185	VAL	3.0
1	A	367	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	100	LEU	2.9
1	B	155	LEU	2.8
1	B	452	GLU	2.7
1	B	591	ARG	2.7
1	A	364	HIS	2.6
1	A	507	ILE	2.6
1	A	35	PHE	2.6
1	B	590	GLY	2.6
1	B	13	LEU	2.6
1	A	55	VAL	2.5
1	A	3	MET	2.4
1	A	31	LEU	2.4
1	B	593	SER	2.4
1	B	7	PHE	2.4
1	B	356	LEU	2.3
1	B	610	GLN	2.3
1	A	586	TYR	2.3
1	B	55	VAL	2.3
1	B	588	GLN	2.3
1	B	31	LEU	2.2
1	A	536	LEU	2.2
1	B	46	LEU	2.2
1	B	16	ILE	2.2
1	B	606	GLY	2.1
1	A	589	LYS	2.1
1	B	368	SER	2.1
1	A	648	GLY	2.1
1	B	200	GLU	2.1
1	B	374	LEU	2.1
1	B	103	GLN	2.1
1	B	363	ARG	2.0
1	B	576	GLY	2.0
1	A	588	GLN	2.0
1	B	364	HIS	2.0
1	B	56	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 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, 95^{th} 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	B	801	5/5	0.77	0.25	164,166,166,167	0
2	SO4	B	802	5/5	0.77	0.23	164,164,165,165	0
2	SO4	A	803	5/5	0.78	0.27	149,150,151,152	0
2	SO4	A	802	5/5	0.82	0.25	178,179,179,180	0
2	SO4	A	801	5/5	0.88	0.48	147,147,149,151	0
2	SO4	A	805	5/5	0.95	0.25	216,218,219,219	5
2	SO4	A	804	5/5	0.98	0.25	124,128,128,128	5

6.5 Other polymers (i)

There are no such residues in this entry.