



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:33 am GMT

PDB ID : 4AG6
Title : Structure of VirB4 of Thermoanaerobacter pseudethanolicus
Authors : Wallden, K.; Williams, R.; Yan, J.; Lian, P.W.; Wang, L.; Thalassinou, K.; Orlova, E.V.; Waksman, G.
Deposited on : 2012-01-24
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

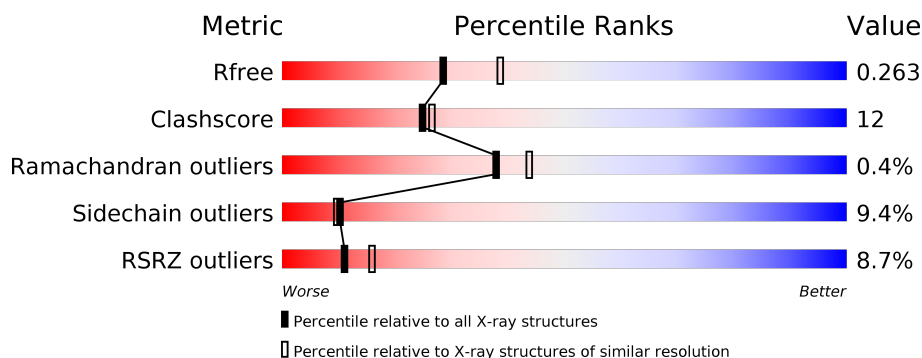
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	392	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>5%</div> </div> </div>
1	B	392	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>•</div> </div> </div>
1	C	392	<div> <div>9%</div> <div> <div></div> <div>43%</div> <div>19%</div> <div>•</div> <div>36%</div> </div> </div>
1	D	392	<div> <div>13%</div> <div> <div></div> <div>34%</div> <div>14%</div> <div>•</div> <div>52%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9178 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 TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	Se	0	1	0
			2921	1855	503	554	3	6			
1	B	376	Total	C	N	O	S	Se	0	1	0
			2950	1876	508	557	3	6			
1	C	252	Total	C	N	O	S	Se	0	0	0
			1802	1163	300	335	2	2			
1	D	190	Total	C	N	O	S	Se	0	0	0
			1199	757	201	239	1	1			

- 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		

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

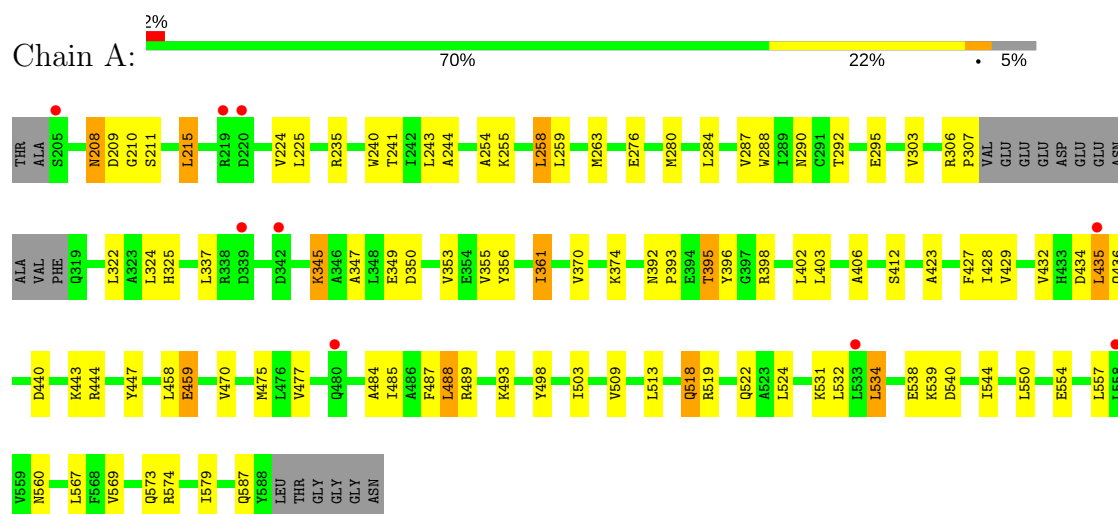
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	126	Total O 126 126	0	0
3	B	118	Total O 118 118	0	0
3	C	12	Total O 12 12	0	0
3	D	5	Total O 5 5	0	0

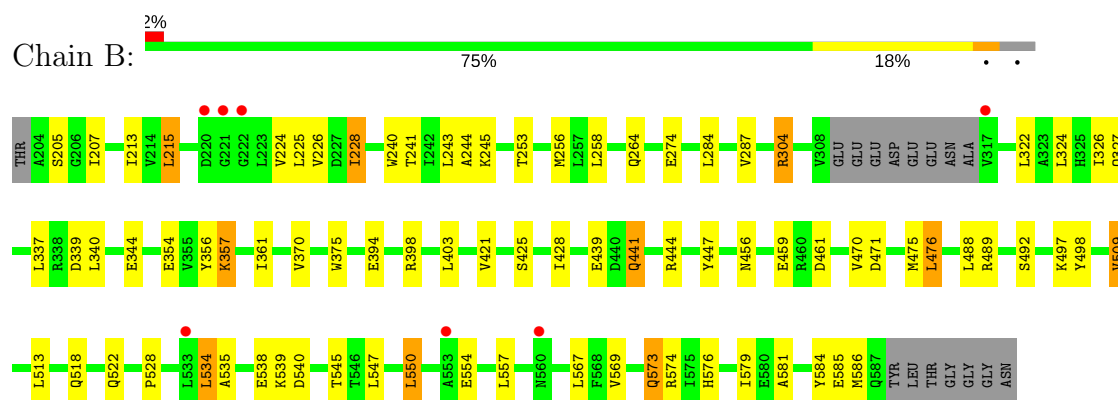
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

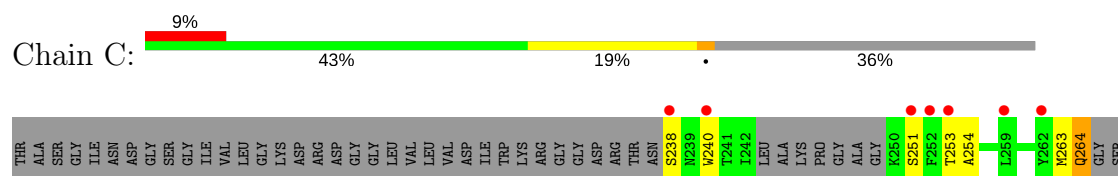
• Molecule 1: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN

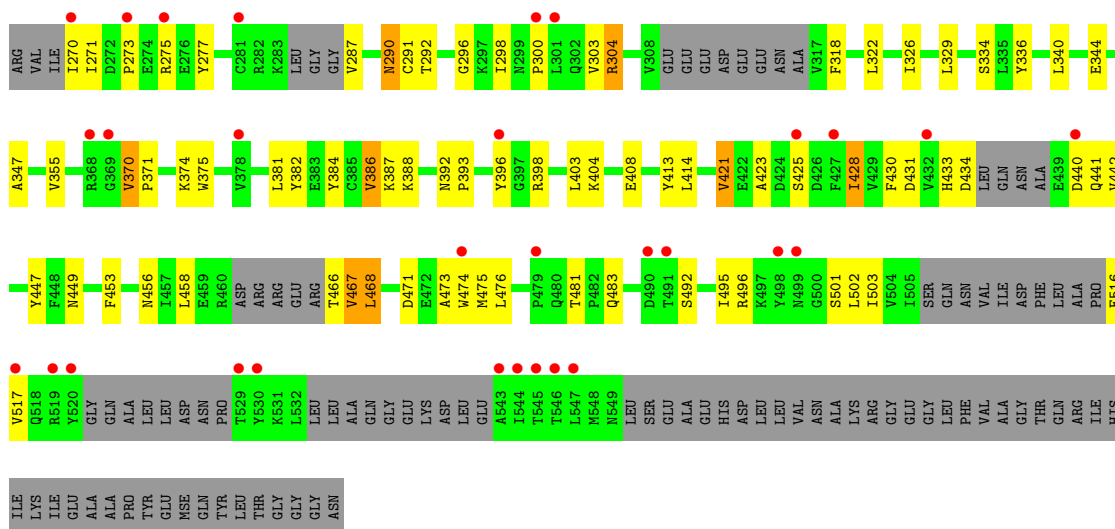


• Molecule 1: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN

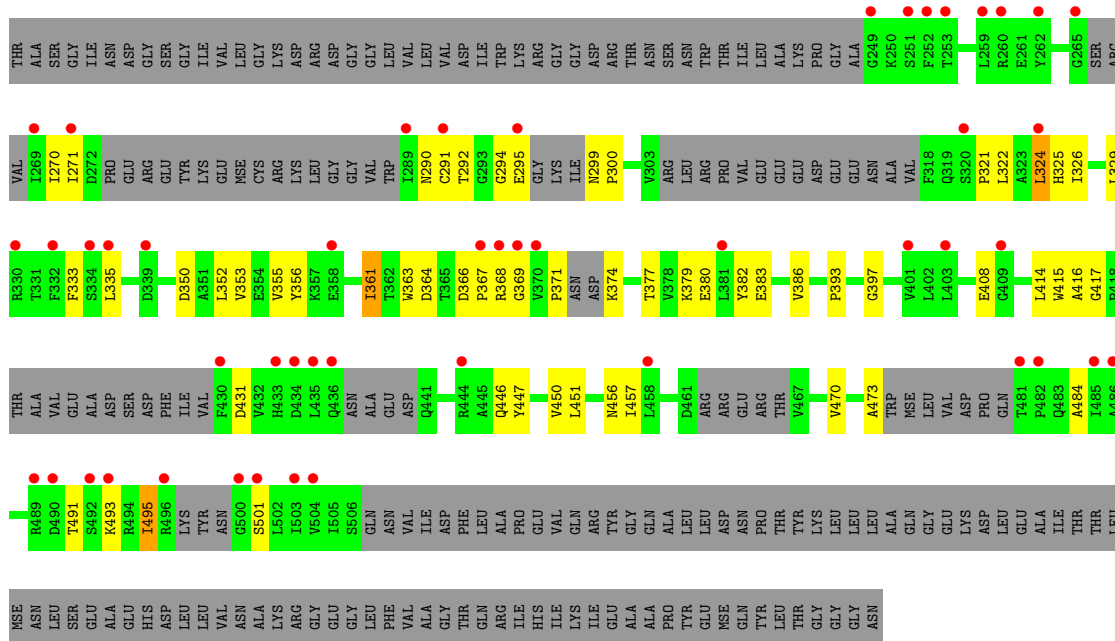
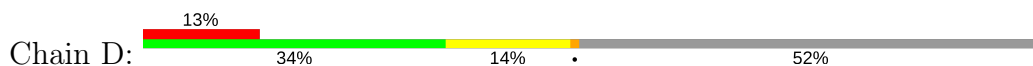


• Molecule 1: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN





● Molecule 1: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.29Å 112.77Å 156.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.35 19.96 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.96-2.35) 96.0 (19.96-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.35Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.226 , 0.266 0.224 , 0.263	Depositor DCC
R_{free} test set	3902 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9178	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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	0.46	0/2972	0.61	0/4029
1	B	0.44	0/3001	0.59	0/4065
1	C	0.32	0/1831	0.50	0/2495
1	D	0.28	0/1207	0.45	0/1654
All	All	0.40	0/9011	0.56	0/12243

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	2921	0	2856	63	0
1	B	2950	0	2912	56	0
1	C	1802	0	1565	59	0
1	D	1199	0	905	38	0
2	A	15	0	0	0	0
2	B	25	0	0	0	0
2	C	5	0	0	0	0
3	A	126	0	0	3	0
3	B	118	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	0	0	0
3	D	5	0	0	0	0
All	All	9178	0	8238	209	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 12.

All (209) 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:334:SER:HB3	1:C:481:THR:HG21	1.37	1.07
1:C:492:SER:HB3	1:C:502:LEU:HD23	1.46	0.94
1:A:432:VAL:O	1:A:435:LEU:HG	1.77	0.84
1:B:228:ILE:HD11	1:B:240:TRP:HZ2	1.47	0.79
1:C:492:SER:O	1:C:495:ILE:HG12	1.83	0.78
1:B:569:VAL:HG22	1:B:574:ARG:HG2	1.68	0.75
1:B:253:THR:HG23	1:B:579:ILE:HG21	1.72	0.71
1:C:334:SER:HB3	1:C:481:THR:CG2	2.18	0.71
1:B:226:VAL:HG22	1:B:228:ILE:HD12	1.71	0.70
1:A:292:THR:HG21	1:A:434:ASP:HB2	1.73	0.70
1:B:538:GLU:HG2	1:B:539:LYS:HG3	1.75	0.69
1:B:439:GLU:HB3	1:B:441:GLN:OE1	1.93	0.68
1:D:356:TYR:CD1	1:D:361:ILE:HD11	2.29	0.68
1:D:329:LEU:HD23	1:D:333:PHE:HE2	1.59	0.67
1:D:447:TYR:O	1:D:450:VAL:HG12	1.93	0.67
1:A:345:LYS:HB2	1:A:345:LYS:NZ	2.09	0.66
1:A:488:LEU:HD13	1:A:524:LEU:HD21	1.79	0.64
1:D:325:HIS:O	1:D:329:LEU:HD12	1.97	0.64
1:B:228:ILE:HD11	1:B:240:TRP:CZ2	2.31	0.64
1:B:228:ILE:HG12	1:B:240:TRP:HE1	1.62	0.64
1:A:395:THR:HG21	1:D:363:TRP:HB3	1.81	0.63
1:A:444:ARG:HG2	1:A:475:MSE:O	1.99	0.62
1:B:444:ARG:HG2	1:B:475:MSE:O	2.00	0.62
1:C:495:ILE:HG13	1:C:496:ARG:N	2.14	0.62
1:C:516:GLU:HG3	1:C:517:VAL:N	2.13	0.62
1:A:370:VAL:HG13	1:A:374:LYS:HD3	1.83	0.61
1:C:441:GLN:HG2	1:C:442:VAL:N	2.15	0.61
1:D:299:ASN:ND2	1:D:377:THR:HG22	2.15	0.61
1:A:509:VAL:HG11	1:A:544:ILE:HD11	1.82	0.61
1:A:361:ILE:O	1:A:361:ILE:HG13	1.99	0.61
1:C:240:TRP:HB2	1:C:503:ILE:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:LEU:HD12	1:C:468:LEU:HB2	1.84	0.60
1:B:241:THR:HG22	1:B:243:LEU:HG	1.84	0.59
1:B:245:LYS:HG2	1:B:535:ALA:O	2.03	0.59
1:A:259:LEU:HD11	1:A:263:MSE:HE3	1.83	0.59
1:B:344:GLU:OE1	1:B:398:ARG:NH1	2.36	0.58
1:C:371:PRO:HD2	1:C:374:LYS:HG3	1.85	0.58
1:A:509:VAL:HG13	1:A:540:ASP:CG	2.24	0.58
1:D:470:VAL:HG12	1:D:470:VAL:O	2.03	0.58
1:B:207:ILE:HG12	1:B:573:GLN:HE21	1.69	0.58
1:D:379:LYS:O	1:D:383:GLU:HG3	2.04	0.58
1:C:271:ILE:HD12	1:C:271:ILE:N	2.18	0.58
1:B:447:TYR:HD2	1:B:475:MSE:HE2	1.68	0.58
1:D:369:GLY:O	1:D:371:PRO:HD3	2.05	0.57
1:A:538[A]:GLU:HG2	1:A:539:LYS:N	2.19	0.57
1:C:382:TYR:CE1	1:C:404:LYS:HB2	2.40	0.57
1:A:345:LYS:HB2	1:A:345:LYS:HZ3	1.70	0.56
1:C:292:THR:O	1:C:414:LEU:HD23	2.04	0.56
1:D:415:TRP:O	1:D:417:GLY:N	2.39	0.56
1:B:554:GLU:HB3	1:B:567:LEU:HD11	1.85	0.56
1:A:244:ALA:HB2	1:A:534:LEU:HB2	1.86	0.56
1:B:361:ILE:HD13	1:B:375:TRP:CZ3	2.41	0.56
1:A:208:ASN:HD22	1:A:208:ASN:C	2.10	0.55
1:A:459:GLU:HG2	1:A:498:TYR:CZ	2.42	0.55
1:B:522:GLN:HG3	1:B:547:LEU:CD1	2.37	0.55
1:A:569:VAL:HG22	1:A:574:ARG:HD2	1.89	0.54
1:A:435:LEU:HD12	1:A:436:GLN:N	2.23	0.54
1:C:336:TYR:HE1	1:C:442:VAL:HG12	1.72	0.54
1:A:435:LEU:HD13	1:A:443:LYS:HG2	1.89	0.54
1:A:518:GLN:HG3	1:A:519:ARG:N	2.22	0.53
1:C:384:TYR:OH	1:C:388:LYS:HE2	2.07	0.53
1:A:440:ASP:HB3	1:A:444:ARG:NH2	2.24	0.53
1:A:392:ASN:N	1:A:393:PRO:HD3	2.23	0.53
1:C:270:ILE:C	1:C:271:ILE:HD12	2.30	0.52
1:B:538:GLU:HG2	1:B:539:LYS:H	1.73	0.52
1:B:557:LEU:HD11	1:B:576:HIS:CG	2.45	0.52
1:C:292:THR:HG21	1:C:434:ASP:CB	2.40	0.52
1:A:254:ALA:O	1:A:258:LEU:HD22	2.09	0.51
1:B:538:GLU:HG2	1:B:539:LYS:N	2.25	0.51
1:B:344:GLU:OE2	1:B:398:ARG:HD3	2.10	0.51
1:B:522:GLN:HG3	1:B:547:LEU:HD11	1.92	0.51
1:A:423:ALA:HB1	1:A:428:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ALA:HB2	1:B:534:LEU:HB2	1.93	0.51
1:B:584:TYR:CE1	1:B:585:GLU:HG3	2.46	0.51
1:C:334:SER:CB	1:C:481:THR:HG21	2.24	0.51
1:D:371:PRO:HD2	1:D:374:LYS:CB	2.41	0.51
1:C:458:LEU:HD23	1:C:458:LEU:O	2.10	0.50
1:D:470:VAL:HG12	1:D:473:ALA:HB2	1.93	0.50
1:A:458:LEU:O	1:A:458:LEU:HD23	2.11	0.50
1:A:509:VAL:HG13	1:A:540:ASP:OD2	2.09	0.50
1:A:395:THR:HG23	1:D:364:ASP:OD1	2.11	0.50
1:C:423:ALA:HB1	1:C:428:ILE:HD12	1.93	0.50
1:B:228:ILE:CG1	1:B:240:TRP:HE1	2.25	0.50
1:B:241:THR:OG1	1:B:528:PRO:HG2	2.12	0.50
1:D:393:PRO:O	1:D:397:GLY:HA3	2.12	0.49
1:A:306:ARG:HB2	1:A:307:PRO:HD2	1.93	0.49
1:C:458:LEU:CD1	1:C:468:LEU:HB2	2.41	0.49
1:B:226:VAL:CG2	1:B:228:ILE:HD12	2.42	0.49
1:B:394:GLU:HB3	1:C:318:PHE:CD2	2.47	0.49
1:C:322:LEU:O	1:C:326:ILE:HG12	2.13	0.49
1:A:395:THR:CG2	1:D:364:ASP:OD1	2.60	0.49
1:D:294:GLY:O	1:D:295:GLU:C	2.51	0.49
1:A:303:VAL:HG13	1:A:325:HIS:HB2	1.95	0.48
1:A:435:LEU:HD22	1:A:443:LYS:HA	1.95	0.48
1:B:322:LEU:HD11	1:B:356:TYR:CD2	2.48	0.48
1:B:215:LEU:HD22	1:B:579:ILE:CD1	2.43	0.48
1:D:290:ASN:O	1:D:292:THR:N	2.45	0.48
1:B:354:GLU:OE2	1:B:357:LYS:NZ	2.44	0.48
1:B:459:GLU:HG3	1:B:498:TYR:CZ	2.49	0.48
1:C:370:VAL:HG23	1:C:374:LYS:HB2	1.96	0.48
1:A:322:LEU:HD13	1:A:361:ILE:HD11	1.96	0.48
1:A:208:ASN:ND2	1:A:209:ASP:O	2.47	0.48
1:D:495:ILE:O	1:D:495:ILE:HG22	2.14	0.48
1:A:435:LEU:HD12	1:A:435:LEU:C	2.34	0.48
1:A:347:ALA:HB1	1:A:396:TYR:CZ	2.49	0.47
1:C:495:ILE:HD12	1:C:501:SER:HA	1.96	0.47
1:B:545:THR:HA	1:B:550:LEU:HB2	1.96	0.47
1:B:447:TYR:CD2	1:B:475:MSE:HE2	2.49	0.47
1:A:353:VAL:HG11	1:D:350:ASP:OD1	2.15	0.47
1:C:466:THR:O	1:C:467:VAL:CB	2.61	0.47
1:C:447:TYR:OH	1:C:471:ASP:O	2.31	0.47
1:C:384:TYR:CE1	1:C:388:LYS:HG3	2.49	0.47
1:D:321:PRO:HG2	1:D:367:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLN:NE2	3:A:2002:HOH:O	2.41	0.47
1:C:344:GLU:OE1	1:C:398:ARG:NH1	2.48	0.47
1:C:474:TRP:C	1:C:476:LEU:H	2.18	0.47
1:B:339:ASP:CG	1:B:398:ARG:HH22	2.18	0.46
1:C:473:ALA:O	1:C:476:LEU:HB3	2.15	0.46
1:D:329:LEU:HD23	1:D:333:PHE:CE2	2.44	0.46
1:C:300:PRO:O	1:C:329:LEU:HD21	2.15	0.46
1:A:447:TYR:HD2	1:A:475:MSE:HE2	1.80	0.46
1:A:489:ARG:HD2	1:A:493:LYS:HE3	1.96	0.46
1:B:581:ALA:HB3	1:B:586:MSE:HE2	1.97	0.46
1:B:509:VAL:HG13	1:B:540:ASP:CG	2.34	0.46
1:C:355:VAL:HG21	1:C:381:LEU:HA	1.98	0.46
1:D:299:ASN:HA	1:D:300:PRO:HD3	1.80	0.46
1:B:447:TYR:CE1	1:B:476:LEU:HD22	2.51	0.46
1:C:290:ASN:O	1:C:296:GLY:HA3	2.16	0.46
1:A:288:TRP:CZ3	1:A:290:ASN:HB2	2.50	0.46
1:A:470:VAL:HG23	1:A:470:VAL:O	2.16	0.46
1:B:287:VAL:HG12	1:B:425:SER:HB3	1.98	0.46
1:C:495:ILE:HG21	1:C:502:LEU:CB	2.46	0.46
1:A:241:THR:HG22	1:A:243:LEU:HG	1.97	0.45
1:A:459:GLU:HG2	1:A:498:TYR:OH	2.15	0.45
1:A:306:ARG:NH2	3:A:2067:HOH:O	2.43	0.45
1:A:337:LEU:HD22	1:A:402:LEU:HB3	1.98	0.45
1:C:303:VAL:HB	1:C:375:TRP:CH2	2.51	0.45
1:D:322:LEU:HD11	1:D:356:TYR:CD2	2.51	0.45
1:B:459:GLU:HG3	1:B:498:TYR:OH	2.17	0.45
1:A:240:TRP:HB2	1:A:503:ILE:HG12	1.98	0.45
1:C:238:SER:O	1:C:501:SER:HB2	2.17	0.45
1:D:321:PRO:HA	1:D:324:LEU:HD12	1.99	0.45
1:B:256:MSE:HA	1:B:256:MSE:HE2	1.99	0.45
1:B:461:ASP:OD1	1:B:461:ASP:O	2.35	0.45
1:D:446:GLN:OE1	1:D:446:GLN:HA	2.17	0.45
1:A:435:LEU:CD1	1:A:435:LEU:C	2.86	0.44
1:C:287:VAL:HG23	1:C:425:SER:OG	2.17	0.44
1:A:209:ASP:O	1:A:210:GLY:C	2.56	0.44
1:C:386:VAL:HG12	1:C:387:LYS:N	2.32	0.44
1:B:274:GLU:OE2	1:B:471:ASP:OD2	2.36	0.44
1:B:322:LEU:O	1:B:326:ILE:HG12	2.18	0.44
1:D:382:TYR:O	1:D:386:VAL:HG23	2.18	0.44
1:A:587:GLN:H	1:A:587:GLN:HG3	1.62	0.44
1:C:370:VAL:HA	1:C:371:PRO:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ARG:HG3	1:C:431:ASP:OD2	2.18	0.43
1:D:415:TRP:C	1:D:417:GLY:H	2.20	0.43
1:D:450:VAL:HG13	1:D:451:LEU:N	2.33	0.43
1:C:292:THR:O	1:C:413:TYR:CD2	2.71	0.43
1:A:484:ALA:O	1:A:487:PHE:HB3	2.18	0.43
1:C:277:TYR:N	1:C:277:TYR:CD1	2.86	0.43
1:A:255:LYS:HE2	1:A:276:GLU:O	2.18	0.43
1:A:322:LEU:HD11	1:A:356:TYR:CD2	2.54	0.43
1:B:213:ILE:HG13	1:B:213:ILE:O	2.19	0.43
1:A:349:GLU:O	1:A:353:VAL:HG23	2.19	0.43
1:A:235:ARG:HB3	3:A:2010:HOH:O	2.19	0.43
1:C:347:ALA:HB1	1:C:396:TYR:CZ	2.54	0.43
1:A:531:LYS:HB2	1:A:569:VAL:HB	2.01	0.42
1:B:304:ARG:HB2	1:B:456:ASN:OD1	2.19	0.42
1:A:215:LEU:HA	1:A:215:LEU:HD23	1.85	0.42
1:B:207:ILE:CG1	1:B:573:GLN:HE21	2.30	0.42
1:D:335:LEU:HD21	1:D:484:ALA:HB2	2.02	0.42
1:A:554:GLU:HB3	1:A:567:LEU:HD11	2.01	0.42
1:C:291:CYS:SG	1:C:430:PHE:HD1	2.43	0.42
1:C:304:ARG:HB2	1:C:456:ASN:CG	2.40	0.42
1:A:350:ASP:OD1	1:D:353:VAL:HG11	2.20	0.42
1:A:406:ALA:O	1:A:412:SER:HA	2.20	0.41
1:D:366:ASP:OD1	1:D:368:ARG:HG2	2.20	0.41
1:B:304:ARG:HB2	1:B:456:ASN:CG	2.41	0.41
1:B:324:LEU:O	1:B:327:GLN:HB2	2.20	0.41
1:B:394:GLU:HB3	1:C:318:PHE:CG	2.56	0.41
1:C:441:GLN:HG2	1:C:442:VAL:H	1.82	0.41
1:C:495:ILE:HD13	1:C:502:LEU:H	1.85	0.41
1:A:477:VAL:HG22	1:A:485:ILE:HG13	2.02	0.41
1:B:339:ASP:CG	1:B:398:ARG:NH2	2.73	0.41
1:C:392:ASN:N	1:C:393:PRO:HD3	2.35	0.41
1:C:251:SER:O	1:C:254:ALA:HB3	2.20	0.41
1:C:304:ARG:NH2	1:C:449:ASN:OD1	2.49	0.41
1:D:355:VAL:HG12	1:D:356:TYR:N	2.35	0.41
1:B:287:VAL:CG1	1:B:428:ILE:HG12	2.50	0.41
1:C:292:THR:O	1:C:413:TYR:CE2	2.74	0.41
1:D:414:LEU:HD22	1:D:446:GLN:NE2	2.36	0.41
1:A:280:MSE:HE2	1:A:427:PHE:CE2	2.56	0.41
1:C:421:VAL:CG2	1:C:453:PHE:CZ	3.04	0.41
1:D:271:ILE:HD11	1:D:451:LEU:HA	2.01	0.41
1:C:298:ILE:HD13	1:C:453:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:GLN:N	1:C:483:GLN:OE1	2.52	0.41
1:B:470:VAL:O	1:B:470:VAL:HG23	2.21	0.40
1:C:386:VAL:CG1	1:C:387:LYS:N	2.83	0.40
1:D:456:ASN:O	1:D:457:ILE:C	2.59	0.40
1:D:493:LYS:C	1:D:495:ILE:H	2.24	0.40
1:C:273:PRO:O	1:C:433:HIS:HA	2.22	0.40
1:D:450:VAL:CG1	1:D:451:LEU:N	2.84	0.40
1:B:339:ASP:OD1	1:B:398:ARG:NH2	2.54	0.40
1:B:584:TYR:CD1	1:B:584:TYR:C	2.94	0.40
1:B:354:GLU:OE2	1:B:357:LYS:HE2	2.22	0.40
1:C:263:MSE:C	1:C:264:GLN:HG2	2.41	0.40
1:D:329:LEU:HD22	1:D:352:LEU:HD11	2.01	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	370/392 (94%)	353 (95%)	17 (5%)	0	100	100
1	B	373/392 (95%)	362 (97%)	11 (3%)	0	100	100
1	C	232/392 (59%)	205 (88%)	26 (11%)	1 (0%)	38	44
1	D	168/392 (43%)	148 (88%)	17 (10%)	3 (2%)	10	7
All	All	1143/1568 (73%)	1068 (93%)	71 (6%)	4 (0%)	38	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	467	VAL
1	D	416	ALA
1	D	291	CYS

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Mol	Chain	Res	Type
1	D	270	ILE

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	302/324 (93%)	273 (90%)	29 (10%)	10	9
1	B	308/324 (95%)	281 (91%)	27 (9%)	12	11
1	C	154/324 (48%)	140 (91%)	14 (9%)	11	11
1	D	79/324 (24%)	70 (89%)	9 (11%)	7	6
All	All	843/1296 (65%)	764 (91%)	79 (9%)	10	10

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	211	SER
1	A	215	LEU
1	A	224	VAL
1	A	225	LEU
1	A	258	LEU
1	A	284	LEU
1	A	287	VAL
1	A	295	GLU
1	A	324	LEU
1	A	345	LYS
1	A	355	VAL
1	A	361	ILE
1	A	395	THR
1	A	398	ARG
1	A	403	LEU
1	A	429	VAL
1	A	435	LEU
1	A	459	GLU
1	A	488	LEU

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Mol	Chain	Res	Type
1	A	513	LEU
1	A	518	GLN
1	A	522	GLN
1	A	532	LEU
1	A	534	LEU
1	A	550	LEU
1	A	557	LEU
1	A	560	ASN
1	A	579	ILE
1	B	205	SER
1	B	215	LEU
1	B	224	VAL
1	B	225	LEU
1	B	228	ILE
1	B	258	LEU
1	B	264	GLN
1	B	284	LEU
1	B	304	ARG
1	B	337	LEU
1	B	340	LEU
1	B	357	LYS
1	B	370	VAL
1	B	403	LEU
1	B	421	VAL
1	B	441	GLN
1	B	476	LEU
1	B	488	LEU
1	B	489	ARG
1	B	492	SER
1	B	497	LYS
1	B	509	VAL
1	B	513	LEU
1	B	518	GLN
1	B	534	LEU
1	B	550	LEU
1	B	573	GLN
1	C	253	THR
1	C	264	GLN
1	C	290	ASN
1	C	304	ARG
1	C	340	LEU
1	C	370	VAL

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Mol	Chain	Res	Type
1	C	386	VAL
1	C	403	LEU
1	C	408	GLU
1	C	421	VAL
1	C	428	ILE
1	C	440	ASP
1	C	468	LEU
1	C	475	MSE
1	D	324	LEU
1	D	326	ILE
1	D	361	ILE
1	D	380	GLU
1	D	408	GLU
1	D	431	ASP
1	D	491	THR
1	D	495	ILE
1	D	501	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	B	518	GLN
1	B	573	GLN
1	C	290	ASN
1	C	327	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

9 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	A	1589	-	4,4,4	0.23	0	6,6,6	0.21	0
2	SO4	A	1590	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	A	1591	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	B	1588	-	4,4,4	0.16	0	6,6,6	0.24	0
2	SO4	B	1589	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	B	1590	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	B	1591	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	B	1592	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	C	1588	-	4,4,4	0.14	0	6,6,6	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1589	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1590	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1591	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1588	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1589	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1590	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1591	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1592	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1588	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/392 (93%)	0.06	9 (2%) 58 68	15, 39, 72, 92	0
1	B	370/392 (94%)	0.09	7 (1%) 67 76	21, 40, 72, 94	0
1	C	247/392 (63%)	0.88	37 (14%) 3 4	38, 83, 123, 147	0
1	D	188/392 (47%)	1.27	49 (26%) 1 1	64, 93, 120, 136	0
All	All	1172/1568 (74%)	0.44	102 (8%) 11 16	15, 52, 114, 147	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	ILE	7.8
1	C	498	TYR	7.5
1	D	370	VAL	6.3
1	D	252	PHE	5.8
1	C	262	TYR	5.6
1	D	492	SER	5.5
1	C	281	CYS	5.4
1	C	252	PHE	5.3
1	C	474	TRP	5.2
1	D	458	LEU	5.2
1	C	251	SER	4.8
1	D	262	TYR	4.8
1	C	544	ILE	4.7
1	C	479	PRO	4.7
1	D	289	ILE	4.7
1	D	251	SER	4.6
1	D	482	PRO	4.4
1	D	368	ARG	4.3
1	D	367	PRO	4.1
1	D	504	VAL	4.0
1	C	369	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	553	ALA	4.0
1	D	291	CYS	3.9
1	D	324	LEU	3.9
1	D	430	PHE	3.8
1	C	517	VAL	3.8
1	D	486	ALA	3.8
1	C	499	ASN	3.7
1	C	270	ILE	3.7
1	D	253	THR	3.7
1	D	434	ASP	3.6
1	B	560	ASN	3.6
1	C	425	SER	3.5
1	B	317	VAL	3.4
1	D	260	ARG	3.4
1	D	493	LYS	3.4
1	D	335	LEU	3.4
1	A	205	SER	3.3
1	C	545	THR	3.3
1	B	220	ASP	3.3
1	D	295	GLU	3.3
1	B	221	GLY	3.2
1	C	432	VAL	3.2
1	C	520	TYR	3.2
1	C	546	THR	3.2
1	C	368	ARG	3.1
1	D	503	ILE	3.0
1	C	273	PRO	3.0
1	C	543	ALA	3.0
1	C	275	ARG	2.9
1	D	401	VAL	2.9
1	D	403	LEU	2.9
1	C	519	ARG	2.8
1	D	339	ASP	2.8
1	A	219	ARG	2.8
1	A	220	ASP	2.7
1	A	558	LEU	2.7
1	C	253	THR	2.7
1	D	444	ARG	2.6
1	D	409	GLY	2.6
1	C	427	PHE	2.6
1	C	530	TYR	2.6
1	C	240	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	378	VAL	2.6
1	D	358	GLU	2.6
1	D	332	PHE	2.6
1	D	320	SER	2.6
1	D	489	ARG	2.5
1	D	249	GLY	2.5
1	C	529	THR	2.5
1	D	369	GLY	2.5
1	C	547	LEU	2.4
1	D	433	HIS	2.4
1	D	334	SER	2.4
1	D	501	SER	2.4
1	A	480	GLN	2.3
1	C	491	THR	2.3
1	D	435	LEU	2.3
1	A	435	LEU	2.3
1	D	381	LEU	2.3
1	C	301	LEU	2.3
1	C	490	ASP	2.3
1	A	533	LEU	2.2
1	A	342	ASP	2.2
1	A	339	ASP	2.2
1	D	490	ASP	2.2
1	C	440	ASP	2.2
1	C	396	TYR	2.1
1	D	330	ARG	2.1
1	D	481	THR	2.1
1	D	496	ARG	2.1
1	C	238	SER	2.1
1	D	265	GLY	2.1
1	B	533	LEU	2.1
1	B	222	GLY	2.1
1	D	259	LEU	2.0
1	D	269	ILE	2.0
1	D	436	GLN	2.0
1	C	300	PRO	2.0
1	C	259	LEU	2.0
1	D	271	ILE	2.0
1	D	500	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1590	5/5	0.92	0.16	0.13	80,80,83,88	0
2	SO4	A	1589	5/5	0.99	0.12	0.04	37,38,42,48	0
2	SO4	B	1591	5/5	0.93	0.17	-0.14	118,118,119,121	0
2	SO4	B	1588	5/5	0.99	0.08	-1.59	37,37,46,48	0
2	SO4	B	1592	5/5	0.70	0.30	-	122,123,125,126	0
2	SO4	C	1588	5/5	0.95	0.29	-	107,108,110,111	0
2	SO4	B	1589	5/5	0.84	0.42	-	83,84,89,92	0
2	SO4	B	1590	5/5	0.95	0.20	-	102,103,104,105	0
2	SO4	A	1591	5/5	0.85	0.19	-	123,123,124,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.