



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:15 PM UTC

PDB ID : 4AG6 / pdb_00004ag6
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

<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

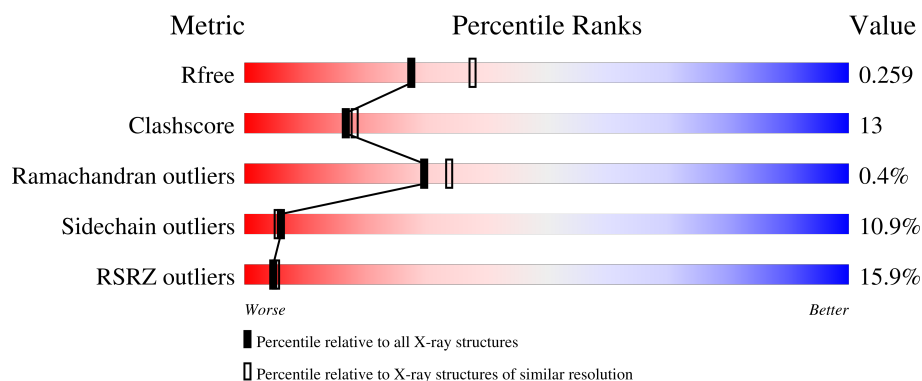
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	392	2% 68% 24% 5%
1	B	392	3% 73% 20% 5%
1	C	392	17% 42% 20% 36%
1	D	392	26% 33% 14% 52%

2 Entry composition [i](#)

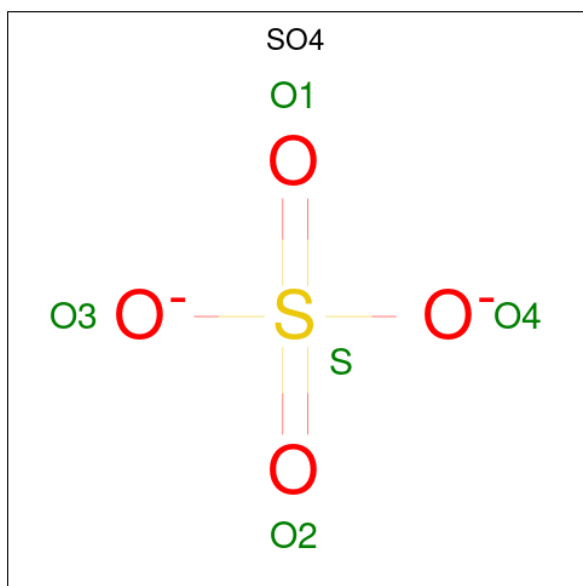
There are 3 unique types of molecules in this entry. The entry contains 9178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (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		

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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

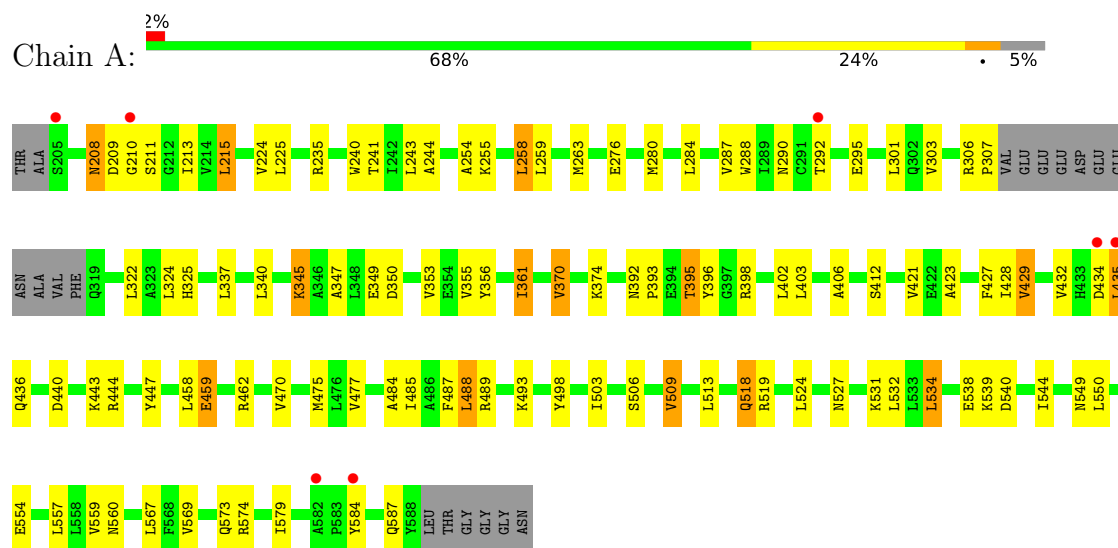
- Molecule 3 is water.

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

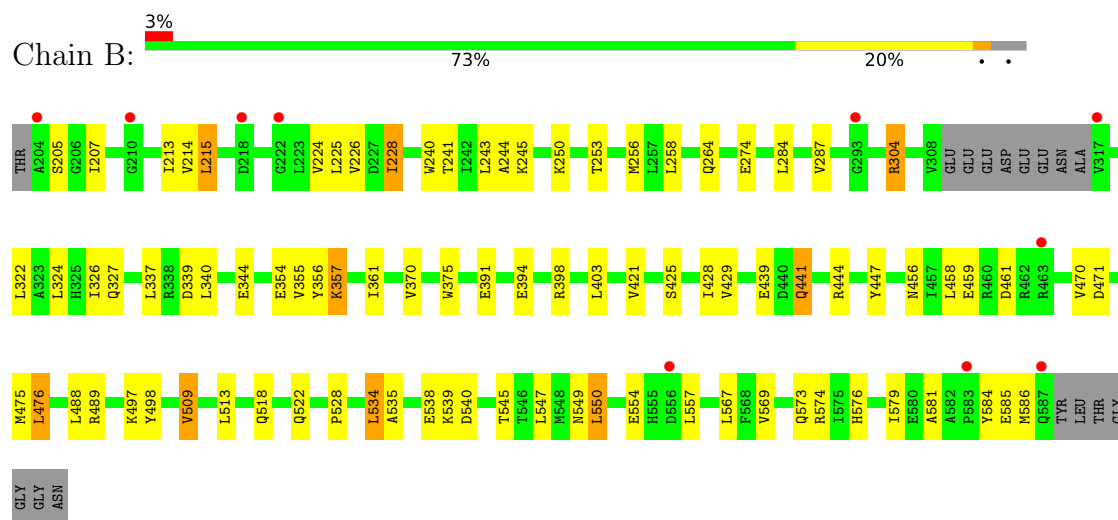
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

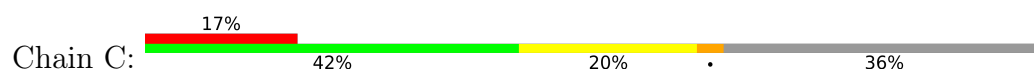
• Molecule 1: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN



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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) 95.8 (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 (Not available) , 0.259	Depositor DCC
R_{free} test set	4030 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 81.1	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

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	0.57	0/2972	0.89	6/4029 (0.1%)
1	B	0.57	0/3001	0.86	0/4065
1	C	0.42	0/1831	0.81	0/2495
1	D	0.39	0/1207	0.81	2/1654 (0.1%)
All	All	0.52	0/9011	0.85	8/12243 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	ASN	CA-C-N	-9.07	110.69	119.76
1	A	527	ASN	C-N-CA	-9.07	110.69	119.76
1	D	370	VAL	N-CA-C	5.72	112.76	107.56
1	A	370	VAL	N-CA-C	5.46	113.33	108.63
1	A	462	ARG	N-CA-C	5.33	117.37	110.65
1	A	506	SER	N-CA-C	5.26	116.52	108.52
1	D	368	ARG	N-CA-C	-5.06	106.53	113.30
1	A	429	VAL	N-CA-C	5.05	115.18	108.11

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	2921	0	2856	64	0
1	B	2950	0	2912	59	0
1	C	1802	0	1565	63	0
1	D	1199	0	905	41	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	1	0
3	C	12	0	0	0	0
3	D	5	0	0	0	0
All	All	9178	0	8238	220	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 13.

All (220) 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:509:VAL:HG13	1:A:540:ASP:CG	2.24	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG13	1:A:361:ILE:O	1.99	0.61
1:C:240:TRP:HB2	1:C:503:ILE:HG12	1.83	0.60
1:C:458:LEU:HD12	1:C:468:LEU:HB2	1.84	0.60
1:A:208:ASN:C	1:A:208:ASN:HD22	2.10	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: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:N	1:C:271:ILE:HD12	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:C:270:ILE:C	1:C:271:ILE:HD12	2.30	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: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:D:294:GLY:O	1:D:295:GLU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASN:N	1:A:393:PRO:HD3	2.23	0.53
1:A:435:LEU:HD12	1:A:435:LEU:C	2.34	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:C:474:TRP:C	1:C:476:LEU:H	2.18	0.51
1:B:339:ASP:CG	1:B:398:ARG:HH22	2.18	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
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:B:509:VAL:HG13	1:B:540:ASP:CG	2.34	0.51
1:C:458:LEU:O	1:C:458:LEU:HD23	2.10	0.50
1:D:470:VAL:HG12	1:D:473:ALA:HB2	1.93	0.50
1:A:395:THR:HG23	1:D:364:ASP:OD1	2.11	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: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:A:435:LEU:C	1:A:435:LEU:CD1	2.86	0.49
1:A:209:ASP:O	1:A:210:GLY:C	2.56	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: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:D:415:TRP:C	1:D:417:GLY:H	2.20	0.48
1:B:250:LYS:NZ	3:B:2018:HOH:O	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:447:TYR:OH	1:C:471:ASP:O	2.31	0.47
1:C:466:THR:O	1:C:467:VAL:CB	2.61	0.47
1:B:339:ASP:CG	1:B:398:ARG:NH2	2.73	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
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:304:ARG:HB2	1:C:456:ASN:CG	2.40	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:B:304:ARG:HB2	1:B:456:ASN:CG	2.41	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: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:D:456:ASN:O	1:D:457:ILE:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:GLU:HG3	1:B:498:TYR:OH	2.17	0.45
1:B:584:TYR:CD1	1:B:584:TYR:C	2.94	0.45
1:C:458:LEU:HD23	1:C:458:LEU:C	2.42	0.45
1:D:493:LYS:C	1:D:495:ILE:H	2.24	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:HE2	1:B:256:MSE:HA	1.99	0.45
1:B:461:ASP:OD1	1:B:461:ASP:O	2.35	0.45
1:D:446:GLN:HA	1:D:446:GLN:OE1	2.17	0.45
1:C:287:VAL:HG23	1:C:425:SER:OG	2.17	0.44
1:B:538:GLU:H	1:B:538:GLU:CD	2.25	0.44
1:C:386:VAL:HG12	1:C:387:LYS:N	2.32	0.44
1:C:263:MSE:C	1:C:264:GLN:HG2	2.41	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:B:458:LEU:HD23	1:B:458:LEU:C	2.43	0.44
1:C:275:ARG:HG3	1:C:431:ASP:OD2	2.18	0.43
1:C:370:VAL:HA	1:C:371:PRO:HD3	1.83	0.43
1:C:292:THR:O	1:C:413:TYR:CD2	2.71	0.43
1:D:327:GLN:O	1:D:328:THR:C	2.59	0.43
1:A:484:ALA:O	1:A:487:PHE:HB3	2.18	0.43
1:C:277:TYR:CD1	1:C:277:TYR:N	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:O	1:B:213:ILE:HG13	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:C:407:ALA:C	1:C:408:GLU:HG3	2.44	0.43
1:A:584:TYR:C	1:A:584:TYR:CD1	2.97	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:HD23	1:A:215:LEU:HA	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:D:450:VAL:HG13	1:D:451:LEU:N	2.33	0.42
1:A:554:GLU:HB3	1:A:567:LEU:HD11	2.01	0.42
1:C:494:ARG:O	1:C:495:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:CYS:SG	1:C:430:PHE:HD1	2.43	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:C:391:GLU:C	1:C:393:PRO:HD3	2.45	0.41
1:D:366:ASP:C	1:D:368:ARG:H	2.28	0.41
1:D:366:ASP:OD1	1:D:368:ARG:HG2	2.20	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: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
1:C:483:GLN:OE1	1:C:483:GLN:N	2.52	0.41
1:D:431:ASP:OD1	1:D:431:ASP:C	2.63	0.41
1:B:470:VAL:HG23	1:B:470:VAL:O	2.21	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:C:431:ASP:OD1	1:C:431:ASP:C	2.64	0.40
1:B:354:GLU:OE2	1:B:357:LYS:HE2	2.22	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 [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	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%)	30	34
1	D	168/392 (43%)	148 (88%)	17 (10%)	3 (2%)	6	5
All	All	1143/1568 (73%)	1068 (93%)	71 (6%)	4 (0%)	30	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	467	VAL
1	D	416	ALA
1	D	291	CYS
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%)	267 (88%)	35 (12%)	5	5
1	B	308/324 (95%)	278 (90%)	30 (10%)	8	7
1	C	154/324 (48%)	138 (90%)	16 (10%)	7	6
1	D	79/324 (24%)	68 (86%)	11 (14%)	3	3
All	All	843/1296 (65%)	751 (89%)	92 (11%)	6	5

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	211	SER
1	A	213	ILE
1	A	215	LEU

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Mol	Chain	Res	Type
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	301	LEU
1	A	324	LEU
1	A	340	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	421	VAL
1	A	429	VAL
1	A	435	LEU
1	A	459	GLU
1	A	488	LEU
1	A	509	VAL
1	A	513	LEU
1	A	518	GLN
1	A	532	LEU
1	A	534	LEU
1	A	549	ASN
1	A	550	LEU
1	A	557	LEU
1	A	559	VAL
1	A	560	ASN
1	A	579	ILE
1	B	205	SER
1	B	214	VAL
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

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Mol	Chain	Res	Type
1	B	340	LEU
1	B	355	VAL
1	B	357	LYS
1	B	370	VAL
1	B	391	GLU
1	B	403	LEU
1	B	421	VAL
1	B	429	VAL
1	B	441	GLN
1	B	476	LEU
1	B	488	LEU
1	B	489	ARG
1	B	497	LYS
1	B	509	VAL
1	B	513	LEU
1	B	518	GLN
1	B	534	LEU
1	B	549	ASN
1	B	550	LEU
1	C	253	THR
1	C	261	GLU
1	C	264	GLN
1	C	270	ILE
1	C	271	ILE
1	C	340	LEU
1	C	370	VAL
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	442	VAL
1	C	468	LEU
1	C	475	MSE
1	D	301	LEU
1	D	324	LEU
1	D	326	ILE
1	D	355	VAL
1	D	361	ILE
1	D	380	GLU
1	D	408	GLU

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Mol	Chain	Res	Type
1	D	431	ASP
1	D	491	THR
1	D	495	ILE
1	D	501	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	480	GLN
1	B	518	GLN
1	B	573	GLN
1	C	290	ASN
1	C	327	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1588	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	B	1591	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	C	1588	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	A	1589	-	4,4,4	0.31	0	6,6,6	0.19	0
2	SO4	B	1590	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	B	1592	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	B	1589	-	4,4,4	0.22	0	6,6,6	0.24	0
2	SO4	A	1590	-	4,4,4	0.23	0	6,6,6	0.18	0
2	SO4	A	1591	-	4,4,4	0.24	0	6,6,6	0.11	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 [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	367/392 (93%)	-0.09	7 (1%) 66 71	15, 39, 72, 92	1 (0%)
1	B	370/392 (94%)	-0.07	10 (2%) 56 63	21, 40, 72, 94	1 (0%)
1	C	247/392 (63%)	1.46	68 (27%) 1 1	38, 83, 123, 147	0
1	D	188/392 (47%)	2.23	101 (53%) 0 0	64, 93, 120, 136	0
All	All	1172/1568 (74%)	0.62	186 (15%) 5 5	15, 52, 114, 147	2 (0%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	281	CYS	8.5
1	D	444	ARG	7.7
1	D	481	THR	7.0
1	D	485	ILE	6.8
1	D	258	LEU	5.9
1	D	504	VAL	5.8
1	D	370	VAL	5.7
1	D	492	SER	5.5
1	C	262	TYR	5.4
1	C	272	ASP	5.1
1	C	498	TYR	5.1
1	C	505	ILE	5.0
1	D	332	PHE	5.0
1	D	503	ILE	4.9
1	C	466	THR	4.9
1	C	257	LEU	4.8
1	D	254	ALA	4.8
1	C	433	HIS	4.7
1	C	252	PHE	4.6
1	C	258	LEU	4.5
1	D	289	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	474	TRP	4.5
1	B	587	GLN	4.4
1	D	264	GLN	4.4
1	D	482	PRO	4.3
1	C	432	VAL	4.3
1	A	205	SER	4.3
1	C	251	SER	4.3
1	D	453	PHE	4.3
1	C	518	GLN	4.3
1	D	334	SER	4.1
1	C	546	THR	4.1
1	D	458	LEU	4.0
1	C	532	LEU	4.0
1	C	472	GLU	3.9
1	D	457	ILE	3.9
1	D	489	ARG	3.9
1	D	496	ARG	3.9
1	D	261	GLU	3.9
1	C	529	THR	3.9
1	D	291	CYS	3.9
1	D	460	ARG	3.9
1	C	530	TYR	3.8
1	C	426	ASP	3.8
1	C	369	GLY	3.8
1	D	323	ALA	3.7
1	D	335	LEU	3.7
1	C	273	PRO	3.7
1	C	490	ASP	3.6
1	D	251	SER	3.6
1	D	430	PHE	3.6
1	C	279	GLU	3.6
1	D	265	GLY	3.5
1	D	488	LEU	3.5
1	D	471	ASP	3.5
1	D	506	SER	3.4
1	D	329	LEU	3.4
1	D	491	THR	3.4
1	D	486	ALA	3.4
1	D	269	ILE	3.3
1	D	262	TYR	3.3
1	D	303	VAL	3.3
1	C	471	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	411	ASP	3.3
1	C	543	ALA	3.3
1	C	491	THR	3.3
1	C	270	ILE	3.2
1	C	308	VAL	3.2
1	D	435	LEU	3.2
1	D	337	LEU	3.2
1	D	367	PRO	3.2
1	C	468	LEU	3.2
1	D	483	GLN	3.2
1	D	331	THR	3.2
1	D	501	SER	3.1
1	D	445	ALA	3.1
1	D	490	ASP	3.1
1	C	492	SER	3.1
1	B	210	GLY	3.0
1	A	584	TYR	3.0
1	C	240	TRP	3.0
1	C	477	VAL	3.0
1	C	253	THR	3.0
1	C	545	THR	3.0
1	D	442	VAL	2.9
1	D	365	THR	2.9
1	C	434	ASP	2.9
1	C	499	ASN	2.9
1	B	204	ALA	2.9
1	C	495	ILE	2.9
1	D	328	THR	2.9
1	C	242	ILE	2.9
1	B	293	GLY	2.9
1	C	259	LEU	2.9
1	D	252	PHE	2.9
1	D	502	LEU	2.9
1	D	467	VAL	2.9
1	D	459	GLU	2.9
1	C	549	ASN	2.9
1	D	451	LEU	2.8
1	C	427	PHE	2.8
1	C	470	VAL	2.8
1	D	494	ARG	2.8
1	D	449	ASN	2.8
1	A	210	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	504	VAL	2.8
1	D	434	ASP	2.7
1	D	330	ARG	2.7
1	D	487	PHE	2.7
1	D	292	THR	2.7
1	D	409	GLY	2.7
1	C	442	VAL	2.7
1	D	257	LEU	2.7
1	D	433	HIS	2.7
1	C	292	THR	2.7
1	C	260	ARG	2.7
1	C	488	LEU	2.7
1	C	254	ALA	2.6
1	D	351	ALA	2.6
1	D	318	PHE	2.6
1	C	531	LYS	2.6
1	B	317	VAL	2.6
1	D	470	VAL	2.6
1	A	292	THR	2.6
1	D	500	GLY	2.6
1	D	401	VAL	2.6
1	D	270	ILE	2.6
1	D	259	LEU	2.5
1	C	282	ARG	2.5
1	C	424	ASP	2.5
1	C	485	ILE	2.5
1	C	496	ARG	2.5
1	D	446	GLN	2.5
1	D	398	ARG	2.5
1	D	324	LEU	2.5
1	D	293	GLY	2.5
1	D	319	GLN	2.5
1	D	452	SER	2.4
1	D	290	ASN	2.4
1	D	322	LEU	2.4
1	C	519	ARG	2.4
1	D	299	ASN	2.4
1	D	338	ARG	2.4
1	D	431	ASP	2.4
1	D	436	GLN	2.4
1	D	300	PRO	2.4
1	C	481	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	405	ARG	2.4
1	C	397	GLY	2.4
1	D	484	ALA	2.3
1	D	505	ILE	2.3
1	B	218	ASP	2.3
1	D	320	SER	2.3
1	B	583	PRO	2.3
1	C	520	TYR	2.3
1	C	238	SER	2.3
1	D	340	LEU	2.3
1	C	413	TYR	2.3
1	A	582	ALA	2.3
1	D	260	ARG	2.3
1	D	271	ILE	2.3
1	D	495	ILE	2.3
1	A	435	LEU	2.2
1	B	556	ASP	2.2
1	D	447	TYR	2.2
1	C	255	LYS	2.2
1	D	406	ALA	2.2
1	D	416	ALA	2.2
1	C	479	PRO	2.2
1	D	455	TRP	2.2
1	C	494	ARG	2.1
1	D	403	LEU	2.1
1	D	327	GLN	2.1
1	D	402	LEU	2.1
1	D	379	LYS	2.1
1	C	483	GLN	2.1
1	A	434	ASP	2.1
1	C	264	GLN	2.1
1	C	277	TYR	2.1
1	C	317	VAL	2.1
1	D	450	VAL	2.1
1	B	222	GLY	2.1
1	D	336	TYR	2.0
1	C	473	ALA	2.0
1	D	364	ASP	2.0
1	B	463	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1592	5/5	0.67	0.14	122,123,125,126	0
2	SO4	A	1591	5/5	0.76	0.15	123,123,124,125	0
2	SO4	C	1588	5/5	0.84	0.08	107,108,110,111	0
2	SO4	B	1591	5/5	0.85	0.12	118,118,119,121	0
2	SO4	B	1589	5/5	0.86	0.20	83,84,89,92	0
2	SO4	A	1590	5/5	0.88	0.19	80,80,83,88	0
2	SO4	B	1590	5/5	0.89	0.09	102,103,104,105	0
2	SO4	B	1588	5/5	0.99	0.05	37,37,46,48	0
2	SO4	A	1589	5/5	0.99	0.06	37,38,42,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.