



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 06:52 PM EST

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

<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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

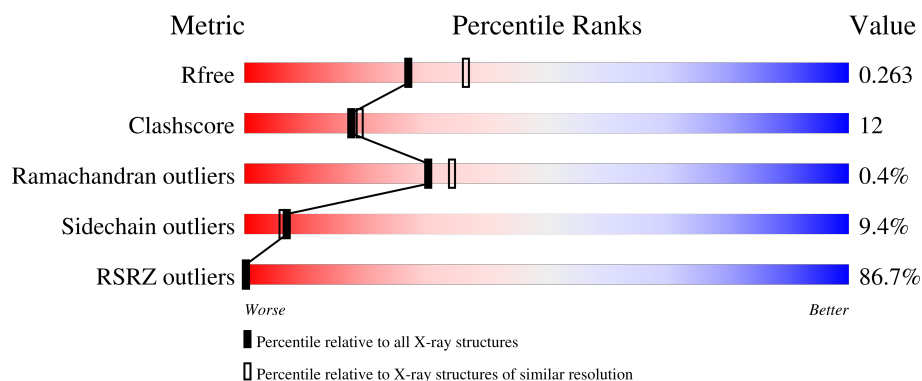
1 Overall quality at a glance

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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div>73%</div> <div>70%</div> <div>22%</div> <div>5%</div> </div>
1	B	392	<div> <div>77%</div> <div>75%</div> <div>18%</div> <div>.</div> </div>
1	C	392	<div> <div>62%</div> <div>43%</div> <div>19%</div> <div>.</div> <div>36%</div> </div>
1	D	392	<div> <div>47%</div> <div>34%</div> <div>14%</div> <div>.</div> <div>52%</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

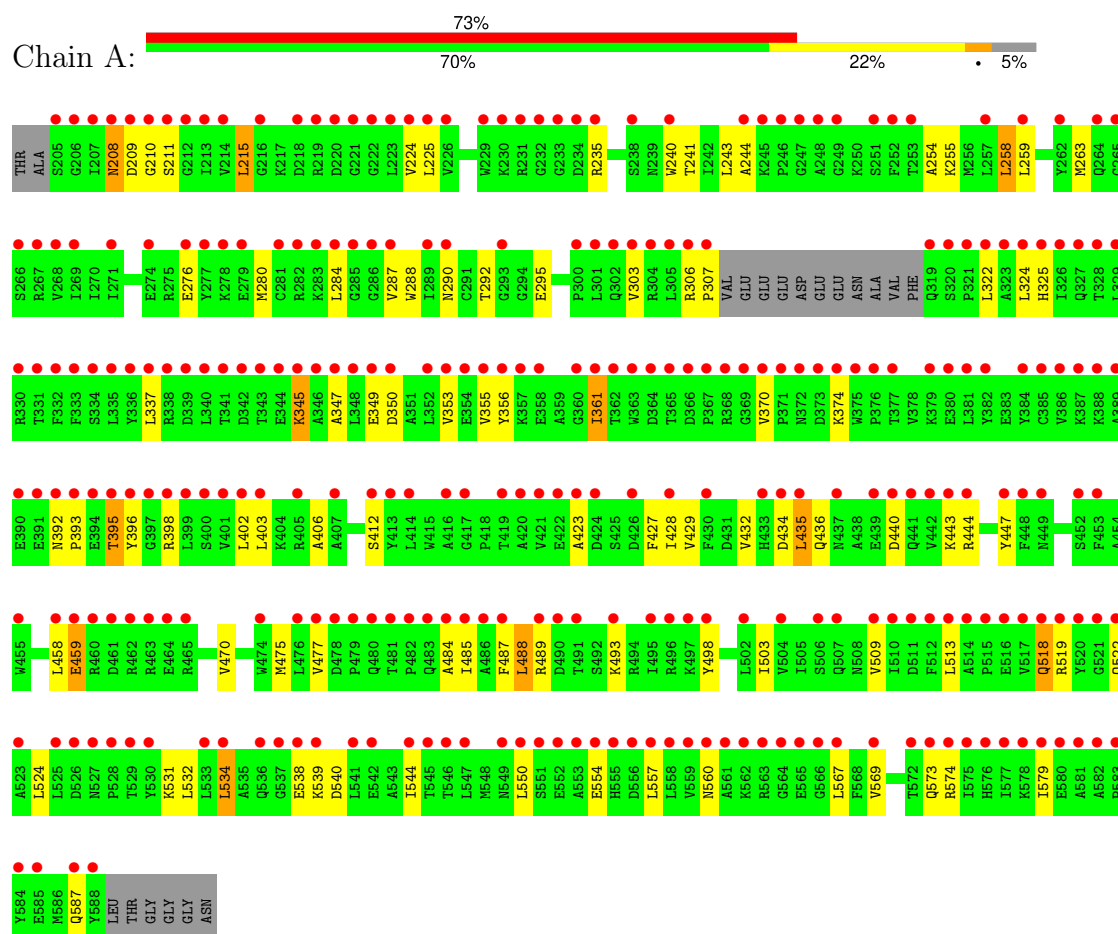
- Molecule 3 is water.

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

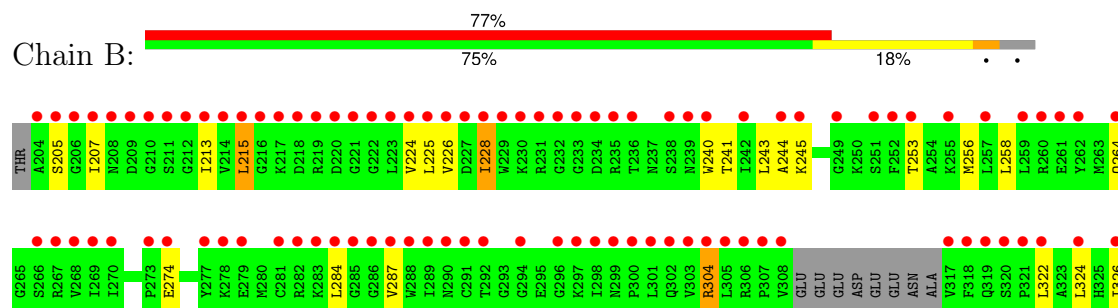
3 Residue-property plots

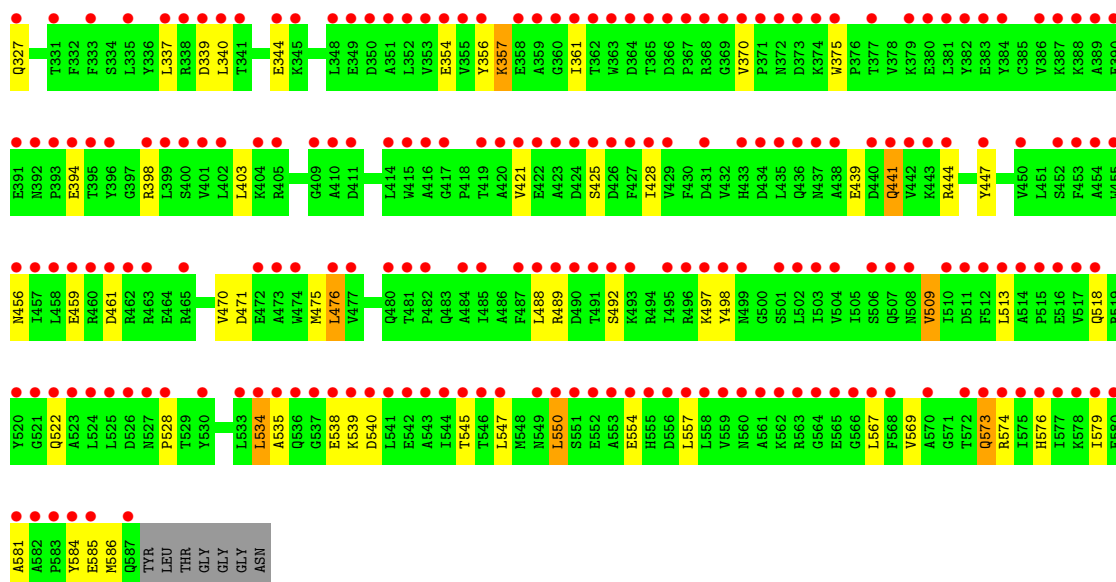
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

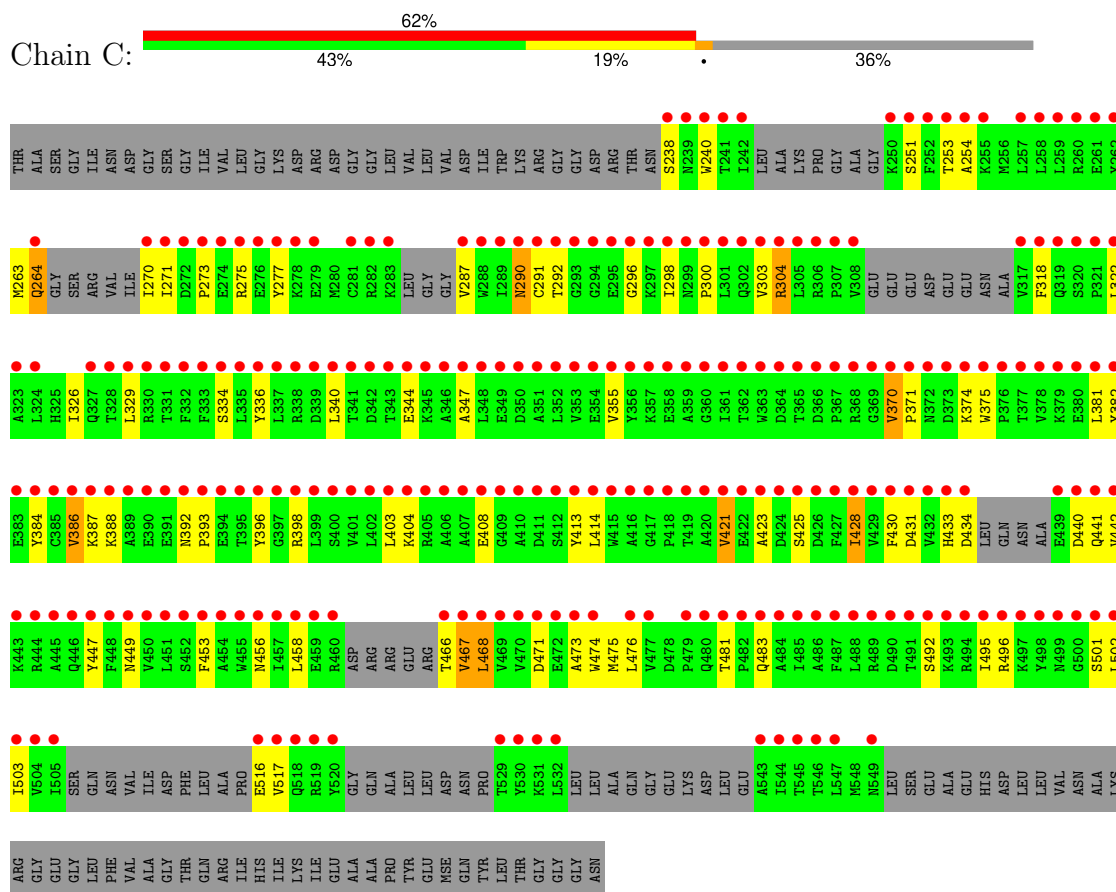


• Molecule 1: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN

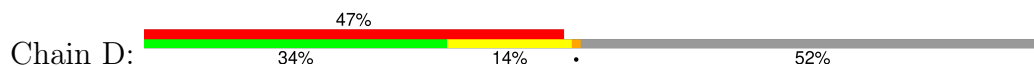




● Molecule 1: TYPE IV SECRETORY PATHWAY VIRB4 COMPONENTS-LIKE PROTEIN



● 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) 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 0.224 , 0.263	Depositor DCC
R_{free} test set	4030 reflections (5.02%)	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)	0.45 , 85.5	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	0.57	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	0.46	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

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:HG13	1:A:361:ILE:O	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: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: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:C	1:A:208:ASN:HD22	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: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: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: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: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: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:A:435:LEU:C	1:A:435:LEU:CD1	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:275:ARG:HG3	1:C:431:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:VAL:HA	1:C:371:PRO:HD3	1.83	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: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: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: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:OE1	1:C:483:GLN:N	2.52	0.41
1:B:470:VAL:HG23	1:B:470:VAL:O	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%)	30	34
1	D	168/392 (43%)	148 (88%)	17 (10%)	3 (2%)	7	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

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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%)	7	6
1	B	308/324 (95%)	281 (91%)	27 (9%)	8	7
1	C	154/324 (48%)	140 (91%)	14 (9%)	7	7
1	D	79/324 (24%)	70 (89%)	9 (11%)	4	4
All	All	843/1296 (65%)	764 (91%)	79 (9%)	7	6

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

Sometimes 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 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	C	1588	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	B	1591	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	1591	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	B	1590	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	B	1588	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	A	1589	-	4,4,4	0.31	0	6,6,6	0.19	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	B	1592	-	4,4,4	0.22	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 ⓘ

Warning: The R factor obtained from EDS is 0.4777, which does not match the depositor's R factor of 0.2262. Please interpret the results in this section carefully.

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%)	3.28	286 (77%) 0 0	15, 39, 72, 92	1 (0%)
1	B	370/392 (94%)	3.39	301 (81%) 0 0	21, 40, 72, 94	1 (0%)
1	C	247/392 (63%)	5.75	244 (98%) 0 0	38, 83, 123, 147	0
1	D	188/392 (47%)	5.80	185 (98%) 0 0	64, 93, 120, 136	0
All	All	1172/1568 (74%)	4.24	1016 (86%) 0 0	15, 52, 114, 147	2 (0%)

All (1016) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	479	PRO	17.3
1	D	505	ILE	14.0
1	C	389	ALA	14.0
1	C	258	LEU	13.7
1	D	397	GLY	13.7
1	C	474	TRP	11.8
1	C	394	GLU	11.7
1	C	401	VAL	11.6
1	C	407	ALA	11.6
1	D	455	TRP	11.3
1	C	490	ASP	11.0
1	D	461	ASP	11.0
1	D	323	ALA	11.0
1	C	433	HIS	10.8
1	D	261	GLU	10.6
1	D	254	ALA	10.6
1	C	431	ASP	10.4
1	C	317	VAL	10.3
1	D	295	GLU	10.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	ARG	10.2
1	C	289	ILE	10.1
1	C	397	GLY	10.0
1	C	252	PHE	10.0
1	B	370	VAL	9.9
1	D	259	LEU	9.8
1	C	250	LYS	9.7
1	C	369	GLY	9.6
1	C	281	CYS	9.6
1	C	410	ALA	9.5
1	C	442	VAL	9.5
1	D	258	LEU	9.5
1	D	483	GLN	9.4
1	A	205	SER	9.3
1	C	393	PRO	9.3
1	C	355	VAL	9.3
1	D	324	LEU	9.3
1	D	368	ARG	9.2
1	D	346	ALA	9.2
1	D	400	SER	9.2
1	C	473	ALA	9.2
1	D	396	TYR	9.1
1	D	365	THR	9.1
1	C	291	CYS	9.1
1	C	262	TYR	9.0
1	D	436	GLN	9.0
1	A	369	GLY	9.0
1	B	463	ARG	9.0
1	C	257	LEU	9.0
1	C	299	ASN	9.0
1	D	490	ASP	9.0
1	C	253	THR	8.9
1	C	341	THR	8.9
1	D	264	GLN	8.9
1	C	260	ARG	8.8
1	D	449	ASN	8.8
1	C	546	THR	8.8
1	C	472	GLU	8.8
1	C	432	VAL	8.8
1	D	395	THR	8.8
1	C	259	LEU	8.7
1	A	397	GLY	8.7

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Mol	Chain	Res	Type	RSRZ
1	B	232	GLY	8.7
1	C	448	PHE	8.7
1	D	364	ASP	8.7
1	C	392	ASN	8.7
1	C	494	ARG	8.6
1	C	545	THR	8.6
1	D	357	LYS	8.5
1	B	296	GLY	8.5
1	A	557	LEU	8.5
1	D	249	GLY	8.5
1	D	255	LYS	8.4
1	C	308	VAL	8.3
1	C	422	GLU	8.3
1	C	476	LEU	8.3
1	C	531	LYS	8.3
1	B	225	LEU	8.2
1	C	504	VAL	8.2
1	D	335	LEU	8.1
1	C	440	ASP	8.1
1	D	430	PHE	8.1
1	D	411	ASP	8.1
1	C	547	LEU	8.1
1	D	265	GLY	8.1
1	D	262	TYR	8.0
1	D	369	GLY	8.0
1	B	560	ASN	8.0
1	C	520	TYR	8.0
1	A	366	ASP	8.0
1	C	272	ASP	8.0
1	C	395	THR	7.9
1	C	466	THR	7.9
1	D	481	THR	7.9
1	D	501	SER	7.9
1	D	351	ALA	7.9
1	D	260	ARG	7.8
1	D	339	ASP	7.8
1	D	342	ASP	7.8
1	C	503	ILE	7.8
1	C	549	ASN	7.8
1	C	273	PRO	7.7
1	D	406	ALA	7.7
1	D	322	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
1	D	370	VAL	7.7
1	D	382	TYR	7.7
1	D	253	THR	7.6
1	C	251	SER	7.6
1	D	251	SER	7.6
1	C	390	GLU	7.6
1	D	328	THR	7.6
1	A	510	ILE	7.6
1	D	460	ARG	7.6
1	B	555	HIS	7.5
1	C	450	VAL	7.5
1	B	553	ALA	7.4
1	D	403	LEU	7.4
1	C	425	SER	7.4
1	D	484	ALA	7.4
1	D	500	GLY	7.4
1	B	585	GLU	7.4
1	B	565	GLU	7.4
1	C	452	SER	7.4
1	D	504	VAL	7.3
1	D	334	SER	7.3
1	C	427	PHE	7.3
1	A	358	GLU	7.3
1	C	404	LYS	7.3
1	C	411	ASP	7.3
1	C	424	ASP	7.3
1	C	296	GLY	7.3
1	D	366	ASP	7.2
1	D	329	LEU	7.2
1	D	389	ALA	7.2
1	C	240	TRP	7.2
1	B	308	VAL	7.1
1	B	549	ASN	7.1
1	D	252	PHE	7.1
1	A	412	SER	7.1
1	D	354	GLU	7.1
1	D	269	ILE	7.1
1	C	293	GLY	7.1
1	D	471	ASP	7.1
1	D	491	THR	7.1
1	C	279	GLU	7.0
1	C	292	THR	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	219	ARG	7.0
1	C	499	ASN	7.0
1	D	393	PRO	6.9
1	A	437	ASN	6.9
1	C	426	ASP	6.9
1	D	443	LYS	6.9
1	C	270	ILE	6.9
1	B	317	VAL	6.9
1	A	367	PRO	6.9
1	D	444	ARG	6.9
1	C	544	ILE	6.8
1	C	402	LEU	6.8
1	B	443	LYS	6.8
1	D	407	ALA	6.8
1	D	290	ASN	6.8
1	D	272	ASP	6.8
1	C	480	GLN	6.8
1	C	429	VAL	6.8
1	C	399	LEU	6.8
1	A	343	THR	6.8
1	C	489	ARG	6.7
1	C	428	ILE	6.7
1	D	433	HIS	6.7
1	D	381	LEU	6.7
1	A	587	GLN	6.7
1	D	404	LYS	6.7
1	D	416	ALA	6.7
1	B	556	ASP	6.7
1	D	341	THR	6.6
1	C	329	LEU	6.6
1	C	337	LEU	6.6
1	B	204	ALA	6.6
1	A	338	ARG	6.6
1	C	443	LYS	6.6
1	D	378	VAL	6.6
1	A	339	ASP	6.5
1	C	420	ALA	6.5
1	D	270	ILE	6.5
1	D	495	ILE	6.5
1	D	294	GLY	6.5
1	A	220	ASP	6.5
1	C	518	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	583	PRO	6.5
1	D	289	ILE	6.5
1	B	584	TYR	6.4
1	B	249	GLY	6.4
1	C	516	GLU	6.4
1	D	349	GLU	6.4
1	A	395	THR	6.4
1	D	434	ASP	6.4
1	C	368	ARG	6.4
1	C	486	ALA	6.4
1	D	502	LEU	6.3
1	B	564	GLY	6.3
1	B	437	ASN	6.3
1	D	291	CYS	6.3
1	B	305	LEU	6.3
1	A	341	THR	6.3
1	A	584	TYR	6.3
1	B	368	ARG	6.3
1	C	371	PRO	6.3
1	B	581	ALA	6.2
1	B	547	LEU	6.2
1	C	449	ASN	6.2
1	C	274	GLU	6.2
1	C	439	GLU	6.2
1	C	543	ALA	6.2
1	C	255	LYS	6.2
1	C	460	ARG	6.2
1	D	355	VAL	6.2
1	C	370	VAL	6.2
1	B	587	GLN	6.1
1	B	208	ASN	6.1
1	B	371	PRO	6.1
1	A	402	LEU	6.1
1	D	361	ILE	6.1
1	C	477	VAL	6.1
1	C	254	ALA	6.1
1	C	287	VAL	6.1
1	C	459	GLU	6.1
1	B	561	ALA	6.1
1	A	307	PRO	6.0
1	B	217	LYS	6.0
1	C	458	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	348	LEU	6.0
1	A	553	ALA	6.0
1	D	459	GLU	6.0
1	B	559	VAL	6.0
1	B	550	LEU	6.0
1	C	505	ILE	5.9
1	A	559	VAL	5.9
1	B	540	ASP	5.9
1	A	546	THR	5.9
1	C	382	TYR	5.9
1	D	413	TYR	5.9
1	A	517	VAL	5.9
1	C	500	GLY	5.9
1	C	430	PHE	5.9
1	D	292	THR	5.9
1	D	374	LYS	5.9
1	B	226	VAL	5.8
1	A	365	THR	5.8
1	C	417	GLY	5.8
1	D	371	PRO	5.8
1	A	393	PRO	5.8
1	B	579	ILE	5.8
1	A	461	ASP	5.7
1	A	344	GLU	5.7
1	A	370	VAL	5.7
1	C	408	GLU	5.7
1	C	530	TYR	5.7
1	C	434	ASP	5.7
1	D	380	GLU	5.7
1	B	224	VAL	5.7
1	A	496	ARG	5.7
1	C	372	ASN	5.7
1	A	362	THR	5.7
1	D	271	ILE	5.7
1	A	368	ARG	5.7
1	A	462	ARG	5.7
1	C	497	LYS	5.6
1	B	210	GLY	5.6
1	D	325	HIS	5.6
1	A	223	LEU	5.6
1	A	244	ALA	5.6
1	C	481	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	261	GLU	5.6
1	D	442	VAL	5.6
1	D	358	GLU	5.6
1	D	468	LEU	5.6
1	B	304	ARG	5.5
1	C	306	ARG	5.5
1	B	220	ASP	5.5
1	C	264	GLN	5.5
1	D	414	LEU	5.5
1	C	469	VAL	5.5
1	A	423	ALA	5.5
1	D	506	SER	5.5
1	C	441	GLN	5.5
1	A	305	LEU	5.5
1	B	223	LEU	5.5
1	C	383	GLU	5.5
1	C	347	ALA	5.5
1	C	484	ALA	5.5
1	D	410	ALA	5.5
1	B	318	PHE	5.5
1	C	318	PHE	5.5
1	D	332	PHE	5.5
1	B	209	ASP	5.4
1	A	564	GLY	5.4
1	C	396	TYR	5.4
1	C	322	LEU	5.4
1	D	257	LEU	5.4
1	C	412	SER	5.4
1	D	319	GLN	5.4
1	C	445	ALA	5.4
1	D	385	CYS	5.4
1	A	382	TYR	5.4
1	B	481	THR	5.4
1	A	285	GLY	5.4
1	C	532	LEU	5.4
1	A	549	ASN	5.4
1	A	560	ASN	5.4
1	C	455	TRP	5.4
1	A	582	ALA	5.3
1	C	271	ILE	5.3
1	B	480[A]	GLN	5.3
1	B	563	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	450	VAL	5.3
1	B	369	GLY	5.3
1	C	377	THR	5.3
1	D	333	PHE	5.3
1	B	460	ARG	5.3
1	C	356	TYR	5.3
1	B	386	VAL	5.3
1	B	229	TRP	5.3
1	D	250	LYS	5.3
1	C	241	THR	5.3
1	B	205	SER	5.3
1	A	579	ILE	5.3
1	C	301	LEU	5.3
1	C	338	ARG	5.3
1	A	539	LYS	5.2
1	A	551	SER	5.2
1	C	350	ASP	5.2
1	B	319	GLN	5.2
1	A	554	GLU	5.2
1	B	363	TRP	5.2
1	D	451	LEU	5.2
1	D	318	PHE	5.2
1	B	580	GLU	5.2
1	A	221	GLY	5.2
1	B	462	ARG	5.2
1	B	575	ILE	5.2
1	B	546	THR	5.2
1	A	248	ALA	5.2
1	C	277	TYR	5.2
1	A	556	ASP	5.1
1	C	423	ALA	5.1
1	D	327	GLN	5.1
1	C	321	PRO	5.1
1	B	402	LEU	5.1
1	B	461	ASP	5.1
1	C	502	LEU	5.1
1	D	352	LEU	5.1
1	C	529	THR	5.1
1	C	421	VAL	5.1
1	A	306	ARG	5.1
1	C	275	ARG	5.1
1	C	374	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	206	GLY	5.1
1	C	307	PRO	5.0
1	D	492	SER	5.0
1	B	230	LYS	5.0
1	C	483	GLN	5.0
1	D	360	GLY	5.0
1	C	386	VAL	5.0
1	D	472	GLU	5.0
1	C	359	ALA	5.0
1	A	403	LEU	5.0
1	C	373	ASP	5.0
1	B	392	ASN	5.0
1	B	562	LYS	5.0
1	B	367	PRO	4.9
1	D	405	ARG	4.9
1	A	391	GLU	4.9
1	A	422	GLU	4.9
1	A	585	GLU	4.9
1	A	420	ALA	4.9
1	C	324	LEU	4.9
1	A	252	PHE	4.9
1	C	491	THR	4.9
1	C	340	LEU	4.9
1	C	385	CYS	4.9
1	C	446	GLN	4.9
1	D	390	GLU	4.9
1	A	550	LEU	4.9
1	B	511	ASP	4.9
1	A	552	GLU	4.8
1	C	519	ARG	4.8
1	D	489	ARG	4.8
1	B	552	GLU	4.8
1	B	353	VAL	4.8
1	D	456	ASN	4.8
1	A	218	ASP	4.8
1	A	349	GLU	4.8
1	B	576	HIS	4.8
1	D	363	TRP	4.8
1	B	436	GLN	4.8
1	B	373	ASP	4.8
1	C	487	PHE	4.7
1	D	447	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	211	SER	4.7
1	B	393	PRO	4.7
1	C	288	TRP	4.7
1	A	580	GLU	4.7
1	B	366	ASP	4.7
1	C	498	TYR	4.7
1	B	473	ALA	4.7
1	D	347	ALA	4.7
1	C	378	VAL	4.7
1	A	575	ILE	4.7
1	B	302	GLN	4.7
1	C	415	TRP	4.7
1	A	324	LEU	4.7
1	A	498	TYR	4.7
1	B	377	THR	4.6
1	B	567	LEU	4.6
1	C	242	ILE	4.6
1	D	394	GLU	4.6
1	B	499	ASN	4.6
1	C	413	TYR	4.6
1	C	294	GLY	4.6
1	B	364	ASP	4.6
1	B	570	ALA	4.6
1	D	398	ARG	4.6
1	C	517	VAL	4.6
1	B	216	GLY	4.6
1	C	276	GLU	4.6
1	A	563	ARG	4.6
1	D	445	ALA	4.6
1	C	353	VAL	4.6
1	D	303	VAL	4.6
1	C	349	GLU	4.5
1	B	578	LYS	4.5
1	D	448	PHE	4.5
1	C	330	ARG	4.5
1	A	392	ASN	4.5
1	C	362	THR	4.5
1	B	421	VAL	4.5
1	A	574	ARG	4.5
1	A	264	GLN	4.5
1	B	557	LEU	4.5
1	C	332	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	375	TRP	4.5
1	A	222	GLY	4.5
1	B	577	ILE	4.5
1	D	384	TYR	4.5
1	B	574	ARG	4.5
1	B	476	LEU	4.5
1	D	320	SER	4.5
1	A	421	VAL	4.4
1	C	409	GLY	4.4
1	B	558	LEU	4.4
1	A	538[A]	GLU	4.4
1	B	321	PRO	4.4
1	D	467	VAL	4.4
1	D	470	VAL	4.4
1	B	215	LEU	4.4
1	C	468	LEU	4.4
1	A	342	ASP	4.4
1	A	481	THR	4.4
1	C	380	GLU	4.4
1	B	497	LYS	4.4
1	C	388	LYS	4.4
1	A	521	GLY	4.4
1	A	361	ILE	4.4
1	B	213	ILE	4.4
1	C	278	LYS	4.4
1	C	298	ILE	4.4
1	C	470	VAL	4.4
1	A	567	LEU	4.4
1	C	331	THR	4.3
1	D	343	THR	4.3
1	B	307	PRO	4.3
1	D	293	GLY	4.3
1	B	518	GLN	4.3
1	A	377	THR	4.3
1	A	398	ARG	4.3
1	B	320	SER	4.3
1	B	278	LYS	4.3
1	C	451	LEU	4.3
1	B	490	ASP	4.3
1	B	498	TYR	4.3
1	B	551	SER	4.3
1	D	487	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	394	GLU	4.3
1	B	538	GLU	4.3
1	A	262	TYR	4.3
1	B	474	TRP	4.3
1	C	492	SER	4.3
1	D	367	PRO	4.3
1	D	446	GLN	4.3
1	D	386	VAL	4.3
1	B	262	TYR	4.2
1	A	347	ALA	4.2
1	A	537	GLY	4.2
1	A	513	LEU	4.2
1	C	290	ASN	4.2
1	D	326	ILE	4.2
1	A	353	VAL	4.2
1	B	541	LEU	4.2
1	B	441	GLN	4.2
1	C	387	LYS	4.2
1	D	418	PRO	4.2
1	B	521	GLY	4.2
1	A	276	GLU	4.2
1	A	394	GLU	4.2
1	B	252	PHE	4.2
1	A	337	LEU	4.2
1	A	518	GLN	4.2
1	D	441	GLN	4.2
1	A	479	PRO	4.2
1	B	447	TYR	4.1
1	D	375	TRP	4.1
1	C	467	VAL	4.1
1	A	374	LYS	4.1
1	C	379	LYS	4.1
1	A	424	ASP	4.1
1	C	453	PHE	4.1
1	B	240	TRP	4.1
1	C	495	ILE	4.1
1	A	331	THR	4.1
1	B	438	ALA	4.1
1	B	283	LYS	4.1
1	B	214	VAL	4.1
1	C	398	ARG	4.1
1	A	390	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	486	ALA	4.1
1	A	340	LEU	4.1
1	A	401	VAL	4.1
1	A	504	VAL	4.1
1	B	287	VAL	4.1
1	B	517	VAL	4.1
1	B	358	GLU	4.1
1	A	376	PRO	4.1
1	A	507	GLN	4.0
1	A	439	GLU	4.0
1	A	520	TYR	4.0
1	D	336	TYR	4.0
1	B	424	ASP	4.0
1	C	471	ASP	4.0
1	A	578	LYS	4.0
1	A	460	ARG	4.0
1	B	389	ALA	4.0
1	B	535	ALA	4.0
1	C	323	ALA	4.0
1	A	435	LEU	4.0
1	C	403	LEU	4.0
1	C	457	ILE	4.0
1	D	401	VAL	4.0
1	C	364	ASP	4.0
1	A	253	THR	4.0
1	B	537	GLY	4.0
1	C	400	SER	4.0
1	D	496	ARG	4.0
1	D	408	GLU	4.0
1	A	357	LYS	3.9
1	C	493	LYS	3.9
1	D	469	VAL	3.9
1	B	327	GLN	3.9
1	B	420	ALA	3.9
1	B	542	GLU	3.9
1	B	388	LYS	3.9
1	B	404	LYS	3.9
1	D	503	ILE	3.9
1	A	588	TYR	3.9
1	A	282	ARG	3.9
1	D	391	GLU	3.9
1	B	339	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	545	THR	3.9
1	A	322	LEU	3.9
1	C	482	PRO	3.9
1	A	210	GLY	3.9
1	A	385	CYS	3.9
1	B	391	GLU	3.9
1	A	259	LEU	3.8
1	B	525	LEU	3.8
1	B	496	ARG	3.8
1	C	319	GLN	3.8
1	B	234	ASP	3.8
1	B	360	GLY	3.8
1	B	379	LYS	3.8
1	A	350	ASP	3.8
1	D	353	VAL	3.8
1	C	384	TYR	3.8
1	C	406	ALA	3.8
1	D	454	ALA	3.8
1	B	513	LEU	3.8
1	B	290	ASN	3.8
1	B	440	ASP	3.8
1	C	295	GLU	3.8
1	B	236	THR	3.8
1	B	544	ILE	3.8
1	D	409	GLY	3.8
1	A	463	ARG	3.7
1	B	356	TYR	3.7
1	B	374	LYS	3.7
1	A	229	TRP	3.7
1	A	442	VAL	3.7
1	D	338	ARG	3.7
1	B	543	ALA	3.7
1	C	416	ALA	3.7
1	B	340	LEU	3.7
1	A	433	HIS	3.7
1	D	457	ILE	3.7
1	A	572	THR	3.7
1	B	362	THR	3.7
1	D	331	THR	3.7
1	B	211	SER	3.7
1	D	412	SER	3.7
1	A	562	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	458	LEU	3.7
1	B	289	ILE	3.7
1	A	235	ARG	3.7
1	A	480	GLN	3.7
1	B	507	GLN	3.7
1	A	371	PRO	3.7
1	A	476	LEU	3.7
1	C	381	LEU	3.7
1	A	373	ASP	3.7
1	A	419	THR	3.6
1	D	415	TRP	3.6
1	B	504	VAL	3.6
1	B	264	GLN	3.6
1	B	255	LYS	3.6
1	A	533	LEU	3.6
1	B	487	PHE	3.6
1	C	485	ILE	3.6
1	A	483	GLN	3.6
1	C	238	SER	3.6
1	C	346	ALA	3.6
1	D	435	LEU	3.6
1	B	398	ARG	3.6
1	C	336	TYR	3.6
1	B	207	ILE	3.6
1	D	383	GLU	3.6
1	C	335	LEU	3.6
1	A	278	LYS	3.6
1	D	493	LYS	3.6
1	C	327	GLN	3.6
1	B	452	SER	3.6
1	C	405	ARG	3.6
1	C	348	LEU	3.6
1	A	484	ALA	3.6
1	A	387	LYS	3.5
1	B	456	ASN	3.5
1	A	319	GLN	3.5
1	B	384	TYR	3.5
1	D	350	ASP	3.5
1	B	361	ILE	3.5
1	B	341	THR	3.5
1	D	362	THR	3.5
1	D	432	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	400	SER	3.5
1	A	455	TRP	3.5
1	B	206	GLY	3.5
1	A	511	ASP	3.5
1	A	384	TYR	3.5
1	B	383	GLU	3.5
1	C	419	THR	3.5
1	B	492	SER	3.5
1	C	418	PRO	3.5
1	A	399	LEU	3.5
1	C	302	GLN	3.5
1	B	417	GLY	3.5
1	B	231	ARG	3.5
1	A	251	SER	3.5
1	C	501	SER	3.5
1	A	225	LEU	3.5
1	B	284	LEU	3.5
1	A	449	ASN	3.5
1	A	561	ALA	3.5
1	A	565	GLU	3.5
1	A	413	TYR	3.5
1	B	534	LEU	3.4
1	A	233	GLY	3.4
1	A	555	HIS	3.4
1	B	472	GLU	3.4
1	C	304	ARG	3.4
1	C	328	THR	3.4
1	D	377	THR	3.4
1	D	399	LEU	3.4
1	B	338	ARG	3.4
1	B	390	GLU	3.4
1	C	297	LYS	3.4
1	A	509	VAL	3.4
1	C	367	PRO	3.4
1	B	335	LEU	3.4
1	A	581	ALA	3.4
1	B	554	GLU	3.4
1	C	366	ASP	3.4
1	B	375	TRP	3.4
1	B	457	ILE	3.4
1	B	453	PHE	3.4
1	B	583	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	300	PRO	3.4
1	A	249	GLY	3.4
1	B	351	ALA	3.4
1	B	428	ILE	3.3
1	B	573	GLN	3.3
1	A	386	VAL	3.3
1	B	238	SER	3.3
1	A	208	ASN	3.3
1	B	299	ASN	3.3
1	C	456	ASN	3.3
1	B	491	THR	3.3
1	C	376	PRO	3.3
1	B	266	SER	3.3
1	A	345	LYS	3.3
1	B	297	LYS	3.3
1	A	523	ALA	3.3
1	A	363	TRP	3.3
1	B	235	ARG	3.3
1	D	376	PRO	3.3
1	B	344	GLU	3.3
1	B	442	VAL	3.3
1	B	301	LEU	3.3
1	B	382	TYR	3.3
1	D	392	ASN	3.3
1	B	253	THR	3.3
1	C	283	LYS	3.3
1	D	344	GLU	3.3
1	A	360	GLY	3.3
1	B	582	ALA	3.3
1	A	334	SER	3.2
1	D	452	SER	3.2
1	A	573	GLN	3.2
1	C	454	ALA	3.2
1	D	330	ARG	3.2
1	A	269	ILE	3.2
1	A	545	THR	3.2
1	C	343	THR	3.2
1	D	482	PRO	3.2
1	A	333	PHE	3.2
1	A	304	ARG	3.2
1	B	218	ASP	3.2
1	C	339	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	LYS	3.2
1	B	365	THR	3.2
1	A	547	LEU	3.2
1	C	305	LEU	3.2
1	A	474	TRP	3.2
1	B	493	LYS	3.2
1	A	459	GLU	3.2
1	A	528	PRO	3.2
1	A	284	LEU	3.2
1	B	455	TRP	3.1
1	C	447	TYR	3.1
1	B	503	ILE	3.1
1	A	372	ASN	3.1
1	A	497	LYS	3.1
1	D	356	TYR	3.1
1	B	528	PRO	3.1
1	B	419	THR	3.1
1	C	365	THR	3.1
1	B	242	ILE	3.1
1	B	324	LEU	3.1
1	C	414	LEU	3.1
1	D	301	LEU	3.1
1	B	527	ASN	3.1
1	A	287	VAL	3.1
1	B	459	GLU	3.1
1	A	336	TYR	3.1
1	A	396	TYR	3.1
1	A	289	ILE	3.1
1	A	506	SER	3.1
1	B	222	GLY	3.1
1	D	337	LEU	3.1
1	D	431	ASP	3.1
1	B	495	ILE	3.0
1	A	566	GLY	3.0
1	B	285	GLY	3.0
1	A	320	SER	3.0
1	D	473	ALA	3.0
1	A	379	LYS	3.0
1	C	352	LEU	3.0
1	B	380	GLU	3.0
1	A	443	LYS	3.0
1	B	482	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	572	THR	3.0
1	A	329	LEU	3.0
1	C	488	LEU	3.0
1	A	453	PHE	3.0
1	B	526	ASP	3.0
1	A	326	ILE	3.0
1	B	566	GLY	3.0
1	A	330	ARG	3.0
1	B	282	ARG	3.0
1	C	351	ALA	3.0
1	A	325	HIS	2.9
1	A	576	HIS	2.9
1	B	228	ILE	2.9
1	C	344	GLU	2.9
1	A	352	LEU	2.9
1	C	360	GLY	2.9
1	B	306	ARG	2.9
1	B	387	LYS	2.9
1	D	359	ALA	2.9
1	A	485	ILE	2.9
1	A	231	ARG	2.9
1	B	506	SER	2.9
1	A	434	ASP	2.9
1	A	490	ASP	2.9
1	C	342	ASP	2.9
1	A	416	ALA	2.9
1	A	417	GLY	2.9
1	A	213	ILE	2.9
1	C	282	ARG	2.9
1	B	303	VAL	2.9
1	C	303	VAL	2.9
1	B	359	ALA	2.9
1	A	279	GLU	2.9
1	A	335	LEU	2.9
1	B	533	LEU	2.9
1	A	375	TRP	2.8
1	A	209	ASP	2.8
1	A	364	ASP	2.8
1	A	355	VAL	2.8
1	B	429	VAL	2.8
1	B	465	ARG	2.8
1	A	300	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	300	PRO	2.8
1	C	300	PRO	2.8
1	B	444	ARG	2.8
1	A	293	GLY	2.8
1	B	221	GLY	2.8
1	A	257	LEU	2.8
1	B	524	LEU	2.8
1	A	527	ASN	2.8
1	D	302	GLN	2.8
1	A	482	PRO	2.8
1	B	349	GLU	2.8
1	A	444	ARG	2.8
1	B	260	ARG	2.8
1	B	405	ARG	2.8
1	B	426	ASP	2.8
1	B	268	VAL	2.8
1	B	244	ALA	2.8
1	D	486	ALA	2.8
1	C	361	ILE	2.7
1	A	519	ARG	2.7
1	C	358	GLU	2.7
1	C	391	GLU	2.7
1	B	410	ALA	2.7
1	A	327	GLN	2.7
1	B	286	GLY	2.7
1	A	458	LEU	2.7
1	B	352	LEU	2.7
1	A	356	TYR	2.7
1	A	323	ALA	2.7
1	A	514	ALA	2.7
1	A	265	GLY	2.7
1	B	233	GLY	2.7
1	A	281	CYS	2.7
1	A	328	THR	2.7
1	A	388	LYS	2.7
1	D	388	LYS	2.7
1	A	267	ARG	2.7
1	A	464	GLU	2.7
1	A	495	ILE	2.7
1	B	251	SER	2.7
1	A	234	ASP	2.7
1	A	530	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	389	ALA	2.7
1	A	542	GLU	2.7
1	A	428	ILE	2.7
1	A	515	PRO	2.7
1	B	431	ASP	2.7
1	A	277	TYR	2.7
1	B	514	ALA	2.7
1	A	212	GLY	2.6
1	A	380	GLU	2.6
1	A	207	ILE	2.6
1	B	425	SER	2.6
1	B	536	GLN	2.6
1	A	477	VAL	2.6
1	B	450	VAL	2.6
1	B	277	TYR	2.6
1	A	502	LEU	2.6
1	B	322	LEU	2.6
1	B	502	LEU	2.6
1	A	400	SER	2.6
1	B	416	ALA	2.6
1	B	423	ALA	2.6
1	A	447	TYR	2.6
1	A	348	LEU	2.6
1	B	395	THR	2.6
1	D	488	LEU	2.6
1	D	321	PRO	2.6
1	B	522	GLN	2.6
1	C	444	ARG	2.6
1	A	232	GLY	2.6
1	A	541	LEU	2.6
1	B	273	PRO	2.6
1	C	334	SER	2.6
1	A	286	GLY	2.5
1	A	448	PHE	2.5
1	B	212	GLY	2.5
1	B	294	GLY	2.5
1	A	558	LEU	2.5
1	B	257	LEU	2.5
1	B	458	LEU	2.5
1	D	299	ASN	2.5
1	A	536	GLN	2.5
1	A	544	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	266	SER	2.5
1	C	496	ARG	2.5
1	A	407	ALA	2.5
1	B	401	VAL	2.5
1	C	333	PHE	2.5
1	D	340	LEU	2.5
1	A	465	ARG	2.5
1	B	269	ILE	2.5
1	B	501	SER	2.5
1	B	488	LEU	2.5
1	D	379	LYS	2.5
1	B	508	ASN	2.5
1	B	326	ILE	2.5
1	A	238	SER	2.5
1	A	440	ASP	2.5
1	A	354	GLU	2.5
1	A	240	TRP	2.5
1	B	409	GLY	2.5
1	C	357	LYS	2.5
1	B	454	ALA	2.5
1	B	337	LEU	2.5
1	B	399	LEU	2.5
1	A	577	ILE	2.4
1	A	478	ASP	2.4
1	A	283	LYS	2.4
1	A	346	ALA	2.4
1	A	321	PRO	2.4
1	B	298	ILE	2.4
1	B	510	ILE	2.4
1	B	516	GLU	2.4
1	B	539	LYS	2.4
1	A	441	GLN	2.4
1	D	402	LEU	2.4
1	B	485	ILE	2.4
1	A	525	LEU	2.4
1	A	226	VAL	2.4
1	A	512	PHE	2.4
1	B	288	TRP	2.4
1	B	333	PHE	2.4
1	B	372	ASN	2.4
1	B	568	PHE	2.4
1	A	529	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	354	GLU	2.4
1	A	526	ASP	2.4
1	B	396	TYR	2.4
1	A	489	ARG	2.4
1	A	569	VAL	2.3
1	A	534	LEU	2.3
1	B	239	ASN	2.3
1	B	435	LEU	2.3
1	B	261	GLU	2.3
1	B	281	CYS	2.3
1	B	291	CYS	2.3
1	A	430	PHE	2.3
1	B	415	TRP	2.3
1	A	414	LEU	2.3
1	A	214	VAL	2.3
1	A	332	PHE	2.3
1	B	267	ARG	2.3
1	B	381	LEU	2.3
1	A	224	VAL	2.3
1	A	246	PRO	2.3
1	B	331	THR	2.3
1	B	512	PHE	2.3
1	C	363	TRP	2.3
1	A	271	ILE	2.3
1	C	239	ASN	2.2
1	A	245	LYS	2.2
1	A	381	LEU	2.2
1	B	414	LEU	2.2
1	B	520	TYR	2.2
1	A	405	ARG	2.2
1	A	487	PHE	2.2
1	B	427	PHE	2.2
1	B	345	LYS	2.2
1	B	422	GLU	2.2
1	A	290	ASN	2.2
1	B	348	LEU	2.2
1	B	515	PRO	2.2
1	B	292	THR	2.2
1	A	302	GLN	2.2
1	A	274	GLU	2.2
1	A	516	GLU	2.2
1	A	301	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	530	TYR	2.2
1	A	522	GLN	2.2
1	B	434	ASP	2.2
1	A	247	GLY	2.1
1	C	345	LYS	2.1
1	A	268	VAL	2.1
1	A	426	ASP	2.1
1	B	350	ASP	2.1
1	B	354	GLU	2.1
1	B	433	HIS	2.1
1	B	245	LYS	2.1
1	D	387	LYS	2.1
1	B	484	ALA	2.1
1	B	227	ASP	2.1
1	A	216	GLY	2.1
1	C	320	SER	2.1
1	D	485	ILE	2.1
1	B	259	LEU	2.1
1	A	452	SER	2.1
1	D	345	LYS	2.1
1	A	491	THR	2.1
1	B	523	ALA	2.1
1	A	303	VAL	2.0
1	B	477	VAL	2.0
1	B	411	ASP	2.0
1	A	493	LYS	2.0
1	B	270	ILE	2.0
1	B	274	GLU	2.0
1	B	279	GLU	2.0
1	B	489	ARG	2.0
1	B	355	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	1591	5/5	0.34	0.29	118,118,119,121	0
2	SO4	B	1590	5/5	0.36	0.23	102,103,104,105	0
2	SO4	B	1592	5/5	0.38	0.45	122,123,125,126	0
2	SO4	A	1591	5/5	0.65	0.35	123,123,124,125	0
2	SO4	A	1590	5/5	0.81	0.29	80,80,83,88	0
2	SO4	A	1589	5/5	0.84	0.27	37,38,42,48	0
2	SO4	C	1588	5/5	0.85	0.19	107,108,110,111	0
2	SO4	B	1589	5/5	0.87	0.19	83,84,89,92	0
2	SO4	B	1588	5/5	0.95	0.12	37,37,46,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.