Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2024 – 02:52 PM EST

PDB ID	:	1DQV
Title	:	CRYSTAL STRUCTURE OF SYNAPTOTAGMIN III C2A/C2B
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Deposited on	:	2000-01-05
Resolution	:	3.20 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:

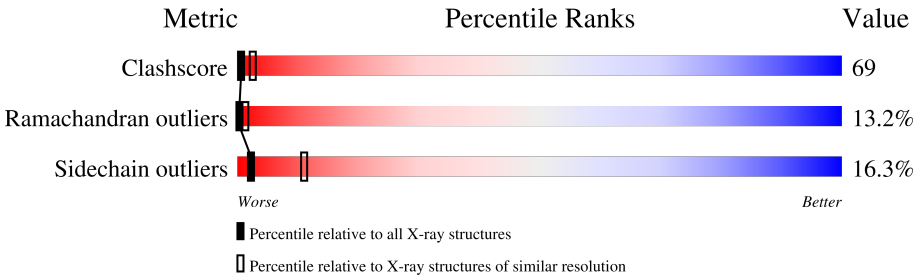
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	296	24% 52% 15% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2195 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.

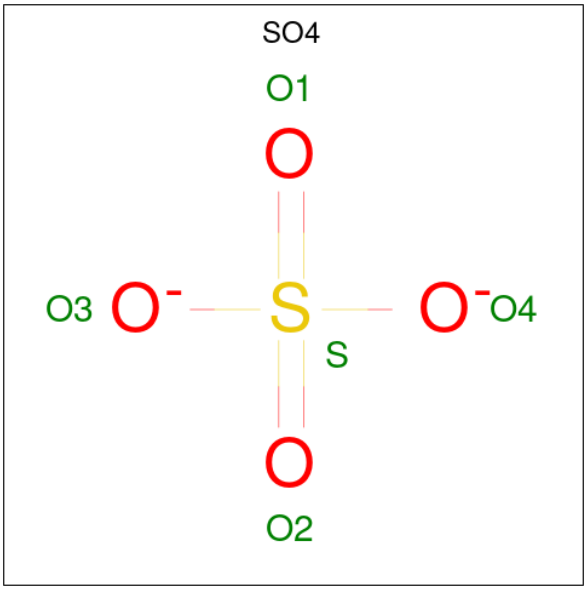
- Molecule 1 is a protein called SYNAPTOTAGMIN III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2186	1399	381	400	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mg	0	0
			4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

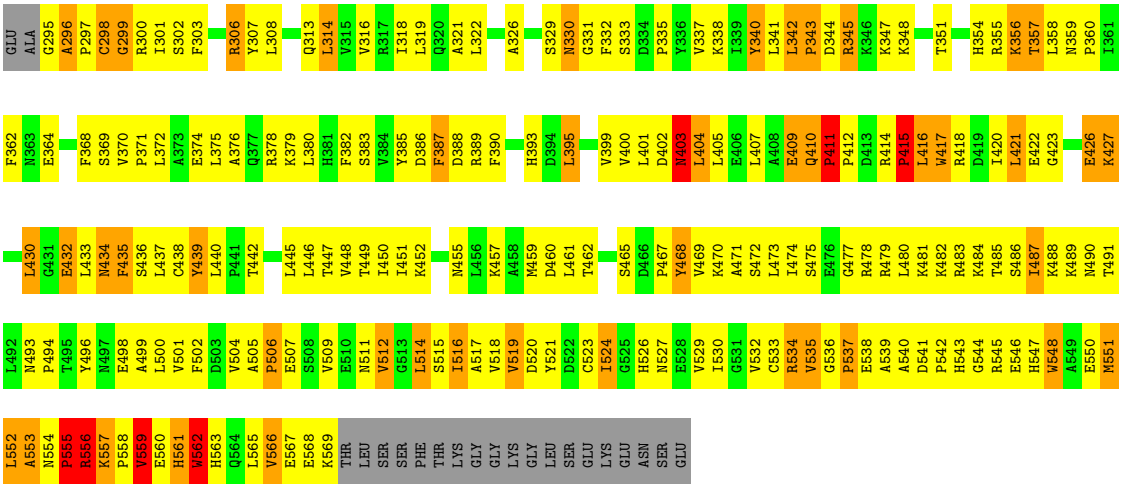
3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: SYNAPTOTAGMIN III

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	125.96Å 125.96Å 118.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	94.3 (50.00-3.20)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.293 , 0.348	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2195	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.43	0/2237	0.74	2/3034 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	559	VAL	N-CA-C	-5.64	95.76	111.00
1	A	386	ASP	N-CA-C	-5.07	97.30	111.00

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	2186	0	2197	301	1
2	A	4	0	0	0	0
3	A	5	0	0	0	0
All	All	2195	0	2197	301	1

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 69.

All (301) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PRO:HG2	1:A:378:ARG:HD2	1.30	1.13
1:A:557:LYS:HB3	1:A:558:PRO:HD3	1.28	1.12
1:A:439:TYR:HB2	1:A:446:LEU:HA	1.25	1.12
1:A:479:ARG:HD2	1:A:482:LYS:HE3	1.39	1.04
1:A:439:TYR:HB3	1:A:551:MET:HE1	1.39	1.02
1:A:371:PRO:HB2	1:A:374:GLU:HB2	1.45	0.98
1:A:382:PHE:HB2	1:A:399:VAL:HG22	1.47	0.95
1:A:548:TRP:O	1:A:551:MET:HB3	1.69	0.93
1:A:342:LEU:HD13	1:A:379:LYS:HD3	1.51	0.92
1:A:516:ILE:HG13	1:A:533:CYS:SG	2.09	0.92
1:A:411:PRO:HD2	1:A:414:ARG:HB2	1.54	0.88
1:A:557:LYS:HB3	1:A:558:PRO:CD	2.04	0.87
1:A:375:LEU:HD22	1:A:404:LEU:HD22	1.56	0.86
1:A:437:LEU:O	1:A:559:VAL:HG21	1.77	0.84
1:A:437:LEU:HD23	1:A:547:HIS:HE1	1.41	0.84
1:A:438:CYS:SG	1:A:556:ARG:HA	2.18	0.84
1:A:471:ALA:HB3	1:A:483:ARG:HB3	1.60	0.83
1:A:558:PRO:O	1:A:559:VAL:HG22	1.79	0.83
1:A:434:ASN:HB2	1:A:562:TRP:HE3	1.43	0.83
1:A:553:ALA:O	1:A:555:PRO:HD3	1.79	0.82
1:A:474:ILE:HD11	1:A:537:PRO:HD2	1.59	0.82
1:A:517:ALA:CB	1:A:532:VAL:HG12	2.09	0.81
1:A:298:CYS:HB2	1:A:420:ILE:HG22	1.61	0.81
1:A:332:PHE:HD1	1:A:356:LYS:HB3	1.46	0.80
1:A:440:LEU:HD21	1:A:555:PRO:HB3	1.64	0.80
1:A:450:ILE:HD11	1:A:500:LEU:HD11	1.65	0.79
1:A:534:ARG:NH2	1:A:541:ASP:HB2	1.98	0.79
1:A:303:PHE:CZ	1:A:401:LEU:HD21	2.18	0.78
1:A:306:ARG:HH12	1:A:412:PRO:HG3	1.46	0.78
1:A:512:VAL:O	1:A:536:GLY:HA2	1.85	0.77
1:A:552:LEU:O	1:A:554:ASN:N	2.17	0.77
1:A:438:CYS:HB2	1:A:556:ARG:HA	1.66	0.76
1:A:512:VAL:O	1:A:537:PRO:HD3	1.86	0.76
1:A:439:TYR:HB2	1:A:446:LEU:CA	2.13	0.75
1:A:470:LYS:HG2	1:A:484:LYS:HG2	1.67	0.75
1:A:556:ARG:O	1:A:558:PRO:HD2	1.85	0.75
1:A:330:ASN:ND2	1:A:332:PHE:H	1.84	0.75
1:A:345:ARG:O	1:A:345:ARG:HD3	1.86	0.75
1:A:544:GLY:O	1:A:547:HIS:HB3	1.85	0.75
1:A:439:TYR:H	1:A:551:MET:HE3	1.51	0.75
1:A:437:LEU:N	1:A:559:VAL:HG21	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASN:HB2	1:A:562:TRP:CE3	2.22	0.74
1:A:440:LEU:CD2	1:A:555:PRO:HB3	2.18	0.73
1:A:306:ARG:NH1	1:A:412:PRO:HG3	2.02	0.73
1:A:470:LYS:O	1:A:516:ILE:HG22	1.88	0.73
1:A:547:HIS:NE2	1:A:559:VAL:O	2.20	0.73
1:A:515:SER:HA	1:A:534:ARG:HA	1.72	0.72
1:A:437:LEU:HB2	1:A:559:VAL:HG11	1.70	0.72
1:A:521:TYR:HA	1:A:527:ASN:OD1	1.89	0.72
1:A:558:PRO:C	1:A:559:VAL:HG22	2.09	0.71
1:A:470:LYS:HD3	1:A:484:LYS:HE2	1.71	0.71
1:A:465:SER:O	1:A:467:PRO:HD3	1.91	0.71
1:A:460:ASP:O	1:A:461:LEU:HB2	1.90	0.71
1:A:479:ARG:HD2	1:A:482:LYS:CE	2.20	0.71
1:A:438:CYS:CB	1:A:556:ARG:HA	2.20	0.70
1:A:504:VAL:HG12	1:A:505:ALA:H	1.57	0.70
1:A:554:ASN:HB3	1:A:556:ARG:HH12	1.56	0.70
1:A:340:TYR:HD2	1:A:348:LYS:HB3	1.56	0.70
1:A:483:ARG:HG3	1:A:500:LEU:HD22	1.72	0.70
1:A:449:THR:HG22	1:A:499:ALA:CB	2.21	0.70
1:A:468:TYR:CE2	1:A:519:VAL:HB	2.26	0.70
1:A:439:TYR:HE2	1:A:509:VAL:HG11	1.57	0.69
1:A:439:TYR:CB	1:A:446:LEU:HA	2.14	0.69
1:A:519:VAL:HG13	1:A:529:VAL:HG22	1.74	0.69
1:A:338:LYS:HE2	1:A:348:LYS:NZ	2.07	0.69
1:A:517:ALA:HB1	1:A:532:VAL:HG12	1.74	0.69
1:A:439:TYR:HB3	1:A:551:MET:CE	2.22	0.68
1:A:535:VAL:O	1:A:548:TRP:HD1	1.76	0.68
1:A:517:ALA:HB2	1:A:532:VAL:HG12	1.76	0.68
1:A:298:CYS:CB	1:A:420:ILE:HG22	2.23	0.68
1:A:437:LEU:HD23	1:A:547:HIS:CE1	2.26	0.68
1:A:307:TYR:OH	1:A:372:LEU:HD23	1.93	0.68
1:A:512:VAL:HB	1:A:537:PRO:HD3	1.74	0.68
1:A:439:TYR:CE2	1:A:509:VAL:HG11	2.28	0.67
1:A:333:SER:O	1:A:335:PRO:HD3	1.95	0.67
1:A:411:PRO:HB2	1:A:412:PRO:CD	2.26	0.66
1:A:389:ARG:HG3	1:A:390:PHE:CE2	2.31	0.66
1:A:296:ALA:H	1:A:297:PRO:HD2	1.60	0.65
1:A:307:TYR:OH	1:A:372:LEU:HA	1.97	0.65
1:A:489:LYS:O	1:A:491:THR:HG22	1.97	0.65
1:A:449:THR:HA	1:A:499:ALA:HA	1.78	0.65
1:A:554:ASN:HB3	1:A:556:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LYS:HE2	1:A:348:LYS:HZ2	1.62	0.65
1:A:298:CYS:O	1:A:299:GLY:O	2.15	0.64
1:A:470:LYS:CD	1:A:484:LYS:HE2	2.27	0.64
1:A:532:VAL:HG22	1:A:567:GLU:O	1.97	0.64
1:A:555:PRO:O	1:A:556:ARG:HB3	1.98	0.63
1:A:434:ASN:HB2	1:A:562:TRP:HB3	1.78	0.63
1:A:298:CYS:HB2	1:A:420:ILE:O	1.99	0.62
1:A:447:THR:CG2	1:A:449:THR:HG23	2.30	0.62
1:A:439:TYR:OH	1:A:506:PRO:HA	2.00	0.61
1:A:301:ILE:HG13	1:A:321:ALA:HB2	1.82	0.61
1:A:512:VAL:HG12	1:A:548:TRP:CD1	2.36	0.61
1:A:434:ASN:CB	1:A:562:TRP:HB3	2.31	0.61
1:A:542:PRO:HA	1:A:545:ARG:HE	1.65	0.61
1:A:451:ILE:HG13	1:A:452:LYS:H	1.66	0.60
1:A:385:TYR:CE2	1:A:395:LEU:HB2	2.36	0.60
1:A:306:ARG:HH11	1:A:306:ARG:HG3	1.67	0.60
1:A:565:LEU:C	1:A:567:GLU:H	2.04	0.60
1:A:483:ARG:CG	1:A:500:LEU:HD22	2.32	0.60
1:A:390:PHE:CD1	1:A:524:ILE:HG21	2.36	0.60
1:A:434:ASN:CG	1:A:451:ILE:HD11	2.22	0.59
1:A:409:GLU:HG2	1:A:410:GLN:HE21	1.66	0.59
1:A:465:SER:C	1:A:467:PRO:HD3	2.22	0.59
1:A:543:HIS:O	1:A:547:HIS:HB2	2.03	0.59
1:A:307:TYR:CZ	1:A:372:LEU:HD23	2.38	0.59
1:A:332:PHE:HA	1:A:358:LEU:HD21	1.85	0.59
1:A:435:PHE:N	1:A:435:PHE:CD2	2.70	0.59
1:A:504:VAL:HG12	1:A:505:ALA:N	2.18	0.59
1:A:468:TYR:HE2	1:A:519:VAL:HB	1.65	0.58
1:A:439:TYR:H	1:A:551:MET:CE	2.14	0.58
1:A:403:ASN:N	1:A:403:ASN:HD22	2.01	0.58
1:A:448:VAL:HB	1:A:500:LEU:HB2	1.86	0.58
1:A:438:CYS:O	1:A:447:THR:HB	2.04	0.58
1:A:460:ASP:O	1:A:461:LEU:CB	2.52	0.58
1:A:535:VAL:O	1:A:548:TRP:CD1	2.57	0.58
1:A:557:LYS:HE2	1:A:558:PRO:HD3	1.86	0.58
1:A:414:ARG:N	1:A:415:PRO:HD3	2.19	0.58
1:A:520:ASP:HB2	1:A:530:ILE:HD11	1.85	0.57
1:A:418:ARG:HH11	1:A:418:ARG:HG2	1.68	0.57
1:A:342:LEU:HB3	1:A:343:PRO:HD3	1.87	0.57
1:A:546:GLU:O	1:A:550:GLU:HG2	2.05	0.57
1:A:437:LEU:CD2	1:A:547:HIS:HE1	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ALA:HB2	1:A:500:LEU:HD13	1.87	0.57
1:A:414:ARG:N	1:A:415:PRO:CD	2.68	0.56
1:A:432:GLU:HB2	1:A:563:HIS:O	2.04	0.56
1:A:414:ARG:O	1:A:415:PRO:C	2.43	0.56
1:A:450:ILE:HD13	1:A:469:VAL:HG21	1.87	0.56
1:A:551:MET:CG	1:A:551:MET:O	2.53	0.56
1:A:551:MET:O	1:A:551:MET:SD	2.63	0.56
1:A:411:PRO:CD	1:A:414:ARG:HB2	2.30	0.56
1:A:435:PHE:CE1	1:A:437:LEU:HD21	2.41	0.56
1:A:449:THR:HG22	1:A:499:ALA:HB2	1.87	0.56
1:A:330:ASN:HD22	1:A:331:GLY:N	2.03	0.56
1:A:523:CYS:SG	1:A:524:ILE:N	2.78	0.55
1:A:387:PHE:C	1:A:387:PHE:CD2	2.79	0.55
1:A:533:CYS:HA	1:A:567:GLU:OE2	2.07	0.55
1:A:514:LEU:O	1:A:534:ARG:O	2.24	0.55
1:A:322:LEU:HA	1:A:359:ASN:OD1	2.07	0.54
1:A:551:MET:O	1:A:552:LEU:HG	2.06	0.54
1:A:560:GLU:O	1:A:561:HIS:CB	2.54	0.54
1:A:557:LYS:O	1:A:559:VAL:HG23	2.07	0.54
1:A:389:ARG:HD2	1:A:389:ARG:O	2.06	0.54
1:A:450:ILE:HD12	1:A:485:THR:CG2	2.37	0.54
1:A:512:VAL:O	1:A:536:GLY:CA	2.54	0.54
1:A:557:LYS:CB	1:A:558:PRO:HD3	2.19	0.54
1:A:450:ILE:CD1	1:A:500:LEU:HD11	2.34	0.54
1:A:557:LYS:O	1:A:559:VAL:CG2	2.56	0.54
1:A:437:LEU:N	1:A:559:VAL:CG2	2.71	0.54
1:A:532:VAL:O	1:A:567:GLU:HB2	2.08	0.53
1:A:437:LEU:HA	1:A:447:THR:O	2.07	0.53
1:A:343:PRO:HB2	1:A:378:ARG:NH1	2.22	0.53
1:A:306:ARG:HD2	1:A:308:LEU:N	2.24	0.53
1:A:437:LEU:N	1:A:437:LEU:HD22	2.24	0.53
1:A:560:GLU:O	1:A:561:HIS:HB3	2.08	0.53
1:A:332:PHE:CD1	1:A:356:LYS:HB3	2.36	0.53
1:A:314:LEU:HD23	1:A:314:LEU:C	2.29	0.52
1:A:314:LEU:C	1:A:314:LEU:CD2	2.78	0.52
1:A:434:ASN:HD22	1:A:435:PHE:N	2.07	0.52
1:A:409:GLU:CG	1:A:410:GLN:HE21	2.22	0.52
1:A:434:ASN:HD22	1:A:435:PHE:H	1.57	0.52
1:A:536:GLY:O	1:A:538:GLU:N	2.33	0.52
1:A:553:ALA:C	1:A:555:PRO:HD3	2.28	0.52
1:A:342:LEU:O	1:A:343:PRO:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASN:CA	1:A:562:TRP:HB3	2.41	0.51
1:A:446:LEU:O	1:A:502:PHE:HB2	2.11	0.51
1:A:470:LYS:CG	1:A:484:LYS:HG2	2.38	0.51
1:A:473:LEU:N	1:A:473:LEU:HD12	2.26	0.51
1:A:501:VAL:O	1:A:501:VAL:HG23	2.11	0.50
1:A:566:VAL:HG12	1:A:566:VAL:O	2.11	0.50
1:A:411:PRO:HB2	1:A:412:PRO:HD2	1.91	0.50
1:A:395:LEU:O	1:A:395:LEU:HD23	2.11	0.50
1:A:438:CYS:SG	1:A:556:ARG:CA	2.94	0.50
1:A:535:VAL:O	1:A:535:VAL:HG12	2.12	0.50
1:A:556:ARG:O	1:A:558:PRO:CD	2.58	0.50
1:A:460:ASP:C	1:A:462:THR:H	2.14	0.50
1:A:438:CYS:O	1:A:447:THR:CB	2.60	0.50
1:A:483:ARG:HG2	1:A:500:LEU:HB3	1.93	0.50
1:A:450:ILE:HD11	1:A:500:LEU:CD1	2.41	0.49
1:A:430:LEU:HD13	1:A:530:ILE:O	2.12	0.49
1:A:409:GLU:HG2	1:A:410:GLN:N	2.27	0.49
1:A:538:GLU:C	1:A:540:ALA:H	2.14	0.49
1:A:558:PRO:C	1:A:559:VAL:CG2	2.79	0.49
1:A:341:LEU:HB3	1:A:378:ARG:HE	1.78	0.49
1:A:344:ASP:OD2	1:A:347:LYS:HB2	2.12	0.49
1:A:330:ASN:HD22	1:A:330:ASN:C	2.15	0.49
1:A:295:GLY:O	1:A:421:LEU:HD12	2.13	0.49
1:A:307:TYR:CE1	1:A:372:LEU:HA	2.48	0.49
1:A:437:LEU:H	1:A:559:VAL:CG2	2.25	0.49
1:A:416:LEU:N	1:A:416:LEU:HD23	2.28	0.49
1:A:343:PRO:CG	1:A:378:ARG:HD2	2.22	0.48
1:A:435:PHE:N	1:A:435:PHE:HD2	2.09	0.48
1:A:506:PRO:O	1:A:509:VAL:HG13	2.13	0.48
1:A:354:HIS:HD2	1:A:362:PHE:CE2	2.31	0.48
1:A:437:LEU:H	1:A:559:VAL:HG21	1.78	0.48
1:A:450:ILE:HD13	1:A:469:VAL:CG2	2.43	0.48
1:A:342:LEU:C	1:A:342:LEU:HD23	2.34	0.48
1:A:506:PRO:O	1:A:509:VAL:HG22	2.14	0.48
1:A:473:LEU:HD22	1:A:478:ARG:HG2	1.94	0.48
1:A:471:ALA:HA	1:A:516:ILE:HG22	1.96	0.48
1:A:519:VAL:HA	1:A:529:VAL:HA	1.96	0.48
1:A:533:CYS:HA	1:A:567:GLU:CD	2.34	0.48
1:A:538:GLU:C	1:A:540:ALA:N	2.68	0.47
1:A:356:LYS:C	1:A:357:THR:HG22	2.34	0.47
1:A:470:LYS:HD2	1:A:482:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:HA	1:A:383:SER:O	2.14	0.47
1:A:329:SER:C	1:A:331:GLY:H	2.18	0.47
1:A:382:PHE:HD1	1:A:399:VAL:CG2	2.27	0.47
1:A:565:LEU:O	1:A:567:GLU:N	2.44	0.47
1:A:517:ALA:HA	1:A:532:VAL:HA	1.95	0.47
1:A:345:ARG:O	1:A:345:ARG:CD	2.59	0.46
1:A:529:VAL:HG21	1:A:569:LYS:NZ	2.30	0.46
1:A:355:ARG:O	1:A:357:THR:HG22	2.15	0.46
1:A:314:LEU:HD22	1:A:316:VAL:HG23	1.96	0.46
1:A:434:ASN:OD1	1:A:451:ILE:HD11	2.16	0.46
1:A:496:TYR:O	1:A:498:GLU:HG3	2.16	0.46
1:A:520:ASP:OD1	1:A:520:ASP:C	2.53	0.46
1:A:299:GLY:O	1:A:420:ILE:HB	2.15	0.46
1:A:354:HIS:HD2	1:A:362:PHE:HE2	1.64	0.45
1:A:433:LEU:C	1:A:433:LEU:HD23	2.36	0.45
1:A:542:PRO:O	1:A:546:GLU:HG3	2.16	0.45
1:A:303:PHE:CD1	1:A:303:PHE:C	2.89	0.45
1:A:439:TYR:N	1:A:551:MET:CE	2.79	0.45
1:A:318:ILE:HG22	1:A:362:PHE:HD1	1.82	0.45
1:A:400:VAL:HG23	1:A:400:VAL:O	2.17	0.45
1:A:434:ASN:ND2	1:A:435:PHE:N	2.64	0.45
1:A:403:ASN:N	1:A:403:ASN:ND2	2.65	0.45
1:A:338:LYS:HD2	1:A:385:TYR:HE1	1.81	0.45
1:A:409:GLU:O	1:A:410:GLN:HB3	2.17	0.45
1:A:313:GLN:HA	1:A:369:SER:HA	1.99	0.45
1:A:534:ARG:CZ	1:A:541:ASP:HB2	2.45	0.45
1:A:437:LEU:N	1:A:437:LEU:CD2	2.80	0.44
1:A:340:TYR:CD2	1:A:348:LYS:HB3	2.45	0.44
1:A:341:LEU:O	1:A:343:PRO:HD2	2.17	0.44
1:A:538:GLU:O	1:A:540:ALA:N	2.50	0.44
1:A:351:THR:HA	1:A:364:GLU:OE1	2.18	0.44
1:A:409:GLU:HG2	1:A:410:GLN:HG3	2.00	0.44
1:A:439:TYR:HA	1:A:445:LEU:O	2.16	0.44
1:A:468:TYR:CE2	1:A:519:VAL:CB	2.99	0.44
1:A:314:LEU:HD11	1:A:404:LEU:HD21	1.99	0.44
1:A:322:LEU:HD12	1:A:417:TRP:CZ3	2.52	0.43
1:A:471:ALA:HA	1:A:516:ILE:CG2	2.48	0.43
1:A:435:PHE:CE1	1:A:516:ILE:HD11	2.53	0.43
1:A:479:ARG:CD	1:A:482:LYS:HE3	2.28	0.43
1:A:302:SER:O	1:A:319:LEU:HB2	2.18	0.43
1:A:403:ASN:O	1:A:407:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:HG22	1:A:351:THR:CG2	2.49	0.43
1:A:330:ASN:ND2	1:A:330:ASN:C	2.72	0.43
1:A:494:PRO:HB2	1:A:496:TYR:CE1	2.53	0.43
1:A:511:ASN:C	1:A:512:VAL:HG23	2.39	0.43
1:A:568:GLU:O	1:A:569:LYS:HG2	2.18	0.43
1:A:512:VAL:CG2	1:A:537:PRO:HG3	2.49	0.43
1:A:337:VAL:HG22	1:A:351:THR:HG23	2.00	0.43
1:A:468:TYR:HB2	1:A:486:SER:O	2.18	0.43
1:A:410:GLN:NE2	1:A:410:GLN:O	2.52	0.43
1:A:534:ARG:HH21	1:A:541:ASP:HB2	1.81	0.43
1:A:390:PHE:O	1:A:461:LEU:HG	2.19	0.42
1:A:345:ARG:HG3	1:A:345:ARG:HH11	1.84	0.42
1:A:434:ASN:HA	1:A:562:TRP:HB3	2.01	0.42
1:A:446:LEU:HD23	1:A:446:LEU:C	2.40	0.42
1:A:371:PRO:HD2	1:A:374:GLU:CD	2.39	0.42
1:A:480:LEU:O	1:A:481:LYS:HD2	2.20	0.42
1:A:469:VAL:HG12	1:A:518:VAL:HA	2.01	0.42
1:A:546:GLU:C	1:A:548:TRP:N	2.71	0.42
1:A:306:ARG:NH1	1:A:306:ARG:HG3	2.32	0.42
1:A:426:GLU:O	1:A:427:LYS:HB2	2.20	0.42
1:A:565:LEU:C	1:A:567:GLU:N	2.72	0.42
1:A:296:ALA:C	1:A:298:CYS:N	2.73	0.42
1:A:341:LEU:HD12	1:A:368:PHE:HD2	1.84	0.42
1:A:459:MET:HB2	1:A:520:ASP:OD2	2.19	0.42
1:A:307:TYR:C	1:A:307:TYR:CD2	2.91	0.41
1:A:472:SER:O	1:A:514:LEU:HD12	2.20	0.41
1:A:467:PRO:HD2	1:A:488:LYS:O	2.19	0.41
1:A:432:GLU:HA	1:A:565:LEU:HG	2.03	0.41
1:A:370:VAL:HG13	1:A:371:PRO:HD2	2.02	0.41
1:A:437:LEU:O	1:A:559:VAL:CG2	2.59	0.41
1:A:437:LEU:HD11	1:A:514:LEU:HD23	2.02	0.41
1:A:307:TYR:OH	1:A:372:LEU:CA	2.67	0.41
1:A:447:THR:HG23	1:A:449:THR:HG23	2.02	0.41
1:A:478:ARG:HG3	1:A:478:ARG:O	2.21	0.41
1:A:551:MET:CE	1:A:551:MET:O	2.68	0.41
1:A:371:PRO:O	1:A:374:GLU:N	2.49	0.41
1:A:388:ASP:H	1:A:393:HIS:CD2	2.39	0.41
1:A:407:LEU:C	1:A:409:GLU:N	2.71	0.41
1:A:418:ARG:HG2	1:A:418:ARG:NH1	2.33	0.41
1:A:307:TYR:CZ	1:A:372:LEU:HA	2.55	0.41
1:A:472:SER:HB3	1:A:482:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:GLY:C	1:A:479:ARG:N	2.73	0.41
1:A:430:LEU:CD2	1:A:457:LYS:HD2	2.51	0.41
1:A:436:SER:HB2	1:A:557:LYS:O	2.21	0.41
1:A:449:THR:HG22	1:A:499:ALA:HB1	2.02	0.41
1:A:303:PHE:CE1	1:A:401:LEU:HD21	2.54	0.40
1:A:329:SER:C	1:A:331:GLY:N	2.74	0.40
1:A:411:PRO:HD2	1:A:414:ARG:CB	2.37	0.40
1:A:529:VAL:HG21	1:A:569:LYS:HZ3	1.85	0.40
1:A:326:ALA:HB1	1:A:331:GLY:O	2.20	0.40
1:A:382:PHE:CB	1:A:399:VAL:HG22	2.32	0.40
1:A:414:ARG:O	1:A:414:ARG:HG3	2.21	0.40
1:A:447:THR:HG22	1:A:449:THR:HG23	2.02	0.40
1:A:533:CYS:HA	1:A:567:GLU:OE1	2.21	0.40
1:A:534:ARG:HD2	1:A:538:GLU:CB	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:CD1	1:A:487:ILE:CD1[9_765]	1.83	0.37

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	273/296 (92%)	178 (65%)	59 (22%)	36 (13%)	0 1

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLY
1	A	342	LEU

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Mol	Chain	Res	Type
1	A	409	GLU
1	A	411	PRO
1	A	427	LYS
1	A	442	THR
1	A	506	PRO
1	A	555	PRO
1	A	556	ARG
1	A	557	LYS
1	A	559	VAL
1	A	561	HIS
1	A	566	VAL
1	A	402	ASP
1	A	417	TRP
1	A	490	ASN
1	A	514	LEU
1	A	524	ILE
1	A	535	VAL
1	A	553	ALA
1	A	562	TRP
1	A	296	ALA
1	A	356	LYS
1	A	376	ALA
1	A	410	GLN
1	A	415	PRO
1	A	426	GLU
1	A	475	SER
1	A	539	ALA
1	A	403	ASN
1	A	430	LEU
1	A	507	GLU
1	A	537	PRO
1	A	552	LEU
1	A	343	PRO
1	A	423	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	239/257 (93%)	200 (84%)	39 (16%)	2 11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	CYS
1	A	300	ARG
1	A	306	ARG
1	A	314	LEU
1	A	330	ASN
1	A	340	TYR
1	A	345	ARG
1	A	357	THR
1	A	360	PRO
1	A	380	LEU
1	A	387	PHE
1	A	395	LEU
1	A	403	ASN
1	A	404	LEU
1	A	405	LEU
1	A	411	PRO
1	A	415	PRO
1	A	416	LEU
1	A	421	LEU
1	A	422	GLU
1	A	432	GLU
1	A	434	ASN
1	A	435	PHE
1	A	439	TYR
1	A	455	ASN
1	A	468	TYR
1	A	487	ILE
1	A	493	ASN
1	A	512	VAL
1	A	516	ILE
1	A	519	VAL
1	A	526	HIS
1	A	534	ARG
1	A	548	TRP
1	A	551	MET
1	A	555	PRO
1	A	556	ARG
1	A	559	VAL

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Mol	Chain	Res	Type
1	A	562	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
1	A	330	ASN
1	A	354	HIS
1	A	363	ASN
1	A	367	GLN
1	A	377	GLN
1	A	403	ASN
1	A	410	GLN
1	A	434	ASN
1	A	511	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
3	SO4	A	594	-	4,4,4	0.31	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.