Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 08:26 AM EDT

PDB ID	:	1FVH
Title	:	CRYSTAL STRUCTURE ANALYSIS OF NEURONAL SEC1 FROM THE SQUID L. PEALEI
Authors	:	Bracher, A.; Weissenhorn, W.
Deposited on	:	2000-09-19
Resolution	:	2.80 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:

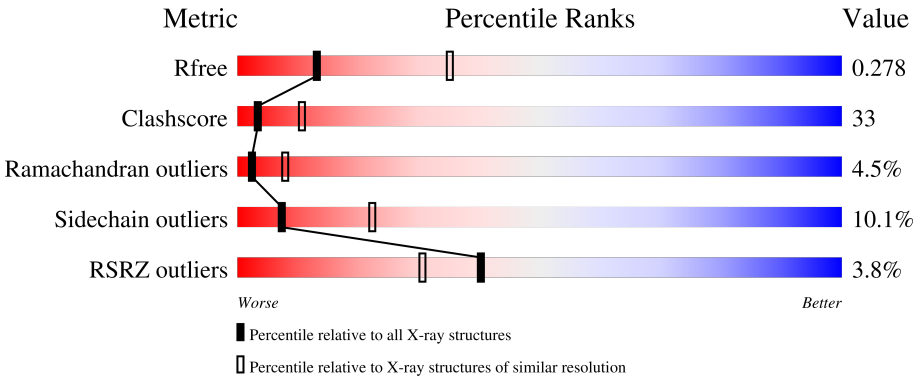
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	591	4% 44% 40% 8% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4449 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 SEC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	546	4412	2794	763	827	28	0	0	0

- Molecule 2 is water.

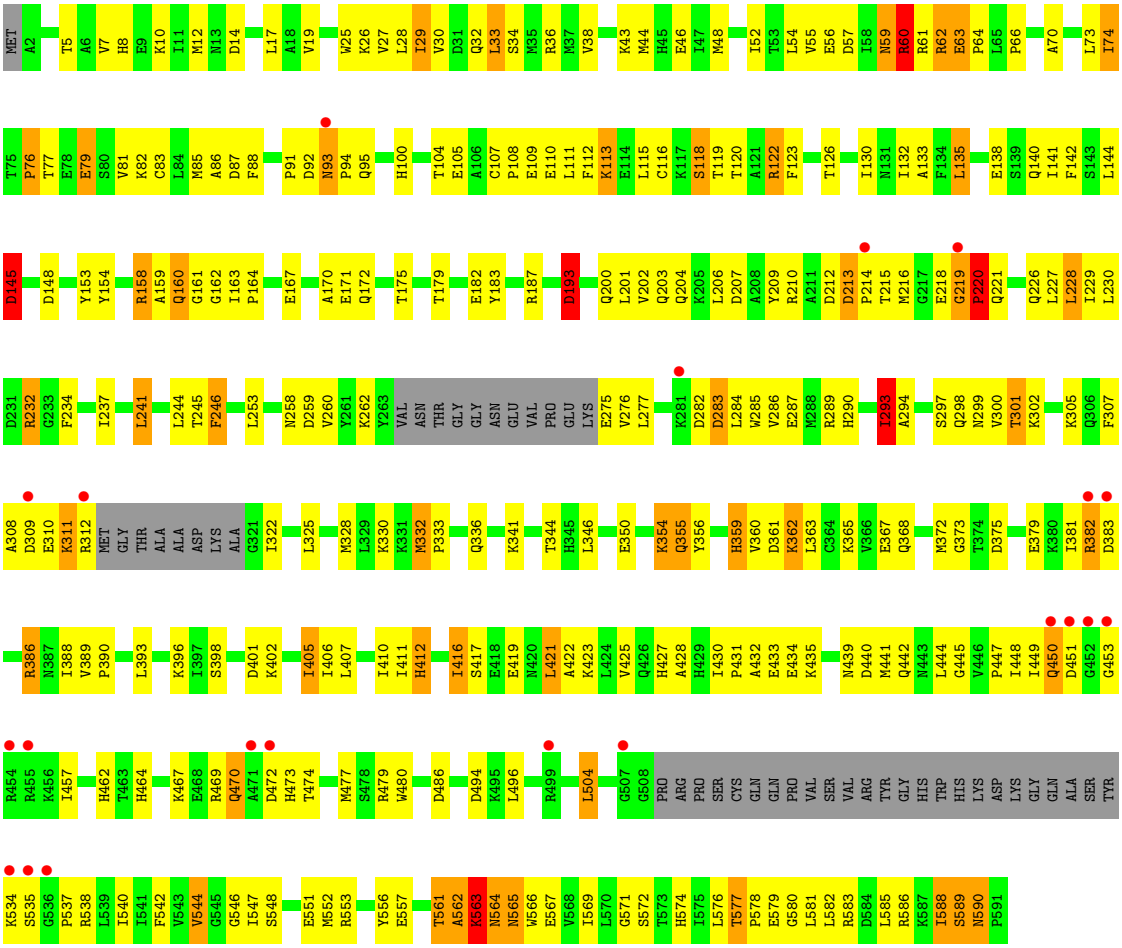
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	37	37	37	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SEC1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.12Å 123.18Å 63.89Å 90.00° 110.49° 90.00°	Depositor
Resolution (Å)	14.91 – 2.80 14.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (14.91-2.80) 86.9 (14.91-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.283 0.233 , 0.278	Depositor DCC
R_{free} test set	923 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4449	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.39	0/4500	0.69	0/6074

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	4412	0	4414	288	0
2	A	37	0	0	0	0
All	All	4449	0	4414	288	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 33.

All (288) 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:163:ILE:HG23	1:A:164:PRO:HD3	1.35	1.04
1:A:122:ARG:H	1:A:122:ARG:HD2	1.22	1.02
1:A:577:THR:HG22	1:A:580:GLY:H	1.25	1.02
1:A:232:ARG:O	1:A:232:ARG:HD3	1.64	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:PRO:HG3	1:A:457:ILE:HB	1.53	0.89
1:A:163:ILE:CG2	1:A:164:PRO:HD3	2.03	0.87
1:A:561:THR:HG23	1:A:562:ALA:H	1.42	0.82
1:A:368:GLN:NE2	1:A:479:ARG:H	1.77	0.82
1:A:10:LYS:HD3	1:A:132:ILE:HD11	1.62	0.82
1:A:182:GLU:OE2	1:A:538:ARG:HD2	1.81	0.80
1:A:113:LYS:HA	1:A:113:LYS:HZ3	1.48	0.77
1:A:93:ASN:N	1:A:94:PRO:HD3	2.00	0.77
1:A:237:ILE:HG22	1:A:241:LEU:HD21	1.66	0.77
1:A:388:ILE:HG23	1:A:405:ILE:HD11	1.69	0.75
1:A:140:GLN:HB2	1:A:556:TYR:CE1	2.22	0.75
1:A:202:VAL:O	1:A:206:LEU:HD12	1.88	0.73
1:A:311:LYS:O	1:A:312:ARG:HB2	1.88	0.73
1:A:588:ILE:HG13	1:A:589:SER:N	2.03	0.73
1:A:141:ILE:HG12	1:A:552:MET:HG2	1.69	0.73
1:A:133:ALA:HB1	1:A:172:GLN:HG2	1.71	0.73
1:A:253:LEU:HB3	1:A:355:GLN:HG2	1.69	0.73
1:A:163:ILE:HG23	1:A:164:PRO:CD	2.18	0.72
1:A:561:THR:O	1:A:563:LYS:HD3	1.88	0.72
1:A:561:THR:HG23	1:A:562:ALA:N	2.03	0.72
1:A:368:GLN:HE21	1:A:479:ARG:H	1.37	0.69
1:A:564:ASN:HB3	1:A:566:TRP:HD1	1.57	0.69
1:A:557:GLU:O	1:A:561:THR:HG22	1.91	0.69
1:A:561:THR:CA	1:A:563:LYS:HD3	2.23	0.69
1:A:561:THR:C	1:A:563:LYS:HD3	2.12	0.69
1:A:276:VAL:HG21	1:A:344:THR:HG21	1.75	0.69
1:A:470:GLN:HG2	1:A:472:ASP:H	1.58	0.69
1:A:363:LEU:O	1:A:367:GLU:HG3	1.93	0.68
1:A:262:LYS:HA	1:A:275:GLU:HA	1.75	0.68
1:A:284:LEU:HD12	1:A:341:LYS:HB3	1.75	0.68
1:A:346:LEU:O	1:A:350:GLU:HG3	1.93	0.68
1:A:577:THR:HG22	1:A:580:GLY:N	2.04	0.68
1:A:561:THR:C	1:A:563:LYS:H	1.98	0.68
1:A:577:THR:CG2	1:A:580:GLY:H	2.04	0.68
1:A:93:ASN:N	1:A:94:PRO:CD	2.56	0.67
1:A:160:GLN:C	1:A:162:GLY:H	1.96	0.67
1:A:113:LYS:HA	1:A:113:LYS:NZ	2.08	0.67
1:A:328:MET:O	1:A:332:MET:HB2	1.93	0.67
1:A:447:PRO:CG	1:A:457:ILE:HB	2.24	0.66
1:A:119:THR:O	1:A:122:ARG:HD3	1.95	0.66
1:A:79:GLU:O	1:A:82:LYS:HB3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HD2	1:A:122:ARG:N	2.06	0.65
1:A:361:ASP:OD2	1:A:362:LYS:HG3	1.97	0.65
1:A:282:ASP:O	1:A:283:ASP:HB3	1.96	0.65
1:A:19:VAL:HG22	1:A:26:LYS:HE2	1.79	0.64
1:A:43:LYS:HB2	1:A:46:GLU:HG3	1.78	0.64
1:A:447:PRO:HG3	1:A:457:ILE:CB	2.26	0.64
1:A:93:ASN:H	1:A:94:PRO:HD3	1.62	0.64
1:A:583:ARG:O	1:A:586:ARG:HB3	1.98	0.64
1:A:52:ILE:HD12	1:A:52:ILE:N	2.13	0.63
1:A:441:MET:CE	1:A:444:LEU:HD22	2.29	0.63
1:A:382:ARG:O	1:A:383:ASP:HB2	1.97	0.63
1:A:368:GLN:HE22	1:A:480:TRP:H	1.44	0.63
1:A:33:LEU:CD2	1:A:135:LEU:HD11	2.29	0.62
1:A:416:ILE:O	1:A:450:GLN:N	2.29	0.62
1:A:202:VAL:HG12	1:A:206:LEU:HD11	1.82	0.62
1:A:451:ASP:C	1:A:453:GLY:H	2.02	0.62
1:A:473:HIS:CD2	1:A:479:ARG:HG2	2.35	0.62
1:A:450:GLN:HG3	1:A:451:ASP:N	2.15	0.62
1:A:200:GLN:HG3	1:A:204:GLN:HE21	1.65	0.61
1:A:585:LEU:O	1:A:588:ILE:HG23	2.00	0.61
1:A:209:TYR:HB3	1:A:216:MET:CE	2.30	0.61
1:A:546:GLY:HA2	1:A:574:HIS:O	2.01	0.61
1:A:237:ILE:HG22	1:A:241:LEU:CD2	2.31	0.61
1:A:332:MET:HB3	1:A:333:PRO:HD3	1.83	0.61
1:A:218:GLU:O	1:A:220:PRO:HD2	2.01	0.60
1:A:542:PHE:HA	1:A:571:GLY:O	2.01	0.60
1:A:109:GLU:HA	1:A:112:PHE:HB3	1.82	0.60
1:A:132:ILE:HG22	1:A:132:ILE:O	2.01	0.60
1:A:115:LEU:O	1:A:118:SER:HB2	2.02	0.60
1:A:293:ILE:HG22	1:A:294:ALA:N	2.17	0.60
1:A:108:PRO:HB2	1:A:110:GLU:OE1	2.02	0.59
1:A:396:LYS:O	1:A:396:LYS:HG2	2.01	0.59
1:A:586:ARG:HG2	1:A:586:ARG:HH11	1.67	0.59
1:A:133:ALA:CB	1:A:172:GLN:HG2	2.33	0.59
1:A:232:ARG:HD3	1:A:232:ARG:C	2.18	0.59
1:A:356:TYR:HA	1:A:360:VAL:HB	1.83	0.59
1:A:32:GLN:O	1:A:36:ARG:HG3	2.02	0.59
1:A:354:LYS:O	1:A:354:LYS:HD3	2.03	0.59
1:A:372:MET:CE	1:A:479:ARG:HB2	2.33	0.59
1:A:439:ASN:O	1:A:448:ILE:HD11	2.03	0.59
1:A:298:GLN:O	1:A:302:LYS:HG2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD23	1:A:427:HIS:O	2.02	0.58
1:A:182:GLU:CD	1:A:538:ARG:HD2	2.22	0.58
1:A:219:GLY:O	1:A:221:GLN:N	2.37	0.58
1:A:576:LEU:HD22	1:A:581:LEU:HB2	1.85	0.58
1:A:412:HIS:C	1:A:412:HIS:CD2	2.77	0.58
1:A:54:LEU:HD23	1:A:55:VAL:N	2.19	0.57
1:A:107:CYS:O	1:A:109:GLU:OE2	2.23	0.57
1:A:431:PRO:C	1:A:433:GLU:H	2.07	0.57
1:A:564:ASN:O	1:A:565:ASN:HB2	2.04	0.56
1:A:333:PRO:HA	1:A:336:GLN:HG2	1.86	0.56
1:A:122:ARG:H	1:A:122:ARG:CD	2.06	0.56
1:A:398:SER:HB3	1:A:401:ASP:OD2	2.05	0.56
1:A:228:LEU:HD22	1:A:229:ILE:N	2.21	0.56
1:A:62:ARG:HH12	1:A:87:ASP:CG	2.09	0.56
1:A:144:LEU:HD22	1:A:172:GLN:HB3	1.87	0.55
1:A:110:GLU:HG2	1:A:111:LEU:N	2.21	0.55
1:A:92:ASP:N	1:A:94:PRO:HD3	2.21	0.55
1:A:372:MET:HE1	1:A:479:ARG:HB2	1.87	0.55
1:A:276:VAL:HG12	1:A:277:LEU:N	2.22	0.54
1:A:441:MET:HE1	1:A:444:LEU:HD22	1.88	0.54
1:A:419:GLU:O	1:A:422:ALA:HB3	2.07	0.54
1:A:440:ASP:OD2	1:A:589:SER:HB2	2.07	0.54
1:A:561:THR:CG2	1:A:562:ALA:H	2.17	0.54
1:A:7:VAL:HG13	1:A:132:ILE:HD13	1.88	0.54
1:A:27:VAL:HG23	1:A:29:ILE:HD13	1.90	0.54
1:A:297:SER:O	1:A:300:VAL:HG12	2.08	0.54
1:A:171:GLU:O	1:A:175:THR:HG23	2.07	0.54
1:A:289:ARG:HG3	1:A:290:HIS:CE1	2.42	0.54
1:A:140:GLN:HB3	1:A:141:ILE:HD12	1.89	0.54
1:A:450:GLN:HG3	1:A:451:ASP:H	1.71	0.54
1:A:581:LEU:O	1:A:585:LEU:HD23	2.08	0.54
1:A:167:GLU:HA	1:A:201:LEU:HD12	1.89	0.54
1:A:227:LEU:HA	1:A:540:ILE:O	2.08	0.53
1:A:362:LYS:CB	1:A:362:LYS:NZ	2.72	0.53
1:A:561:THR:O	1:A:563:LYS:N	2.38	0.53
1:A:354:LYS:HD3	1:A:354:LYS:C	2.28	0.53
1:A:469:ARG:NH1	1:A:486:ASP:OD1	2.40	0.53
1:A:289:ARG:HG2	1:A:290:HIS:N	2.23	0.53
1:A:187:ARG:HH11	1:A:226:GLN:HE22	1.57	0.53
1:A:561:THR:HA	1:A:563:LYS:HD3	1.90	0.53
1:A:160:GLN:C	1:A:162:GLY:N	2.62	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:HB3	1:A:95:GLN:HB3	1.92	0.52
1:A:183:TYR:OH	1:A:207:ASP:OD1	2.27	0.52
1:A:73:LEU:HD11	1:A:130:ILE:HD11	1.92	0.52
1:A:88:PHE:HD2	1:A:123:PHE:CD1	2.27	0.52
1:A:589:SER:O	1:A:590:ASN:HB2	2.09	0.52
1:A:83:CYS:O	1:A:86:ALA:HB3	2.10	0.52
1:A:33:LEU:HD23	1:A:36:ARG:HD3	1.92	0.52
1:A:373:GLY:O	1:A:381:ILE:HG12	2.09	0.52
1:A:62:ARG:H	1:A:62:ARG:HD2	1.75	0.52
1:A:564:ASN:HD22	1:A:566:TRP:HE1	1.59	0.51
1:A:431:PRO:O	1:A:433:GLU:N	2.43	0.51
1:A:76:PRO:HG3	1:A:105:GLU:O	2.10	0.51
1:A:362:LYS:NZ	1:A:362:LYS:HB3	2.25	0.51
1:A:450:GLN:CG	1:A:451:ASP:H	2.22	0.51
1:A:44:MET:O	1:A:48:MET:HG2	2.11	0.50
1:A:110:GLU:CG	1:A:111:LEU:N	2.74	0.50
1:A:322:ILE:HD12	1:A:322:ILE:N	2.26	0.50
1:A:203:GLN:HA	1:A:206:LEU:HD12	1.93	0.50
1:A:305:LYS:NZ	1:A:312:ARG:NH2	2.59	0.50
1:A:431:PRO:HB3	1:A:433:GLU:OE2	2.12	0.50
1:A:142:PHE:CZ	1:A:571:GLY:HA3	2.46	0.50
1:A:161:GLY:O	1:A:164:PRO:HD2	2.11	0.50
1:A:203:GLN:HB2	1:A:504:LEU:HD21	1.94	0.50
1:A:564:ASN:O	1:A:565:ASN:CB	2.59	0.49
1:A:12:MET:O	1:A:17:LEU:HB2	2.12	0.49
1:A:79:GLU:O	1:A:82:LYS:N	2.45	0.49
1:A:118:SER:HB3	1:A:120:THR:H	1.76	0.49
1:A:259:ASP:O	1:A:277:LEU:HD12	2.12	0.49
1:A:286:VAL:HA	1:A:289:ARG:HD2	1.94	0.49
1:A:325:LEU:N	1:A:325:LEU:HD12	2.27	0.49
1:A:421:LEU:O	1:A:425:VAL:HG23	2.12	0.49
1:A:10:LYS:O	1:A:14:ASP:HB2	2.12	0.49
1:A:36:ARG:HH12	1:A:145:ASP:CG	2.16	0.49
1:A:451:ASP:C	1:A:453:GLY:N	2.66	0.49
1:A:372:MET:HE1	1:A:480:TRP:N	2.28	0.49
1:A:416:ILE:HG23	1:A:417:SER:N	2.28	0.49
1:A:586:ARG:HG2	1:A:586:ARG:NH1	2.28	0.49
1:A:30:VAL:HG12	1:A:73:LEU:HB3	1.95	0.49
1:A:361:ASP:CG	1:A:362:LYS:H	2.17	0.48
1:A:538:ARG:HG2	1:A:538:ARG:HH11	1.75	0.48
1:A:375:ASP:OD2	1:A:379:GLU:HB2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:HA	1:A:14:ASP:OD2	2.13	0.48
1:A:187:ARG:CZ	1:A:496:LEU:HD23	2.44	0.48
1:A:57:ASP:HB3	1:A:60:ARG:HG3	1.96	0.48
1:A:407:LEU:O	1:A:411:ILE:HG13	2.13	0.48
1:A:410:ILE:CG2	1:A:448:ILE:HA	2.43	0.48
1:A:410:ILE:HG21	1:A:448:ILE:HA	1.95	0.48
1:A:325:LEU:N	1:A:325:LEU:CD1	2.77	0.47
1:A:187:ARG:HH12	1:A:496:LEU:HB3	1.78	0.47
1:A:462:HIS:HB3	1:A:464:HIS:CE1	2.49	0.47
1:A:170:ALA:HB2	1:A:201:LEU:HB3	1.95	0.47
1:A:425:VAL:HG11	1:A:435:LYS:HG3	1.96	0.47
1:A:305:LYS:HZ2	1:A:312:ARG:NH2	2.13	0.47
1:A:228:LEU:HD13	1:A:230:LEU:HG	1.97	0.47
1:A:289:ARG:HG2	1:A:290:HIS:H	1.80	0.47
1:A:203:GLN:HA	1:A:206:LEU:CD1	2.44	0.47
1:A:215:THR:O	1:A:218:GLU:HB2	2.15	0.47
1:A:311:LYS:O	1:A:312:ARG:CB	2.60	0.47
1:A:5:THR:O	1:A:8:HIS:HB3	2.15	0.47
1:A:77:THR:O	1:A:81:VAL:HG23	2.15	0.46
1:A:431:PRO:C	1:A:433:GLU:N	2.69	0.46
1:A:442:GLN:HB2	1:A:448:ILE:HD11	1.96	0.46
1:A:406:ILE:O	1:A:410:ILE:HG13	2.14	0.46
1:A:561:THR:C	1:A:563:LYS:N	2.67	0.46
1:A:356:TYR:CE1	1:A:361:ASP:HB3	2.51	0.46
1:A:282:ASP:HB3	1:A:285:TRP:HB3	1.98	0.46
1:A:535:SER:OG	1:A:565:ASN:ND2	2.49	0.46
1:A:33:LEU:HD21	1:A:135:LEU:HD11	1.98	0.46
1:A:308:ALA:C	1:A:310:GLU:H	2.18	0.46
1:A:74:ILE:HD13	1:A:74:ILE:H	1.81	0.46
1:A:202:VAL:O	1:A:206:LEU:CD1	2.63	0.45
1:A:286:VAL:HG12	1:A:286:VAL:O	2.16	0.45
1:A:538:ARG:HG2	1:A:538:ARG:NH1	2.32	0.45
1:A:34:SER:O	1:A:38:VAL:HG23	2.15	0.45
1:A:300:VAL:HG13	1:A:301:THR:N	2.32	0.45
1:A:91:PRO:C	1:A:93:ASN:H	2.18	0.45
1:A:154:TYR:CD1	1:A:444:LEU:HG	2.51	0.45
1:A:228:LEU:HD11	1:A:230:LEU:HD21	1.99	0.45
1:A:148:ASP:OD1	1:A:158:ARG:NH2	2.50	0.45
1:A:359:HIS:CD2	1:A:360:VAL:HG23	2.52	0.45
1:A:63:GLU:HA	1:A:64:PRO:HD3	1.81	0.45
1:A:100:HIS:HA	1:A:126:THR:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TYR:HB2	1:A:216:MET:HG2	1.99	0.45
1:A:538:ARG:NH1	1:A:567:GLU:OE1	2.44	0.45
1:A:64:PRO:O	1:A:66:PRO:HD3	2.16	0.45
1:A:138:GLU:HB3	1:A:556:TYR:OH	2.17	0.45
1:A:563:LYS:HE2	1:A:563:LYS:HB2	1.80	0.45
1:A:262:LYS:CB	1:A:275:GLU:HB3	2.48	0.44
1:A:445:GLY:O	1:A:457:ILE:HG21	2.17	0.44
1:A:299:ASN:N	1:A:299:ASN:HD22	2.16	0.44
1:A:449:ILE:O	1:A:450:GLN:O	2.35	0.44
1:A:450:GLN:CG	1:A:451:ASP:N	2.78	0.44
1:A:142:PHE:CE1	1:A:571:GLY:HA3	2.52	0.44
1:A:154:TYR:CE1	1:A:444:LEU:HG	2.53	0.44
1:A:286:VAL:HG13	1:A:289:ARG:NH1	2.33	0.44
1:A:381:ILE:HD11	1:A:412:HIS:CE1	2.53	0.44
1:A:135:LEU:HD13	1:A:135:LEU:N	2.33	0.44
1:A:54:LEU:HD23	1:A:54:LEU:C	2.38	0.44
1:A:144:LEU:O	1:A:145:ASP:C	2.56	0.44
1:A:444:LEU:N	1:A:444:LEU:HD12	2.33	0.44
1:A:135:LEU:HD21	1:A:145:ASP:HB2	1.99	0.43
1:A:423:LYS:HA	1:A:423:LYS:HD3	1.84	0.43
1:A:544:VAL:O	1:A:544:VAL:HG22	2.19	0.43
1:A:29:ILE:CD1	1:A:29:ILE:N	2.81	0.43
1:A:212:ASP:O	1:A:213:ASP:CB	2.66	0.43
1:A:245:THR:HG21	1:A:553:ARG:NH2	2.33	0.43
1:A:27:VAL:HG22	1:A:70:ALA:HA	2.00	0.43
1:A:402:LYS:HD3	1:A:428:ALA:HB1	2.01	0.43
1:A:85:MET:SD	1:A:118:SER:OG	2.77	0.42
1:A:310:GLU:C	1:A:311:LYS:HG2	2.39	0.42
1:A:362:LYS:HB3	1:A:362:LYS:HZ3	1.83	0.42
1:A:56:GLU:OE2	1:A:62:ARG:HB2	2.19	0.42
1:A:193:ASP:OD1	1:A:193:ASP:N	2.49	0.42
1:A:210:ARG:HE	1:A:214:PRO:HA	1.83	0.42
1:A:27:VAL:HG23	1:A:29:ILE:CD1	2.49	0.42
1:A:113:LYS:NZ	1:A:116:CYS:HB2	2.34	0.42
1:A:118:SER:C	1:A:120:THR:H	2.21	0.42
1:A:365:LYS:HB3	1:A:477:MET:HE1	2.01	0.42
1:A:368:GLN:O	1:A:372:MET:HB2	2.19	0.42
1:A:54:LEU:CD2	1:A:56:GLU:HG2	2.50	0.42
1:A:365:LYS:HB3	1:A:477:MET:CE	2.48	0.42
1:A:59:ASN:O	1:A:61:ARG:N	2.52	0.42
1:A:245:THR:CG2	1:A:553:ARG:NH2	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:MET:HE3	1:A:479:ARG:HB2	2.01	0.42
1:A:402:LYS:O	1:A:406:ILE:HG13	2.19	0.42
1:A:451:ASP:O	1:A:453:GLY:N	2.53	0.42
1:A:467:LYS:HE2	1:A:469:ARG:NH1	2.35	0.42
1:A:548:SER:OG	1:A:551:GLU:HG3	2.20	0.42
1:A:470:GLN:NE2	1:A:472:ASP:O	2.45	0.42
1:A:284:LEU:HD12	1:A:341:LYS:CB	2.47	0.41
1:A:386:ARG:HG3	1:A:386:ARG:HH11	1.85	0.41
1:A:412:HIS:C	1:A:412:HIS:HD2	2.22	0.41
1:A:561:THR:CG2	1:A:562:ALA:N	2.73	0.41
1:A:567:GLU:HG2	1:A:569:ILE:CD1	2.50	0.41
1:A:227:LEU:HD23	1:A:227:LEU:O	2.20	0.41
1:A:232:ARG:NH2	1:A:551:GLU:OE1	2.49	0.41
1:A:170:ALA:CB	1:A:201:LEU:HB3	2.49	0.41
1:A:258:ASN:O	1:A:259:ASP:HB2	2.20	0.41
1:A:307:PHE:CD1	1:A:307:PHE:C	2.94	0.41
1:A:360:VAL:O	1:A:361:ASP:C	2.58	0.41
1:A:289:ARG:CG	1:A:290:HIS:N	2.84	0.41
1:A:537:PRO:O	1:A:566:TRP:HA	2.20	0.41
1:A:10:LYS:HD2	1:A:179:THR:HG23	2.02	0.41
1:A:28:LEU:C	1:A:29:ILE:HD12	2.40	0.41
1:A:389:VAL:HB	1:A:390:PRO:HD3	2.03	0.41
1:A:534:LYS:HG2	1:A:534:LYS:O	2.20	0.41
1:A:93:ASN:O	1:A:94:PRO:C	2.58	0.41
1:A:361:ASP:CG	1:A:362:LYS:N	2.74	0.41
1:A:382:ARG:O	1:A:383:ASP:CB	2.68	0.41
1:A:386:ARG:HH11	1:A:386:ARG:CG	2.34	0.41
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.97	0.41
1:A:577:THR:O	1:A:578:PRO:C	2.57	0.40
1:A:564:ASN:HB3	1:A:566:TRP:CD1	2.46	0.40
1:A:579:GLU:O	1:A:582:LEU:HB2	2.21	0.40
1:A:308:ALA:C	1:A:310:GLU:N	2.75	0.40
1:A:19:VAL:HG23	1:A:100:HIS:CE1	2.56	0.40
1:A:120:THR:O	1:A:120:THR:HG22	2.21	0.40
1:A:298:GLN:HG2	1:A:299:ASN:ND2	2.37	0.40
1:A:430:ILE:CG2	1:A:434:GLU:HB2	2.51	0.40
1:A:547:ILE:HG23	1:A:572:SER:HB2	2.01	0.40
1:A:276:VAL:CG1	1:A:277:LEU:N	2.83	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	538/591 (91%)	455 (85%)	59 (11%)	24 (4%)	2 8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	193	ASP
1	A	213	ASP
1	A	219	GLY
1	A	220	PRO
1	A	311	LYS
1	A	330	LYS
1	A	450	GLN
1	A	564	ASN
1	A	59	ASN
1	A	60	ARG
1	A	145	ASP
1	A	159	ALA
1	A	432	ALA
1	A	562	ALA
1	A	561	THR
1	A	563	LYS
1	A	565	ASN
1	A	246	PHE
1	A	590	ASN
1	A	93	ASN
1	A	332	MET
1	A	76	PRO
1	A	293	ILE

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	487/523 (93%)	438 (90%)	49 (10%)	7 22

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	TRP
1	A	29	ILE
1	A	33	LEU
1	A	60	ARG
1	A	62	ARG
1	A	63	GLU
1	A	74	ILE
1	A	104	THR
1	A	113	LYS
1	A	118	SER
1	A	122	ARG
1	A	135	LEU
1	A	145	ASP
1	A	153	TYR
1	A	158	ARG
1	A	160	GLN
1	A	193	ASP
1	A	220	PRO
1	A	228	LEU
1	A	232	ARG
1	A	234	PHE
1	A	241	LEU
1	A	244	LEU
1	A	246	PHE
1	A	260	VAL
1	A	283	ASP
1	A	287	GLU
1	A	293	ILE
1	A	301	THR
1	A	309	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	354	LYS
1	A	355	GLN
1	A	359	HIS
1	A	362	LYS
1	A	382	ARG
1	A	386	ARG
1	A	405	ILE
1	A	412	HIS
1	A	416	ILE
1	A	421	LEU
1	A	470	GLN
1	A	474	THR
1	A	494	ASP
1	A	504	LEU
1	A	544	VAL
1	A	563	LYS
1	A	577	THR
1	A	588	ILE
1	A	589	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	165	ASN
1	A	204	GLN
1	A	226	GLN
1	A	247	GLN
1	A	258	ASN
1	A	299	ASN
1	A	336	GLN
1	A	355	GLN
1	A	357	GLN
1	A	359	HIS
1	A	368	GLN
1	A	384	HIS
1	A	387	ASN
1	A	395	GLN
1	A	412	HIS
1	A	439	ASN
1	A	442	GLN
1	A	443	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	465	ASN
1	A	473	HIS
1	A	476	GLN
1	A	560	GLN
1	A	564	ASN
1	A	565	ASN
1	A	574	HIS
1	A	590	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)

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	546/591 (92%)	-0.14	21 (3%) 40 30	32, 59, 90, 110	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	SER	5.0
1	A	454	ARG	3.8
1	A	455	ARG	3.8
1	A	453	GLY	3.6
1	A	534	LYS	3.5
1	A	93	ASN	3.1
1	A	214	PRO	3.1
1	A	309	ASP	2.7
1	A	383	ASP	2.5
1	A	451	ASP	2.5
1	A	536	GLY	2.4
1	A	507	GLY	2.3
1	A	472	ASP	2.3
1	A	450	GLN	2.3
1	A	219	GLY	2.3
1	A	382	ARG	2.3
1	A	471	ALA	2.1
1	A	281	LYS	2.1
1	A	312	ARG	2.1
1	A	499	ARG	2.1
1	A	452	GLY	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.