



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:44 PM UTC

PDB ID : 2XHE / pdb_00002xhe
Title : Crystal structure of the Unc18-syntaxin 1 complex from *Monosiga brevicollis*
Authors : Burkhardt, P.; Stegmann, C.M.; Wahl, M.C.; Fasshauer, D.
Deposited on : 2010-06-14
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

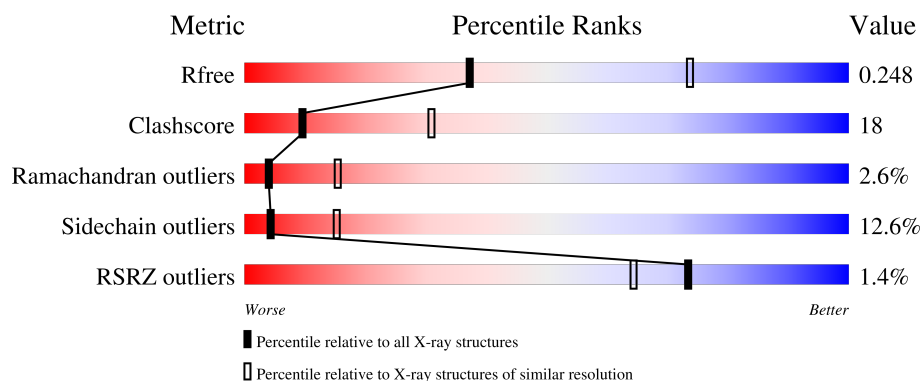
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	650	52%26%9%13%
2	B	279	3% 51%23%•21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6315 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 UNC18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	S	0	0	1
			4466	2805	780	856	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A9V0L3

- Molecule 2 is a protein called SYNTAXIN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1801	1095	342	356	8			

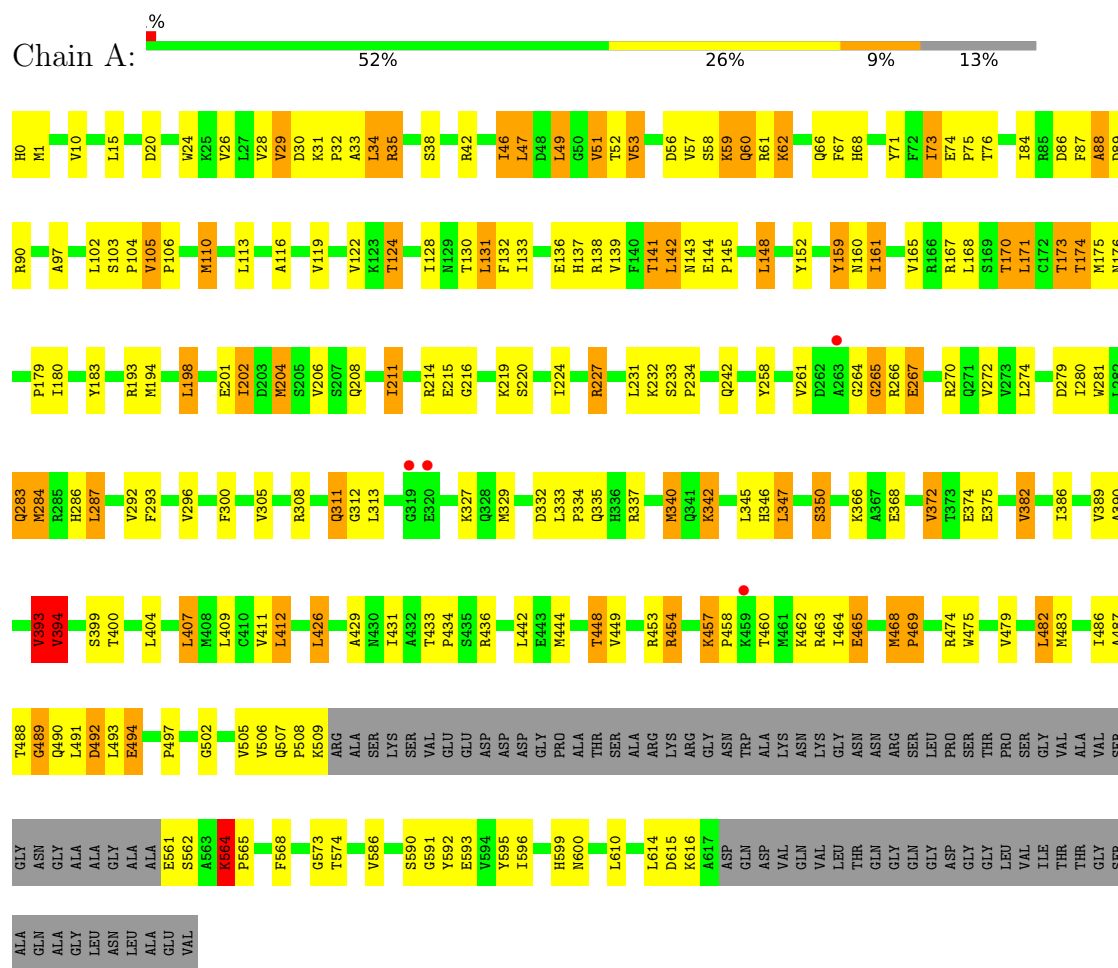
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	2	Total	O	0	0
			2	2		

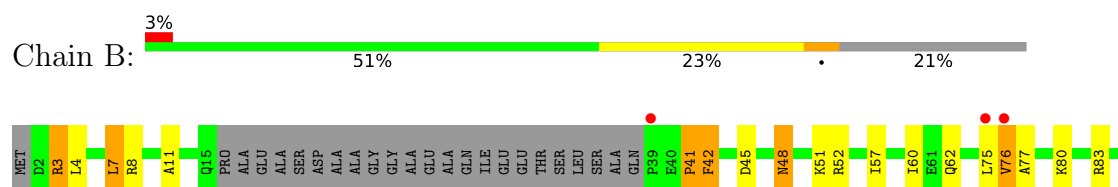
3 Residue-property plots

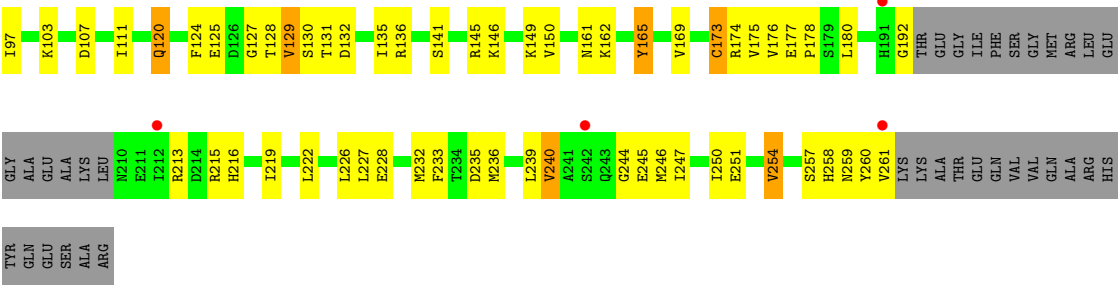
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: UNC18



• Molecule 2: SYNTAXIN1





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	146.20Å 146.20Å 214.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.60 – 2.80 34.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.60-2.80) 99.9 (34.60-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.250 0.190 , 0.248	Depositor DCC
R_{free} test set	1726 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6315	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

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	0.54	1/4541 (0.0%)	0.90	10/6140 (0.2%)
2	B	0.42	0/1817	0.76	0/2430
All	All	0.51	1/6358 (0.0%)	0.86	10/8570 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	616	LYS	C-N	-6.37	1.24	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	VAL	CB-CA-C	-7.09	102.43	112.22
1	A	49	LEU	N-CA-C	-6.51	103.75	112.94
1	A	564	LYS	CA-C-N	6.13	126.04	119.85
1	A	564	LYS	C-N-CA	6.13	126.04	119.85
1	A	457	LYS	CA-C-N	6.02	126.04	119.90
1	A	457	LYS	C-N-CA	6.02	126.04	119.90
1	A	393	VAL	N-CA-C	5.77	118.26	111.05
1	A	468	MET	CA-C-N	5.41	126.61	119.84
1	A	468	MET	C-N-CA	5.41	126.61	119.84
1	A	159	TYR	N-CA-C	5.22	116.97	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	590	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4466	0	4493	176	0
2	B	1801	0	1779	56	0
3	A	46	0	0	4	0
3	B	2	0	0	0	0
All	All	6315	0	6272	223	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 18.

All (223) 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:444:MET:HE1	1:A:615:ASP:HB3	1.43	0.97
1:A:561:GLU:HG2	1:A:562:SER:H	1.31	0.95
1:A:337:ARG:CZ	2:B:240:VAL:HG11	2.02	0.89
1:A:296:VAL:HG12	1:A:347:LEU:HD13	1.63	0.80
1:A:283:GLN:HG3	1:A:284:MET:HE3	1.63	0.79
1:A:167:ARG:O	1:A:170:THR:HB	1.85	0.77
1:A:145:PRO:HA	1:A:600:ASN:HD22	1.49	0.76
2:B:75:LEU:HD23	2:B:76:VAL:HG12	1.67	0.76
2:B:76:VAL:HG13	2:B:77:ALA:H	1.50	0.75
1:A:57:VAL:HG21	1:A:73:ILE:HD11	1.68	0.75
1:A:346:HIS:O	1:A:350:SER:HB2	1.87	0.74
1:A:444:MET:CE	1:A:615:ASP:HB3	2.18	0.73
1:A:286:HIS:HE1	3:A:2005:HOH:O	1.71	0.73
1:A:284:MET:HG3	1:A:292:VAL:HG22	1.69	0.72
1:A:227:ARG:O	1:A:227:ARG:HD3	1.90	0.72
1:A:131:LEU:H	1:A:170:THR:HG21	1.53	0.71
2:B:235:ASP:O	2:B:239:LEU:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:HD2	1:A:170:THR:HG22	1.57	0.69
1:A:179:PRO:HD2	1:A:202:ILE:HD12	1.73	0.69
1:A:564:LYS:HD2	1:A:591:GLY:O	1.94	0.68
2:B:124:PHE:HB2	2:B:258:HIS:HE2	1.59	0.67
2:B:192:GLY:HA2	2:B:216:HIS:ND1	2.10	0.67
1:A:202:ILE:O	1:A:206:VAL:HG23	1.94	0.66
1:A:561:GLU:HG2	1:A:562:SER:N	2.07	0.66
1:A:130:THR:HG22	1:A:174:THR:CG2	2.26	0.65
1:A:342:LYS:HE3	3:A:2029:HOH:O	1.95	0.65
2:B:239:LEU:HD13	2:B:239:LEU:O	1.97	0.65
2:B:161:ASN:O	2:B:165:TYR:HB2	1.96	0.65
1:A:261:VAL:HG12	1:A:266:ARG:HA	1.80	0.64
1:A:53:VAL:HG13	2:B:135:ILE:HG13	1.79	0.64
1:A:284:MET:HE2	1:A:287:LEU:CD2	2.28	0.64
1:A:198:LEU:O	1:A:202:ILE:HG23	1.98	0.63
1:A:266:ARG:H	1:A:266:ARG:HD2	1.62	0.63
2:B:57:ILE:HG23	2:B:150:VAL:HG21	1.81	0.62
1:A:130:THR:HA	1:A:170:THR:HG23	1.81	0.61
1:A:444:MET:HE1	1:A:615:ASP:CB	2.26	0.61
1:A:374:GLU:C	1:A:382:VAL:HG13	2.25	0.61
1:A:35:ARG:HE	1:A:35:ARG:HA	1.65	0.60
1:A:488:THR:HG22	1:A:488:THR:O	2.02	0.60
2:B:76:VAL:HG13	2:B:77:ALA:N	2.17	0.60
1:A:372:VAL:HG13	1:A:475:TRP:CE3	2.37	0.59
2:B:125:GLU:C	2:B:127:GLY:H	2.08	0.59
2:B:169:VAL:HG11	2:B:215:ARG:HH11	1.67	0.59
1:A:206:VAL:HG22	1:A:211:ILE:HG13	1.83	0.59
1:A:10:VAL:HG11	1:A:128:ILE:HG23	1.84	0.58
2:B:174:ARG:C	2:B:176:VAL:H	2.12	0.58
1:A:31:LYS:HB2	1:A:32:PRO:HD3	1.85	0.58
1:A:300:PHE:CE1	1:A:340:MET:HE3	2.38	0.58
1:A:58:SER:O	1:A:59:LYS:HB2	2.03	0.57
2:B:107:ASP:O	2:B:111:ILE:HG13	2.03	0.57
1:A:266:ARG:HD2	1:A:266:ARG:N	2.18	0.57
1:A:242:GLN:HG3	1:A:281:TRP:CZ2	2.40	0.57
1:A:52:THR:HG23	1:A:53:VAL:HG22	1.86	0.57
1:A:132:PHE:HD2	1:A:170:THR:CG2	2.18	0.56
1:A:312:GLY:C	1:A:313:LEU:HG	2.31	0.56
1:A:426:LEU:HD23	1:A:436:ARG:HD3	1.87	0.56
1:A:161:ILE:HD12	1:A:194:MET:HB2	1.88	0.56
1:A:180:ILE:HD13	1:A:219:LYS:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HG3	1:A:102:LEU:HD12	1.86	0.56
1:A:390:ALA:O	1:A:394:VAL:HG22	2.05	0.56
1:A:145:PRO:CA	1:A:600:ASN:HD22	2.19	0.56
2:B:165:TYR:O	2:B:219:ILE:HD11	2.05	0.56
1:A:300:PHE:HE1	1:A:340:MET:HE3	1.71	0.56
1:A:46:ILE:HG23	1:A:51:VAL:CG2	2.36	0.55
1:A:148:LEU:HD13	1:A:614:LEU:HD21	1.88	0.55
2:B:41:PRO:O	2:B:42:PHE:HB3	2.05	0.55
2:B:244:GLY:HA2	2:B:247:ILE:HG22	1.89	0.55
1:A:179:PRO:CD	1:A:202:ILE:HD12	2.38	0.54
1:A:170:THR:O	1:A:174:THR:CG2	2.55	0.54
2:B:3:ARG:H	2:B:3:ARG:HD2	1.72	0.54
1:A:165:VAL:HG12	1:A:201:GLU:HG3	1.90	0.54
1:A:0:HIS:O	1:A:1:MET:HB2	2.07	0.53
1:A:20:ASP:HB2	1:A:68:HIS:CD2	2.43	0.53
1:A:284:MET:HE2	1:A:287:LEU:HD22	1.91	0.53
1:A:493:LEU:HD21	1:A:502:GLY:O	2.08	0.53
1:A:568:PHE:HD1	1:A:595:TYR:HB2	1.72	0.53
2:B:129:VAL:HG12	2:B:130:SER:N	2.24	0.53
1:A:30:ASP:O	1:A:34:LEU:HB2	2.07	0.53
1:A:412:LEU:HD13	1:A:442:LEU:HD13	1.91	0.53
2:B:169:VAL:HG11	2:B:215:ARG:NH1	2.23	0.53
1:A:60:GLN:HG2	1:A:86:ASP:OD2	2.09	0.52
1:A:227:ARG:HD3	1:A:227:ARG:C	2.21	0.52
1:A:561:GLU:CG	1:A:562:SER:H	2.12	0.52
1:A:170:THR:O	1:A:174:THR:HG23	2.09	0.52
1:A:103:SER:HB2	1:A:104:PRO:HD2	1.91	0.52
2:B:141:SER:HB3	2:B:145:ARG:HH12	1.75	0.52
1:A:173:THR:HA	1:A:211:ILE:CG2	2.39	0.52
1:A:407:LEU:HD23	1:A:431:ILE:CD1	2.40	0.52
1:A:463:ARG:O	1:A:464:ILE:HB	2.10	0.51
1:A:492:ASP:HB3	1:A:494:GLU:HG2	1.92	0.51
1:A:53:VAL:HG13	2:B:135:ILE:CG1	2.40	0.51
2:B:125:GLU:C	2:B:127:GLY:N	2.69	0.51
1:A:66:GLN:H	1:A:66:GLN:CD	2.18	0.51
1:A:87:PHE:O	1:A:88:ALA:C	2.53	0.51
1:A:180:ILE:CD1	1:A:219:LYS:HD3	2.41	0.51
1:A:453:ARG:O	1:A:454:ARG:HB3	2.10	0.51
1:A:29:VAL:HG22	1:A:33:ALA:HB3	1.93	0.50
1:A:171:LEU:O	1:A:175:MET:HB2	2.11	0.50
1:A:232:LYS:HD3	1:A:372:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:HG11	1:A:345:LEU:HD22	1.92	0.50
2:B:80:LYS:HA	2:B:83:ARG:HB2	1.92	0.50
2:B:244:GLY:C	2:B:246:MET:H	2.19	0.50
1:A:75:PRO:HG3	1:A:103:SER:O	2.10	0.50
1:A:375:GLU:O	1:A:474:ARG:NH2	2.45	0.50
1:A:214:ARG:O	1:A:215:GLU:HB2	2.11	0.50
2:B:232:MET:SD	2:B:236:MET:HG3	2.51	0.50
1:A:131:LEU:CD1	1:A:167:ARG:HA	2.41	0.50
1:A:215:GLU:OE1	1:A:219:LYS:HE2	2.11	0.49
1:A:264:GLY:O	1:A:265:GLY:C	2.55	0.49
1:A:280:ILE:O	1:A:284:MET:HB2	2.12	0.49
1:A:296:VAL:CG1	1:A:347:LEU:HD13	2.37	0.49
1:A:58:SER:O	1:A:59:LYS:CB	2.60	0.49
1:A:308:ARG:NH1	1:A:313:LEU:HB3	2.27	0.49
1:A:491:LEU:HB3	3:A:2043:HOH:O	2.12	0.49
2:B:124:PHE:HD1	2:B:258:HIS:CD2	2.31	0.49
1:A:161:ILE:HD11	1:A:193:ARG:HD2	1.93	0.49
1:A:311:GLN:HB3	1:A:312:GLY:H	1.51	0.48
1:A:87:PHE:O	1:A:89:ASP:N	2.47	0.48
1:A:487:ALA:HA	1:A:592:TYR:CE1	2.49	0.48
1:A:148:LEU:HD22	1:A:152:TYR:HD2	1.77	0.48
1:A:308:ARG:NH2	1:A:332:ASP:OD2	2.47	0.48
1:A:464:ILE:O	1:A:465:GLU:HB2	2.13	0.48
1:A:84:ILE:O	1:A:88:ALA:HB2	2.14	0.48
1:A:198:LEU:HD12	1:A:224:ILE:HD11	1.95	0.47
1:A:258:TYR:OH	1:A:270:ARG:HD3	2.13	0.47
2:B:244:GLY:O	2:B:245:GLU:HG2	2.14	0.47
2:B:124:PHE:CD1	2:B:258:HIS:CD2	3.03	0.47
1:A:132:PHE:CD2	1:A:170:THR:HG22	2.45	0.47
1:A:141:THR:HG23	1:A:143:ASN:H	1.79	0.47
1:A:142:LEU:HB2	1:A:599:HIS:HA	1.97	0.47
1:A:486:ILE:C	1:A:488:THR:H	2.22	0.47
1:A:283:GLN:CG	1:A:284:MET:HE3	2.40	0.47
1:A:487:ALA:HA	1:A:592:TYR:CD1	2.50	0.46
2:B:129:VAL:HG12	2:B:130:SER:H	1.81	0.46
1:A:35:ARG:HA	1:A:35:ARG:NE	2.31	0.46
1:A:292:VAL:O	1:A:293:PHE:C	2.59	0.46
1:A:426:LEU:HB3	1:A:436:ARG:CZ	2.46	0.46
1:A:284:MET:HA	1:A:287:LEU:HD22	1.98	0.46
1:A:35:ARG:HB3	1:A:133:ILE:HD12	1.97	0.45
1:A:47:LEU:HD12	1:A:47:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LYS:HA	1:A:62:LYS:HD2	1.69	0.45
1:A:165:VAL:CG1	1:A:201:GLU:HG3	2.45	0.45
2:B:80:LYS:O	2:B:80:LYS:HG2	2.15	0.45
1:A:266:ARG:O	1:A:267:GLU:C	2.59	0.45
2:B:244:GLY:CA	2:B:247:ILE:HG22	2.45	0.45
1:A:75:PRO:HB3	1:A:105:VAL:HA	1.98	0.45
1:A:159:TYR:O	1:A:160:ASN:HB3	2.16	0.45
1:A:183:TYR:O	1:A:497:PRO:HD2	2.17	0.45
1:A:433:THR:OG1	1:A:434:PRO:HD3	2.16	0.45
2:B:120:GLN:CD	2:B:120:GLN:H	2.25	0.45
2:B:60:ILE:HG23	2:B:97:ILE:HG23	1.97	0.45
1:A:29:VAL:HG22	1:A:33:ALA:CB	2.46	0.45
1:A:176:ASN:HA	1:A:211:ILE:HG22	1.98	0.45
1:A:74:GLU:HB3	1:A:76:THR:HG23	1.98	0.45
1:A:75:PRO:CG	1:A:103:SER:O	2.65	0.44
1:A:334:PRO:HB2	2:B:233:PHE:HB3	1.99	0.44
1:A:10:VAL:CG1	1:A:128:ILE:HG23	2.47	0.44
1:A:489:GLY:O	1:A:507:GLN:HB3	2.17	0.44
1:A:508:PRO:O	1:A:509:LYS:C	2.60	0.44
1:A:489:GLY:HA2	1:A:505:VAL:HG12	1.98	0.44
1:A:483:MET:HB3	1:A:586:VAL:HG11	1.99	0.44
1:A:179:PRO:HA	1:A:220:SER:O	2.17	0.44
1:A:493:LEU:HD12	1:A:493:LEU:N	2.33	0.44
1:A:407:LEU:CD2	1:A:431:ILE:CD1	2.95	0.44
1:A:87:PHE:CZ	1:A:97:ALA:HB2	2.53	0.43
1:A:292:VAL:HG12	1:A:350:SER:OG	2.18	0.43
2:B:45:ASP:O	2:B:48:ASN:HB2	2.18	0.43
1:A:368:GLU:O	1:A:372:VAL:HB	2.18	0.43
1:A:38:SER:OG	2:B:251:GLU:HG3	2.18	0.43
1:A:227:ARG:O	1:A:227:ARG:CD	2.64	0.43
2:B:215:ARG:O	2:B:219:ILE:HD13	2.19	0.43
1:A:130:THR:HG22	1:A:174:THR:HG21	2.01	0.43
1:A:131:LEU:HD13	1:A:167:ARG:HG2	2.00	0.43
1:A:116:ALA:O	1:A:119:VAL:HG12	2.18	0.43
2:B:4:LEU:HD11	2:B:8:ARG:NH1	2.34	0.43
2:B:177:GLU:HA	2:B:178:PRO:HD3	1.86	0.43
1:A:24:TRP:HB2	1:A:67:PHE:CE1	2.54	0.43
1:A:119:VAL:HG21	2:B:11:ALA:CB	2.48	0.43
1:A:148:LEU:HD23	1:A:573:GLY:HA3	2.00	0.43
1:A:468:MET:HA	1:A:469:PRO:HD2	1.79	0.43
1:A:366:LYS:HE2	1:A:366:LYS:HB3	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:TYR:O	2:B:261:VAL:HB	2.19	0.42
1:A:138:ARG:NH2	1:A:593:GLU:OE2	2.51	0.42
1:A:139:VAL:HA	1:A:596:ILE:O	2.19	0.42
2:B:162:LYS:O	2:B:162:LYS:HG2	2.19	0.42
1:A:28:VAL:HG11	1:A:71:TYR:CE2	2.53	0.42
1:A:26:VAL:HG22	1:A:53:VAL:HG23	2.01	0.42
1:A:233:SER:HB2	1:A:234:PRO:HD3	2.00	0.42
2:B:125:GLU:O	2:B:127:GLY:N	2.53	0.42
1:A:206:VAL:C	1:A:208:GLN:H	2.27	0.42
1:A:312:GLY:O	1:A:313:LEU:HG	2.19	0.42
1:A:74:GLU:HA	1:A:75:PRO:HD3	1.92	0.42
2:B:254:VAL:O	2:B:254:VAL:CG2	2.68	0.42
1:A:38:SER:HA	2:B:250:ILE:HD12	2.02	0.41
1:A:110:MET:HG3	2:B:7:LEU:HD23	2.02	0.41
1:A:426:LEU:HD12	1:A:426:LEU:HA	1.90	0.41
2:B:132:ASP:O	2:B:136:ARG:HG3	2.20	0.41
1:A:56:ASP:O	1:A:58:SER:O	2.39	0.41
1:A:286:HIS:CE1	3:A:2005:HOH:O	2.58	0.41
1:A:61:ARG:HB3	2:B:259:ASN:HA	2.02	0.41
1:A:490:GLN:OE1	1:A:507:GLN:HB2	2.21	0.41
1:A:87:PHE:CE2	1:A:97:ALA:HB2	2.55	0.41
1:A:204:MET:HE3	1:A:204:MET:HB3	1.77	0.41
1:A:105:VAL:HA	1:A:106:PRO:HD3	1.91	0.41
1:A:393:VAL:HG13	1:A:429:ALA:HA	2.02	0.41
2:B:222:LEU:O	2:B:226:LEU:HG	2.21	0.41
1:A:10:VAL:HG11	1:A:128:ILE:CG2	2.48	0.41
1:A:148:LEU:HD22	1:A:152:TYR:CD2	2.56	0.41
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.89	0.41
1:A:564:LYS:HA	1:A:565:PRO:HD3	1.81	0.41
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.92	0.41
1:A:482:LEU:HA	1:A:482:LEU:HD12	1.77	0.41
2:B:130:SER:O	2:B:131:THR:C	2.64	0.41
1:A:457:LYS:HA	1:A:458:PRO:HD3	1.84	0.40
2:B:259:ASN:CG	2:B:260:TYR:H	2.29	0.40
2:B:213:ARG:HB2	2:B:213:ARG:CZ	2.50	0.40
1:A:89:ASP:CG	1:A:90:ARG:H	2.29	0.40
1:A:136:GLU:O	1:A:137:HIS:C	2.64	0.40
1:A:491:LEU:O	1:A:492:ASP:C	2.64	0.40
1:A:132:PHE:CD1	1:A:132:PHE:C	3.00	0.40
1:A:283:GLN:HG3	1:A:284:MET:CE	2.44	0.40
2:B:169:VAL:O	2:B:173:CYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:THR:OG1	2:B:258:HIS:CD2	2.75	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	563/650 (87%)	504 (90%)	45 (8%)	14 (2%)	4	16
2	B	214/279 (77%)	180 (84%)	28 (13%)	6 (3%)	4	14
All	All	777/929 (84%)	684 (88%)	73 (9%)	20 (3%)	4	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ALA
2	B	180	LEU
1	A	59	LYS
1	A	62	LYS
1	A	124	THR
1	A	265	GLY
1	A	267	GLU
1	A	448	THR
1	A	465	GLU
1	A	492	ASP
2	B	42	PHE
2	B	76	VAL
2	B	129	VAL
1	A	454	ARG
1	A	489	GLY
1	A	469	PRO
1	A	564	LYS

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Mol	Chain	Res	Type
2	B	41	PRO
2	B	175	VAL
1	A	216	GLY

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	499/557 (90%)	428 (86%)	71 (14%)	3	12
2	B	200/242 (83%)	183 (92%)	17 (8%)	10	31
All	All	699/799 (88%)	611 (87%)	88 (13%)	4	15

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	29	VAL
1	A	34	LEU
1	A	35	ARG
1	A	42	ARG
1	A	46	ILE
1	A	47	LEU
1	A	51	VAL
1	A	53	VAL
1	A	60	GLN
1	A	73	ILE
1	A	105	VAL
1	A	110	MET
1	A	113	LEU
1	A	122	VAL
1	A	124	THR
1	A	131	LEU
1	A	141	THR
1	A	142	LEU
1	A	144	GLU

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Mol	Chain	Res	Type
1	A	148	LEU
1	A	161	ILE
1	A	168	LEU
1	A	170	THR
1	A	171	LEU
1	A	173	THR
1	A	174	THR
1	A	198	LEU
1	A	202	ILE
1	A	204	MET
1	A	211	ILE
1	A	227	ARG
1	A	231	LEU
1	A	274	LEU
1	A	279	ASP
1	A	283	GLN
1	A	284	MET
1	A	287	LEU
1	A	305	VAL
1	A	311	GLN
1	A	327	LYS
1	A	329	MET
1	A	333	LEU
1	A	335	GLN
1	A	340	MET
1	A	342	LYS
1	A	347	LEU
1	A	350	SER
1	A	372	VAL
1	A	382	VAL
1	A	386	ILE
1	A	389	VAL
1	A	393	VAL
1	A	394	VAL
1	A	399	SER
1	A	400	THR
1	A	407	LEU
1	A	409	LEU
1	A	411	VAL
1	A	412	LEU
1	A	426	LEU
1	A	448	THR

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Mol	Chain	Res	Type
1	A	449	VAL
1	A	460	THR
1	A	462	LYS
1	A	479	VAL
1	A	482	LEU
1	A	494	GLU
1	A	506	VAL
1	A	574	THR
1	A	610	LEU
2	B	3	ARG
2	B	7	LEU
2	B	48	ASN
2	B	51	LYS
2	B	52	ARG
2	B	62	GLN
2	B	103	LYS
2	B	120	GLN
2	B	146	LYS
2	B	149	LYS
2	B	165	TYR
2	B	173	CYS
2	B	227	LEU
2	B	228	GLU
2	B	240	VAL
2	B	254	VAL
2	B	257	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	335	GLN
1	A	424	ASN
1	A	588	GLN
1	A	600	ASN
2	B	102	ASN
2	B	243	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	567/650 (87%)	-0.38	4 (0%) 84 77	44, 87, 153, 237	0
2	B	220/279 (78%)	0.02	7 (3%) 50 40	69, 125, 210, 247	0
All	All	787/929 (84%)	-0.27	11 (1%) 73 64	44, 95, 186, 247	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	261	VAL	3.9
1	A	263	ALA	3.0
2	B	39	PRO	2.9
2	B	242	SER	2.8
2	B	191	HIS	2.8
1	A	320	GLU	2.5
2	B	75	LEU	2.4
1	A	319	GLY	2.3
2	B	76	VAL	2.2
1	A	459	LYS	2.1
2	B	212	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.