



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 PM UTC

PDB ID : 3I2W / pdb_00003i2w
Title : Crystal structure of EFC/F-BAR domain of Drosophila Syndapin/PACSIN
Authors : Edeling, M.A.; Owen, D.J.; Traub, L.M.
Deposited on : 2009-06-29
Resolution : 2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

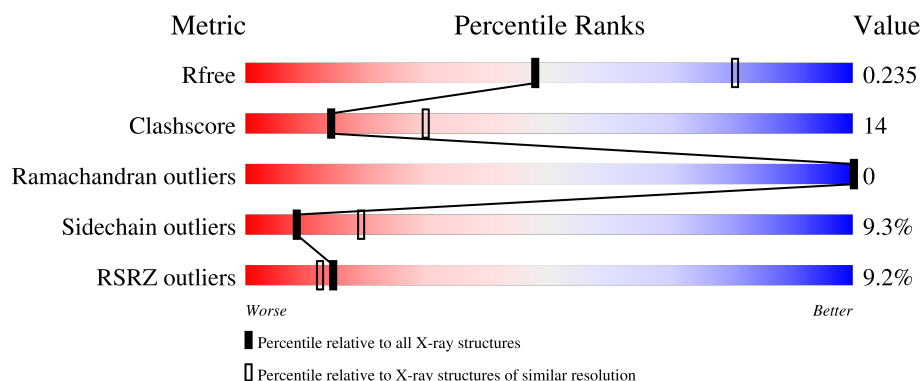
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	290	
1	B	290	

2 Entry composition [i](#)

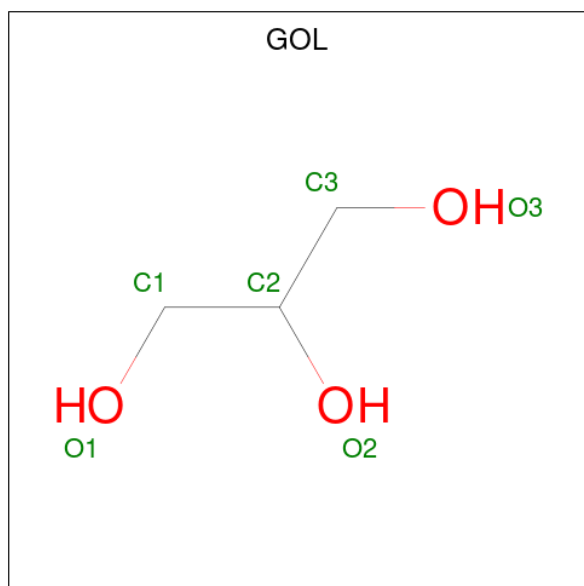
There are 4 unique types of molecules in this entry. The entry contains 4731 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Syndapin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	Se	0	0	0
			2252	1423	390	428	6	5			
1	B	285	Total	C	N	O	S	Se	0	0	0
			2360	1480	415	453	6	6			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Na 2	0	0
3	B	1	Total 1	Na 1	0	0

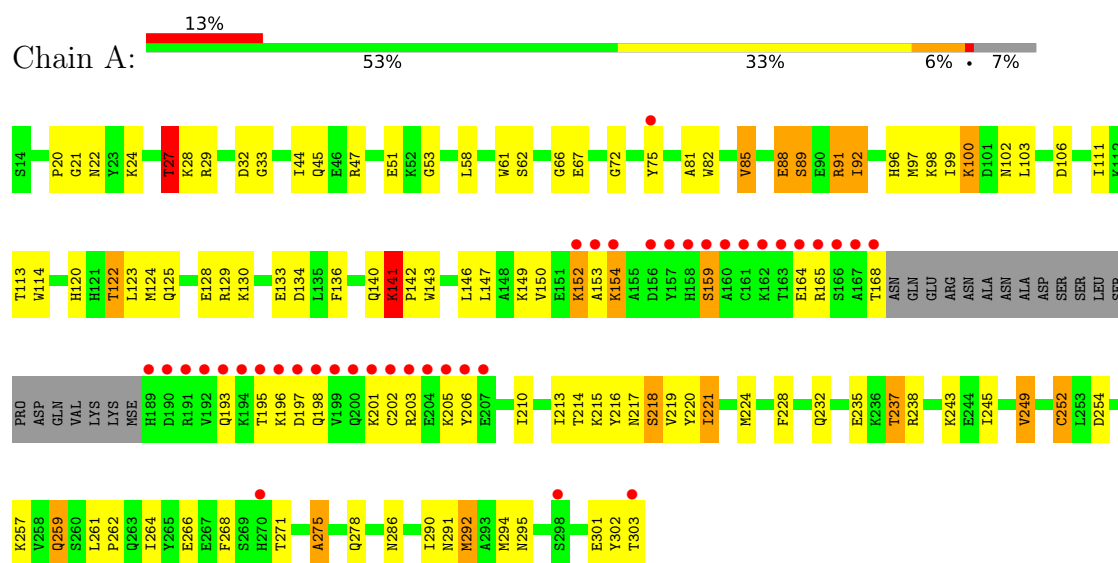
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total 51	O 51	0	0
4	B	53	Total 53	O 53	0	0

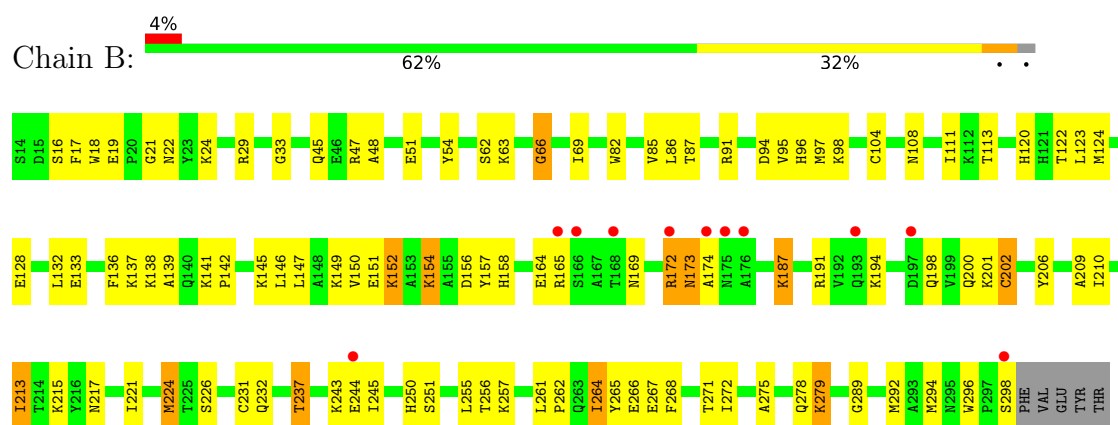
3 Residue-property plots

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

• Molecule 1: Syndapin



• Molecule 1: Syndapin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.59Å 85.53Å 192.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 2.67 39.07 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.07-2.67) 99.7 (39.07-2.67)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.234 , 0.258 (Not available) , 0.235	Depositor DCC
R_{free} test set	1522 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4731	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL

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	1.36	15/2296 (0.7%)	1.35	18/3080 (0.6%)
1	B	1.45	12/2403 (0.5%)	1.37	15/3222 (0.5%)
All	All	1.41	27/4699 (0.6%)	1.36	33/6302 (0.5%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	MSE	SE-CE	-9.31	1.67	1.95
1	A	292	MSE	SE-CE	-6.80	1.75	1.95
1	B	124	MSE	SE-CE	-6.79	1.75	1.95
1	B	294	MSE	CG-SE	-6.62	1.75	1.95
1	B	294	MSE	SE-CE	-6.61	1.75	1.95
1	A	294	MSE	SE-CE	-6.39	1.76	1.95
1	A	224	MSE	SE-CE	-6.24	1.76	1.95
1	A	221	ILE	CA-CB	-6.04	1.46	1.54
1	B	210	ILE	CA-CB	-5.98	1.47	1.54
1	A	295	ASN	CA-C	-5.90	1.45	1.52
1	A	271	THR	C-O	-5.79	1.17	1.24
1	A	124	MSE	CG-SE	-5.68	1.78	1.95
1	B	226	SER	N-CA	-5.67	1.39	1.46
1	A	292	MSE	CG-SE	-5.67	1.78	1.95
1	A	294	MSE	CG-SE	-5.61	1.78	1.95
1	A	62	SER	N-CA	-5.58	1.39	1.46
1	B	237	THR	N-CA	-5.58	1.39	1.46
1	B	62	SER	N-CA	-5.57	1.39	1.46
1	B	244	GLU	CD-OE2	5.45	1.35	1.25
1	B	69	ILE	CA-CB	-5.34	1.47	1.54
1	A	159	SER	CB-OG	5.33	1.52	1.42
1	A	58	LEU	N-CA	-5.22	1.40	1.46
1	B	133	GLU	CA-C	-5.20	1.46	1.52
1	A	124	MSE	SE-CE	-5.06	1.80	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	ASN	C-O	-5.04	1.18	1.24
1	A	91	ARG	N-CA	-5.03	1.40	1.46
1	A	134	ASP	CA-C	-5.01	1.46	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	GLU	N-CA-C	-9.11	100.48	111.69
1	A	89	SER	N-CA-C	-7.80	102.86	111.36
1	B	158	HIS	N-CA-C	-7.39	103.21	112.90
1	B	296	TRP	CA-C-N	-7.15	112.61	119.76
1	B	296	TRP	C-N-CA	-7.15	112.61	119.76
1	B	54	TYR	N-CA-C	-6.73	103.87	111.14
1	A	249	VAL	N-CA-C	-6.73	103.76	110.62
1	B	202	CYS	N-CA-C	6.33	117.85	111.07
1	B	18	TRP	CA-C-N	6.33	129.19	120.39
1	B	18	TRP	C-N-CA	6.33	129.19	120.39
1	A	27	THR	N-CA-CB	-6.10	101.10	110.13
1	A	97	MSE	N-CA-C	-6.04	104.27	111.69
1	B	209	ALA	N-CA-C	-6.03	104.27	111.69
1	A	290	ILE	N-CA-C	5.88	119.29	111.17
1	B	66	GLY	N-CA-C	-5.86	105.70	112.50
1	A	85	VAL	CB-CA-C	-5.71	104.57	111.88
1	B	137	LYS	N-CA-C	-5.70	105.14	111.36
1	A	47	ARG	N-CA-C	-5.68	105.01	111.14
1	A	228	PHE	N-CA-C	-5.61	105.31	111.82
1	A	141	LYS	N-CA-C	5.46	119.91	112.55
1	A	72	GLY	CA-C-N	5.43	125.05	119.56
1	A	72	GLY	C-N-CA	5.43	125.05	119.56
1	B	82	TRP	N-CA-C	-5.38	105.42	111.28
1	A	88	GLU	N-CA-C	-5.34	105.63	111.82
1	A	275	ALA	N-CA-C	-5.33	102.16	110.10
1	B	251	SER	CA-CB-OG	-5.25	100.60	111.10
1	A	136	PHE	CA-C-N	5.23	127.29	120.28
1	A	136	PHE	C-N-CA	5.23	127.29	120.28
1	B	104	CYS	N-CA-C	5.19	118.77	112.23
1	A	66	GLY	N-CA-C	-5.19	106.50	112.73
1	A	237	THR	CA-C-N	5.17	127.20	120.28
1	A	237	THR	C-N-CA	5.17	127.20	120.28
1	B	174	ALA	N-CA-C	-5.03	107.22	113.55

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	2252	0	2207	75	0
1	B	2360	0	2316	65	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	51	0	0	1	0
4	B	53	0	0	3	0
All	All	4731	0	4539	131	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 14.

All (131) 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:27:THR:CG2	1:A:133:GLU:OE2	2.17	0.93
1:A:29:ARG:HH22	1:A:232:GLN:HE21	1.17	0.90
1:B:29:ARG:HH22	1:B:232:GLN:HE21	1.20	0.88
1:A:27:THR:HG23	1:A:133:GLU:OE2	1.73	0.88
1:A:91:ARG:HE	1:A:264:ILE:HG12	1.37	0.88
1:B:146:LEU:HB2	1:B:213:ILE:HD12	1.61	0.82
1:B:139:ALA:CB	1:B:224:MSE:CE	2.58	0.82
1:A:152:LYS:HG2	1:A:153:ALA:N	1.95	0.81
1:B:169:ASN:O	1:B:172:ARG:HB3	1.83	0.78
1:A:164:GLU:OE2	1:A:196:LYS:HG2	1.83	0.78
1:B:21:GLY:O	1:B:24:LYS:HG3	1.84	0.78
1:A:20:PRO:HA	1:A:140:GLN:NE2	2.00	0.76
1:B:139:ALA:HB1	1:B:224:MSE:HE2	1.68	0.76
1:B:139:ALA:HB3	1:B:224:MSE:CE	2.16	0.75
1:B:122:THR:HG22	1:B:123:LEU:HG	1.69	0.73
1:B:139:ALA:CB	1:B:224:MSE:HE2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ARG:HH22	1:B:232:GLN:NE2	1.88	0.72
1:B:120:HIS:HD2	1:B:128:GLU:OE2	1.72	0.72
1:B:139:ALA:HB3	1:B:224:MSE:HE1	1.72	0.71
1:A:51:GLU:OE1	1:A:96:HIS:HD2	1.74	0.71
1:A:102:ASN:O	1:A:106:ASP:HB3	1.92	0.70
1:A:149:LYS:O	1:A:150:VAL:C	2.32	0.69
1:A:27:THR:HG21	1:A:133:GLU:OE2	1.94	0.66
1:A:20:PRO:HA	1:A:140:GLN:HE22	1.60	0.65
1:B:139:ALA:HB1	1:B:224:MSE:CE	2.24	0.65
1:A:302:TYR:HE2	1:B:165:ARG:HH11	1.43	0.65
1:A:53:GLY:HA3	2:A:1:GOL:H12	1.81	0.63
1:B:111:ILE:HD11	1:B:245:ILE:HG21	1.80	0.63
1:A:21:GLY:O	1:A:24:LYS:HG3	2.00	0.61
1:A:193:GLN:HA	1:A:196:LYS:HE2	1.81	0.61
1:A:235:GLU:OE1	1:A:238:ARG:NH2	2.32	0.61
1:A:29:ARG:HH22	1:A:232:GLN:NE2	1.96	0.60
1:B:217:ASN:O	1:B:221:ILE:HG13	2.01	0.60
1:A:286:ASN:HD22	1:A:291:ASN:HB2	1.66	0.60
1:B:146:LEU:HB2	1:B:213:ILE:CD1	2.30	0.60
1:B:152:LYS:HE2	1:B:156:ASP:OD2	2.01	0.60
1:B:132:LEU:HD23	1:B:231:CYS:SG	2.42	0.59
1:A:111:ILE:HD11	1:A:245:ILE:HG21	1.85	0.59
1:A:220:TYR:O	1:A:221:ILE:C	2.42	0.59
1:A:235:GLU:CD	1:A:238:ARG:NH2	2.63	0.57
1:A:262:PRO:HA	1:B:256:THR:HG21	1.86	0.57
1:A:286:ASN:ND2	1:A:291:ASN:HD22	2.05	0.55
1:B:172:ARG:HG3	1:B:173:ASN:HD22	1.72	0.54
1:A:88:GLU:HG3	1:A:89:SER:N	2.23	0.53
1:B:132:LEU:HD12	1:B:132:LEU:N	2.23	0.53
1:B:172:ARG:CG	1:B:173:ASN:HD22	2.22	0.53
1:A:261:LEU:N	1:A:262:PRO:CD	2.71	0.53
1:A:125:GLN:HG3	1:A:130:LYS:NZ	2.24	0.53
1:A:61:TRP:HH2	1:A:85:VAL:HG11	1.73	0.52
1:A:259:GLN:O	1:A:262:PRO:HD2	2.10	0.52
1:B:122:THR:O	1:B:123:LEU:C	2.51	0.52
1:B:200:GLN:O	1:B:201:LYS:C	2.52	0.52
1:A:122:THR:O	1:A:123:LEU:C	2.53	0.51
1:B:149:LYS:O	1:B:150:VAL:C	2.49	0.51
1:A:75:TYR:CD1	1:A:75:TYR:N	2.78	0.50
1:A:149:LYS:HA	1:A:152:LYS:HD2	1.92	0.50
1:B:33:GLY:HA3	4:B:340:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLY:HA2	1:B:86:LEU:CD1	2.41	0.50
1:A:154:LYS:HB2	1:A:206:TYR:CE1	2.47	0.50
1:A:33:GLY:HA3	4:A:342:HOH:O	2.11	0.49
1:A:125:GLN:HG3	1:A:130:LYS:HE2	1.95	0.49
1:A:120:HIS:ND1	1:A:128:GLU:OE2	2.34	0.49
1:B:139:ALA:C	1:B:224:MSE:HE3	2.38	0.49
1:A:154:LYS:HB2	1:A:206:TYR:HE1	1.78	0.48
1:B:51:GLU:OE1	1:B:96:HIS:HD2	1.96	0.48
1:B:45:GLN:O	1:B:48:ALA:HB3	2.14	0.48
1:A:27:THR:HG23	1:A:129:ARG:HE	1.77	0.48
1:A:164:GLU:OE2	1:A:196:LYS:CG	2.59	0.48
1:A:88:GLU:OE2	1:B:47:ARG:NH2	2.40	0.47
1:A:217:ASN:O	1:A:218:SER:C	2.56	0.47
1:A:125:GLN:HG3	1:A:130:LYS:CE	2.44	0.47
1:A:165:ARG:HD3	1:A:165:ARG:HA	1.78	0.46
1:A:61:TRP:HH2	1:A:85:VAL:CG1	2.27	0.46
1:A:243:LYS:HG3	1:B:275:ALA:HB3	1.97	0.46
1:A:292:MSE:SE	1:B:17:PHE:H	2.48	0.46
1:A:114:TRP:HZ2	1:A:237:THR:HG22	1.80	0.45
1:B:145:LYS:O	1:B:146:LEU:C	2.58	0.45
1:A:213:ILE:O	1:A:216:TYR:N	2.46	0.45
1:B:198:GLN:OE1	1:B:198:GLN:HA	2.15	0.45
1:A:210:ILE:HD13	1:B:298:SER:HA	1.99	0.45
1:A:81:ALA:O	1:A:82:TRP:C	2.57	0.44
1:B:141:LYS:HB3	1:B:142:PRO:HD3	1.99	0.44
1:A:22:ASN:C	1:A:24:LYS:H	2.23	0.44
1:A:195:THR:HA	1:A:198:GLN:HB3	1.99	0.44
1:A:141:LYS:O	1:A:142:PRO:C	2.60	0.44
1:A:254:ASP:OD1	1:A:254:ASP:C	2.60	0.44
1:B:271:THR:O	1:B:272:ILE:C	2.60	0.44
1:B:91:ARG:HB3	1:B:264:ILE:HG12	2.00	0.44
1:B:172:ARG:CG	1:B:173:ASN:ND2	2.80	0.44
1:B:94:ASP:O	1:B:95:VAL:C	2.58	0.44
1:B:122:THR:HG22	1:B:123:LEU:N	2.33	0.44
1:A:249:VAL:O	1:A:252:CYS:HB2	2.18	0.43
1:B:154:LYS:HB2	1:B:206:TYR:CZ	2.53	0.43
1:B:257:LYS:HE3	4:B:352:HOH:O	2.18	0.43
1:A:152:LYS:HG2	1:A:153:ALA:H	1.80	0.43
1:B:255:LEU:HD23	1:B:255:LEU:HA	1.88	0.43
1:A:53:GLY:HA3	2:A:1:GOL:C1	2.47	0.43
1:B:154:LYS:HB2	1:B:206:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:NH2	1:A:232:GLN:HE21	2.00	0.43
1:A:213:ILE:CG2	1:A:214:THR:N	2.82	0.43
1:B:261:LEU:HD12	1:B:261:LEU:HA	1.65	0.43
1:B:16:SER:O	1:B:19:GLU:HB2	2.19	0.42
1:A:92:ILE:HD12	1:A:92:ILE:HA	1.76	0.42
1:A:216:TYR:O	1:A:219:VAL:N	2.47	0.42
1:B:97:MSE:HE3	4:B:334:HOH:O	2.20	0.42
1:B:157:TYR:HB2	1:B:202:CYS:HB3	2.02	0.42
1:A:213:ILE:O	1:A:214:THR:C	2.62	0.42
1:B:136:PHE:O	1:B:224:MSE:HE1	2.20	0.42
1:A:216:TYR:O	1:A:217:ASN:C	2.62	0.42
1:B:132:LEU:CD2	1:B:231:CYS:SG	3.08	0.42
1:B:261:LEU:O	1:B:262:PRO:C	2.63	0.41
1:A:44:ILE:O	1:A:45:GLN:C	2.62	0.41
1:B:157:TYR:O	1:B:157:TYR:CG	2.73	0.41
1:B:278:GLN:O	1:B:279:LYS:C	2.61	0.41
1:B:289:GLY:O	1:B:292:MSE:HG3	2.20	0.41
1:A:142:PRO:HB2	1:A:216:TYR:CE2	2.56	0.41
1:A:20:PRO:HD3	1:A:143:TRP:HZ3	1.84	0.41
1:A:275:ALA:HB3	1:B:243:LYS:HG3	2.01	0.41
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.94	0.41
1:A:146:LEU:HB2	1:A:213:ILE:HG13	2.03	0.41
1:A:254:ASP:HA	1:B:265:TYR:CE1	2.55	0.41
1:B:268:PHE:CD1	1:B:268:PHE:O	2.74	0.41
1:A:22:ASN:C	1:A:24:LYS:N	2.76	0.41
1:A:32:ASP:O	1:A:33:GLY:C	2.62	0.41
1:B:22:ASN:C	1:B:24:LYS:H	2.29	0.41
1:B:265:TYR:O	1:B:266:GLU:C	2.64	0.41
1:B:187:LYS:HE2	1:B:191:ARG:HH21	1.86	0.41
1:A:99:ILE:O	1:A:100:LYS:C	2.62	0.40
1:A:261:LEU:H	1:A:262:PRO:CD	2.35	0.40
1:B:147:LEU:O	1:B:151:GLU:HG2	2.22	0.40
1:A:268:PHE:CD2	1:B:250:HIS:HD2	2.39	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	266/290 (92%)	244 (92%)	22 (8%)	0	100	100
1	B	283/290 (98%)	261 (92%)	22 (8%)	0	100	100
All	All	549/580 (95%)	505 (92%)	44 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	247/259 (95%)	219 (89%)	28 (11%)	5	13
1	B	260/259 (100%)	241 (93%)	19 (7%)	13	29
All	All	507/518 (98%)	460 (91%)	47 (9%)	8	19

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	28	LYS
1	A	67	GLU
1	A	92	ILE
1	A	98	LYS
1	A	100	LYS
1	A	113	THR
1	A	122	THR

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Mol	Chain	Res	Type
1	A	141	LYS
1	A	147	LEU
1	A	152	LYS
1	A	154	LYS
1	A	159	SER
1	A	168	THR
1	A	197	ASP
1	A	201	LYS
1	A	202	CYS
1	A	203	ARG
1	A	205	LYS
1	A	215	LYS
1	A	218	SER
1	A	252	CYS
1	A	257	LYS
1	A	259	GLN
1	A	266	GLU
1	A	278	GLN
1	A	301	GLU
1	A	303	THR
1	B	63	LYS
1	B	85	VAL
1	B	87	THR
1	B	98	LYS
1	B	113	THR
1	B	138	LYS
1	B	152	LYS
1	B	154	LYS
1	B	164	GLU
1	B	172	ARG
1	B	173	ASN
1	B	187	LYS
1	B	194	LYS
1	B	213	ILE
1	B	215	LYS
1	B	237	THR
1	B	264	ILE
1	B	267	GLU
1	B	279	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	96	HIS
1	A	193	GLN
1	A	198	GLN
1	A	232	GLN
1	A	250	HIS
1	A	259	GLN
1	A	274	ASN
1	A	286	ASN
1	A	287	ASN
1	A	291	ASN
1	B	96	HIS
1	B	102	ASN
1	B	105	ASN
1	B	110	GLN
1	B	120	HIS
1	B	173	ASN
1	B	200	GLN
1	B	232	GLN
1	B	248	ASN
1	B	273	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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
2	GOL	B	2	-	5,5,5	0.24	0	5,5,5	1.39	1 (20%)
2	GOL	A	1	-	5,5,5	0.63	0	5,5,5	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	2	-	-	4/4/4/4	-
2	GOL	A	1	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GOL	C3-C2-C1	-2.69	101.92	111.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	GOL	O1-C1-C2-C3
2	B	2	GOL	O1-C1-C2-C3
2	B	2	GOL	C1-C2-C3-O3
2	A	1	GOL	O1-C1-C2-O2
2	A	1	GOL	O2-C2-C3-O3
2	B	2	GOL	O1-C1-C2-O2
2	B	2	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/290 (91%)	0.64	39 (14%) 6 4	22, 35, 156, 174	1 (0%)
1	B	279/290 (96%)	0.15	11 (3%) 43 38	20, 32, 67, 85	0
All	All	544/580 (93%)	0.39	50 (9%) 14 12	20, 33, 110, 174	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ARG	12.6
1	A	163	THR	8.3
1	A	201	LYS	6.0
1	A	192	VAL	5.9
1	A	189	HIS	5.7
1	A	168	THR	5.5
1	A	162	LYS	5.4
1	A	303	THR	5.0
1	B	174	ALA	4.9
1	A	166	SER	4.8
1	B	175	ASN	4.8
1	A	198	GLN	4.8
1	A	206	TYR	4.7
1	A	199	VAL	4.6
1	A	195	THR	4.5
1	A	159	SER	4.4
1	A	203	ARG	4.4
1	A	158	HIS	4.2
1	A	194	LYS	4.1
1	A	160	ALA	4.0
1	A	167	ALA	4.0
1	A	205	LYS	3.9
1	A	156	ASP	3.8
1	A	270	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	161	CYS	3.8
1	B	298	SER	3.7
1	A	202	CYS	3.6
1	A	157	TYR	3.5
1	A	164	GLU	3.4
1	B	244	GLU	3.3
1	A	190	ASP	3.1
1	A	153	ALA	3.1
1	A	200	GLN	3.1
1	A	154	LYS	3.0
1	A	298	SER	2.9
1	A	152	LYS	2.9
1	A	207	GLU	2.8
1	A	196	LYS	2.5
1	A	197	ASP	2.5
1	B	172	ARG	2.4
1	A	193	GLN	2.4
1	B	176	ALA	2.3
1	B	168	THR	2.3
1	A	75	TYR	2.2
1	B	166	SER	2.2
1	A	165	ARG	2.1
1	B	165	ARG	2.1
1	B	193	GLN	2.1
1	A	204	GLU	2.0
1	B	197	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	3	1/1	0.74	0.22	46,46,46,46	0
2	GOL	A	1	6/6	0.88	0.17	51,53,54,56	0
2	GOL	B	2	6/6	0.95	0.09	27,32,32,35	0
3	NA	B	304	1/1	0.95	0.05	33,33,33,33	0
3	NA	A	304	1/1	0.96	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.