



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:42 AM UTC

PDB ID : 9SOC / pdb_00009soc
Title : Murine RanBP10-Twa1 complex
Authors : van gen Hassend, P.M.; Schindelin, H.
Deposited on : 2025-09-12
Resolution : 3.18 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

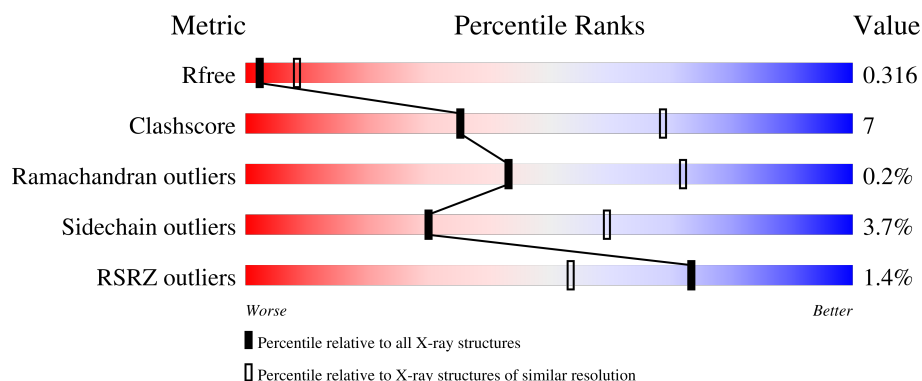
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	595	<div> <div>2%</div> <div>61% 13% 26%</div> </div>
1	C	595	<div> <div>2%</div> <div>60% 13% 26%</div> </div>
2	B	228	<div> <div>2%</div> <div>77% 20%</div> </div>
2	D	228	<div> <div>2%</div> <div>82% 15%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10581 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 Ran-binding protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3449	2171	614	643	21			
1	C	442	Total	C	N	O	S	0	0	0
			3449	2171	614	643	21			

- Molecule 2 is a protein called Glucose-induced degradation protein 8 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1838	1159	313	356	10			
2	D	223	Total	C	N	O	S	0	0	0
			1838	1159	313	356	10			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

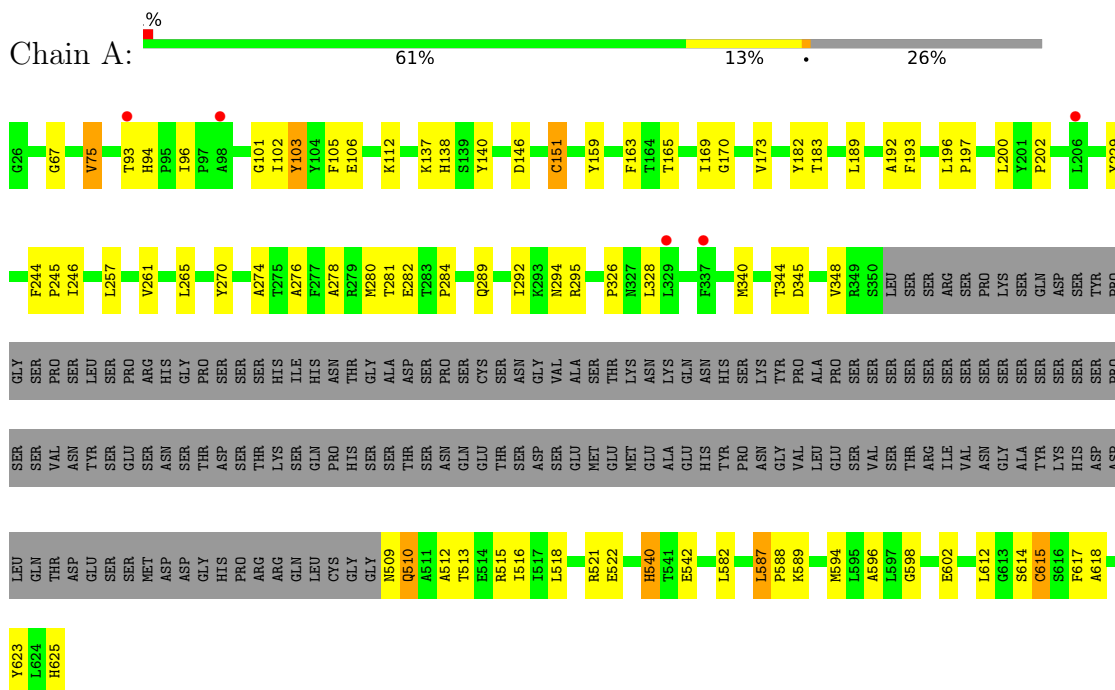
- Molecule 4 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Co	0	0
			1	1		

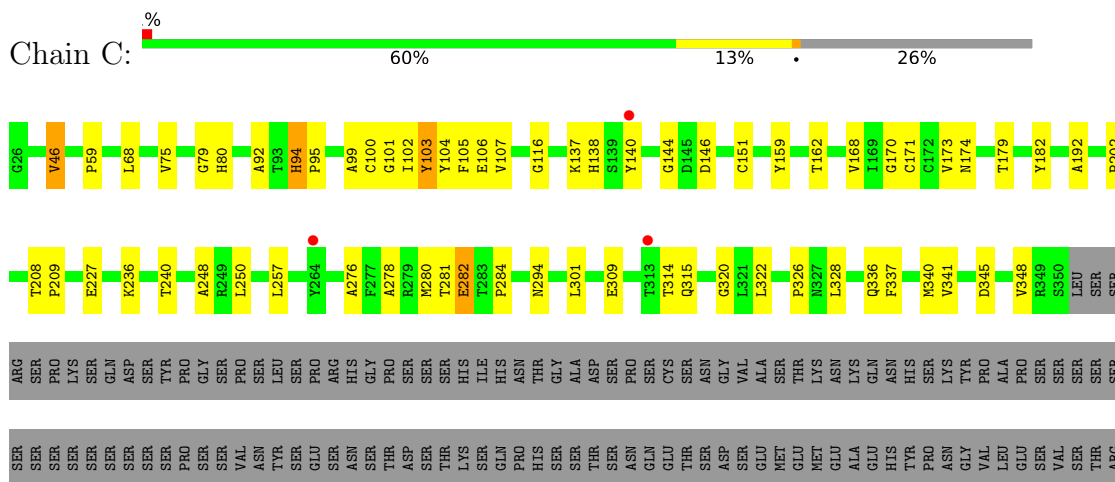
3 Residue-property plots

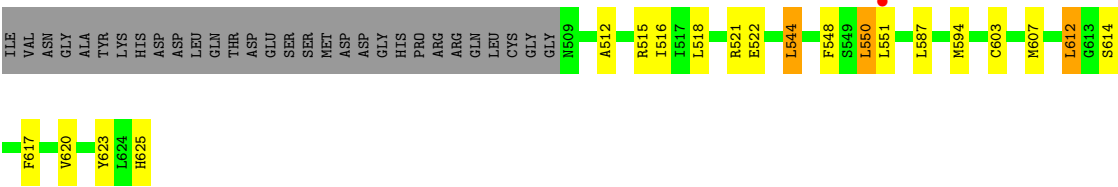
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ran-binding protein 10

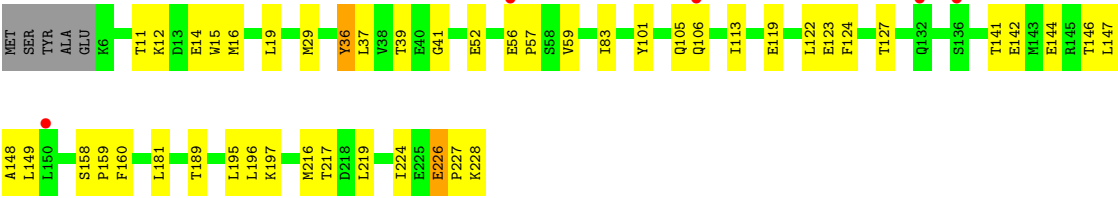
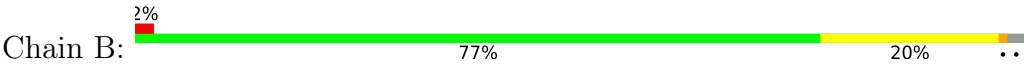


• Molecule 1: Ran-binding protein 10

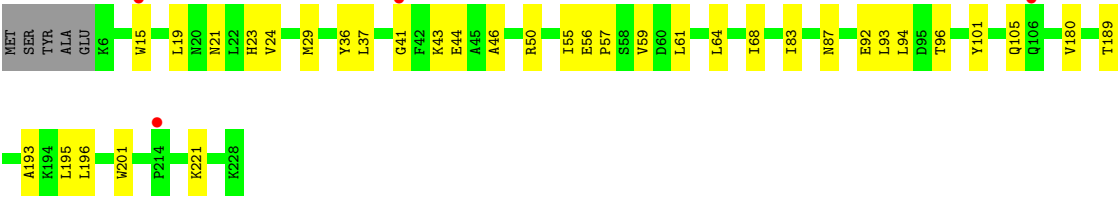
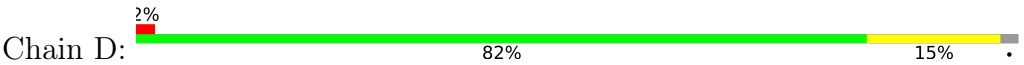




● Molecule 2: Glucose-induced degradation protein 8 homolog



● Molecule 2: Glucose-induced degradation protein 8 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.92Å 124.92Å 479.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.18 20.00 – 3.18	Depositor EDS
% Data completeness (in resolution range)	28.5 (20.00-3.18) 28.5 (20.00-3.18)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.299 , 0.312 0.304 , 0.316	Depositor DCC
R_{free} test set	513 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2573e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, CO

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	0.28	0/3534	0.57	0/4789
1	C	0.27	0/3534	0.53	0/4789
2	B	0.25	0/1867	0.52	0/2512
2	D	0.25	0/1867	0.52	0/2512
All	All	0.27	0/10802	0.54	0/14602

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 [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	3449	0	3354	53	0
1	C	3449	0	3354	60	0
2	B	1838	0	1845	35	0
2	D	1838	0	1845	27	0
3	C	6	0	8	0	0
4	D	1	0	0	0	0
All	All	10581	0	10406	155	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 7.

All (155) 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:596:ALA:HB2	2:B:216:MET:HE1	1.51	0.92
2:B:57:PRO:HB2	2:B:59:VAL:HG22	1.54	0.87
2:B:106:GLN:HG3	2:B:146:THR:HG21	1.68	0.76
1:C:257:LEU:HD22	2:D:196:LEU:HD13	1.67	0.76
2:B:141:THR:HG21	1:C:227:GLU:HG3	1.68	0.73
1:C:345:ASP:O	1:C:348:VAL:HG22	1.88	0.72
1:C:620:VAL:HG23	2:D:195:LEU:HD11	1.73	0.71
1:A:596:ALA:CB	2:B:216:MET:HE1	2.23	0.68
1:A:512:ALA:O	1:A:516:ILE:HG23	1.94	0.67
1:A:509:ASN:ND2	1:A:510:GLN:OE1	2.28	0.66
2:D:24:VAL:HG11	2:D:29:MET:HE3	1.80	0.64
1:A:159:TYR:CE1	1:A:192:ALA:HB2	2.33	0.64
1:A:246:ILE:HG21	2:B:197:LYS:HE2	1.79	0.63
1:C:512:ALA:O	1:C:516:ILE:HG23	1.98	0.63
1:C:102:ILE:HA	1:C:173:VAL:O	1.98	0.63
1:A:257:LEU:HD22	2:B:196:LEU:HD13	1.80	0.62
1:C:623:TYR:HB2	2:D:195:LEU:HD13	1.83	0.61
1:A:623:TYR:HB2	2:B:195:LEU:HD13	1.84	0.59
2:D:92:GLU:O	2:D:96:THR:HG23	2.04	0.58
1:A:163:PHE:CB	1:A:169:ILE:HD11	2.33	0.58
2:B:147:LEU:HD12	2:B:148:ALA:N	2.18	0.58
2:B:101:TYR:O	2:B:105:GLN:HG2	2.04	0.57
1:C:144:GLY:O	1:C:162:THR:OG1	2.21	0.57
1:C:236:LYS:O	1:C:240:THR:HG23	2.06	0.56
2:D:59:VAL:HG23	2:D:61:LEU:H	1.71	0.55
1:C:140:TYR:CD1	1:C:151:CYS:HA	2.41	0.55
2:D:56:GLU:N	2:D:57:PRO:CD	2.70	0.55
2:B:56:GLU:N	2:B:57:PRO:HD2	2.23	0.54
1:C:607:MET:HE1	2:D:201:TRP:CH2	2.42	0.54
1:C:104:TYR:HA	1:C:171:CYS:O	2.08	0.53
1:C:594:MET:HG2	2:D:29:MET:HE1	1.89	0.53
1:A:513:THR:O	1:A:516:ILE:HG12	2.08	0.53
2:D:43:LYS:HD2	2:D:61:LEU:HB3	1.90	0.53
1:A:261:VAL:HG21	2:B:36:TYR:CE2	2.44	0.52
1:A:276:ALA:O	1:A:280:MET:HG2	2.09	0.52
1:C:607:MET:HE3	1:C:612:LEU:HD13	1.92	0.52
1:C:101:GLY:O	1:C:102:ILE:HD13	2.10	0.52
2:D:24:VAL:CG1	2:D:29:MET:HE3	2.39	0.52
1:A:345:ASP:O	1:A:348:VAL:HG22	2.10	0.52
1:C:281:THR:HG23	1:C:282:GLU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:HA	1:A:170:GLY:HA2	1.91	0.51
2:B:144:GLU:HA	2:B:147:LEU:CD2	2.40	0.51
1:C:544:LEU:HD22	1:C:548:PHE:CZ	2.46	0.51
2:D:57:PRO:HB3	2:D:59:VAL:HG22	1.92	0.51
1:A:602:GLU:HG3	2:B:15:TRP:CH2	2.46	0.51
1:C:345:ASP:HB3	1:C:348:VAL:HG13	1.91	0.51
1:C:515:ARG:HA	1:C:518:LEU:HD12	1.93	0.51
1:C:140:TYR:HD1	1:C:151:CYS:HA	1.76	0.50
1:A:270:TYR:CG	2:B:52:GLU:HB3	2.46	0.50
2:D:101:TYR:O	2:D:105:GLN:HG2	2.10	0.50
1:C:116:GLY:HA2	1:C:208:THR:HG21	1.94	0.50
1:C:46:VAL:HG22	1:C:99:ALA:HB3	1.92	0.50
2:B:149:LEU:HD23	2:B:160:PHE:HB2	1.92	0.50
1:A:515:ARG:HA	1:A:518:LEU:HD12	1.92	0.50
2:B:12:LYS:HD2	2:B:226:GLU:HB3	1.93	0.50
1:A:96:ILE:HG13	1:A:202:PRO:HD3	1.94	0.50
1:A:101:GLY:O	1:A:102:ILE:HD13	2.11	0.49
2:D:93:LEU:HD21	2:D:180:VAL:HG22	1.92	0.49
1:A:294:ASN:OD1	1:A:295:ARG:N	2.45	0.49
1:C:103:TYR:CD1	1:C:105:PHE:CZ	3.00	0.49
1:A:140:TYR:CD1	1:A:151:CYS:HA	2.48	0.49
2:D:193:ALA:HA	2:D:196:LEU:HD12	1.94	0.49
2:B:123:GLU:O	2:B:127:THR:HG23	2.12	0.49
2:D:57:PRO:CB	2:D:59:VAL:HG22	2.43	0.49
2:B:119:GLU:HG3	2:B:122:LEU:HD12	1.95	0.48
2:B:141:THR:HG21	1:C:227:GLU:CG	2.39	0.48
1:C:170:GLY:O	1:C:182:TYR:HA	2.12	0.48
1:C:107:VAL:O	1:C:168:VAL:HA	2.14	0.48
2:D:37:LEU:O	2:D:41:GLY:N	2.47	0.48
1:A:102:ILE:CG1	1:A:617:PHE:HZ	2.27	0.48
1:A:163:PHE:CG	1:A:169:ILE:CD1	2.97	0.47
1:C:105:PHE:CZ	1:C:202:PRO:HG3	2.50	0.47
1:A:521:ARG:HG2	1:A:522:GLU:N	2.29	0.47
1:C:250:LEU:HD23	1:C:250:LEU:C	2.39	0.47
1:A:257:LEU:N	1:A:257:LEU:HD23	2.30	0.47
1:C:544:LEU:HD22	1:C:548:PHE:CE2	2.50	0.47
2:B:12:LYS:O	2:B:15:TRP:HB3	2.15	0.47
1:A:278:ALA:HB1	1:A:284:PRO:HD2	1.97	0.47
2:D:24:VAL:HG11	2:D:29:MET:CE	2.45	0.47
2:B:56:GLU:N	2:B:57:PRO:CD	2.78	0.46
1:C:276:ALA:O	1:C:280:MET:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:HE1	1:A:151:CYS:SG	2.37	0.46
1:A:163:PHE:CG	1:A:169:ILE:HD11	2.50	0.46
1:C:314:THR:HG21	1:C:322:LEU:HD21	1.97	0.46
1:A:265:LEU:CD1	1:A:274:ALA:HB2	2.46	0.46
2:B:37:LEU:O	2:B:41:GLY:N	2.49	0.46
1:C:548:PHE:HD1	1:C:551:LEU:HD12	1.80	0.46
1:A:102:ILE:HA	1:A:173:VAL:O	2.15	0.45
1:A:340:MET:SD	1:A:516:ILE:HG22	2.56	0.45
2:B:39:THR:HG23	2:B:181:LEU:HD13	1.98	0.45
1:C:521:ARG:HG2	1:C:522:GLU:N	2.31	0.45
2:B:16:MET:SD	2:B:224:ILE:HG12	2.56	0.45
2:B:144:GLU:O	2:B:147:LEU:HG	2.16	0.45
2:B:11:THR:HB	2:B:14:GLU:HB2	1.99	0.45
1:C:137:LYS:O	1:C:138:HIS:HB2	2.16	0.45
2:D:43:LYS:HA	2:D:46:ALA:HB3	1.99	0.45
1:C:280:MET:HE3	2:D:44:GLU:HB2	1.98	0.45
2:B:144:GLU:HA	2:B:147:LEU:HG	1.99	0.44
1:C:102:ILE:CG1	1:C:617:PHE:HZ	2.29	0.44
1:C:276:ALA:O	1:C:280:MET:HB2	2.17	0.44
1:A:182:TYR:O	1:A:189:LEU:HB2	2.16	0.44
1:A:540:HIS:N	1:A:540:HIS:ND1	2.65	0.44
1:A:103:TYR:CD1	1:A:105:PHE:CZ	3.05	0.44
1:A:112:LYS:HB3	1:A:165:THR:HB	1.99	0.44
1:A:102:ILE:HG13	1:A:617:PHE:HZ	1.82	0.44
1:A:197:PRO:HD2	1:A:200:LEU:HD11	1.99	0.44
1:C:59:PRO:HB3	1:C:68:LEU:HD12	2.00	0.44
1:C:79:GLY:C	1:C:80:HIS:CG	2.96	0.44
1:C:341:VAL:HG11	1:C:550:LEU:CD2	2.48	0.44
1:C:159:TYR:CE1	1:C:192:ALA:HB2	2.53	0.43
1:A:344:THR:O	1:A:345:ASP:HB2	2.18	0.43
1:A:598:GLY:O	1:A:602:GLU:HG2	2.18	0.43
1:A:594:MET:HG2	2:B:29:MET:HE1	1.99	0.43
1:C:94:HIS:HB3	1:C:95:PRO:HD2	2.00	0.43
2:B:158:SER:N	2:B:159:PRO:CD	2.81	0.43
1:A:229:TYR:CE1	1:C:248:ALA:HB2	2.53	0.43
2:B:227:PRO:O	2:B:228:LYS:C	2.60	0.43
1:C:278:ALA:HB1	1:C:284:PRO:HD2	1.99	0.43
1:A:163:PHE:HB3	1:A:169:ILE:HD11	1.99	0.43
2:D:56:GLU:N	2:D:57:PRO:HD3	2.33	0.43
1:C:315:GLN:HA	1:C:320:GLY:HA2	2.01	0.43
2:B:216:MET:HE2	2:B:219:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:ARG:HG2	2:D:55:ILE:HG12	2.01	0.42
1:A:289:GLN:HA	1:A:292:ILE:HD12	2.01	0.42
1:C:100:CYS:C	1:C:102:ILE:H	2.28	0.42
1:C:106:GLU:HA	1:C:170:GLY:HA2	2.02	0.42
2:D:43:LYS:HB2	2:D:64:LEU:HD23	2.01	0.42
1:A:137:LYS:O	1:A:138:HIS:HB2	2.20	0.42
1:A:278:ALA:HB1	1:A:284:PRO:CD	2.50	0.42
1:C:92:ALA:HB2	1:C:202:PRO:HG2	2.02	0.42
2:D:87:ASN:OD1	2:D:94:LEU:HD12	2.20	0.42
1:A:193:PHE:HB2	1:A:196:LEU:HD11	2.02	0.42
2:B:113:ILE:HD13	2:B:149:LEU:CD1	2.50	0.42
1:C:102:ILE:HG12	1:C:617:PHE:HZ	1.85	0.41
1:A:615:CYS:O	1:A:618:ALA:O	2.38	0.41
1:C:301:LEU:HD22	1:C:309:GLU:HB2	2.01	0.41
1:C:345:ASP:CB	1:C:348:VAL:HG13	2.50	0.41
1:A:281:THR:HG23	1:A:282:GLU:N	2.35	0.41
2:B:106:GLN:OE1	2:B:142:GLU:OE1	2.39	0.41
1:C:79:GLY:O	1:C:80:HIS:C	2.64	0.41
1:C:257:LEU:CD2	2:D:196:LEU:HD13	2.45	0.41
2:D:21:ASN:O	2:D:23:HIS:CE1	2.74	0.41
1:C:79:GLY:HA2	1:C:209:PRO:HB2	2.03	0.41
1:C:257:LEU:N	1:C:257:LEU:HD23	2.36	0.41
1:C:336:GLN:HG3	1:C:345:ASP:OD1	2.20	0.41
1:A:93:THR:HG22	1:A:94:HIS:NE2	2.36	0.41
1:C:337:PHE:O	1:C:340:MET:HG2	2.21	0.41
1:C:102:ILE:HG12	1:C:617:PHE:CZ	2.57	0.40
1:A:582:LEU:HD23	1:A:587:LEU:O	2.22	0.40
2:B:124:PHE:HA	2:B:127:THR:OG1	2.21	0.40
1:C:603:CYS:SG	2:D:15:TRP:HH2	2.44	0.40
1:A:67:GLY:O	1:A:75:VAL:HA	2.21	0.40
1:A:588:PRO:O	1:A:589:LYS:C	2.64	0.40
1:C:79:GLY:HA2	1:C:209:PRO:CB	2.51	0.40
1:A:244:PHE:O	1:A:245:PRO:C	2.64	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	438/595 (74%)	424 (97%)	13 (3%)	1 (0%)	43	72
1	C	438/595 (74%)	423 (97%)	14 (3%)	1 (0%)	43	72
2	B	221/228 (97%)	213 (96%)	8 (4%)	0	100	100
2	D	221/228 (97%)	215 (97%)	6 (3%)	0	100	100
All	All	1318/1646 (80%)	1275 (97%)	41 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	PRO
1	A	326	PRO

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	368/507 (73%)	354 (96%)	14 (4%)	29	59
1	C	368/507 (73%)	352 (96%)	16 (4%)	26	56
2	B	203/207 (98%)	197 (97%)	6 (3%)	36	63
2	D	203/207 (98%)	197 (97%)	6 (3%)	36	63
All	All	1142/1428 (80%)	1100 (96%)	42 (4%)	30	59

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	103	TYR
1	A	146	ASP
1	A	151	CYS
1	A	183	THR
1	A	328	LEU
1	A	510	GLN
1	A	540	HIS
1	A	542	GLU
1	A	587	LEU
1	A	612	LEU
1	A	614	SER
1	A	615	CYS
1	A	625	HIS
2	B	19	LEU
2	B	36	TYR
2	B	83	ILE
2	B	189	THR
2	B	217	THR
2	B	226	GLU
1	C	46	VAL
1	C	75	VAL
1	C	94	HIS
1	C	103	TYR
1	C	146	ASP
1	C	174	ASN
1	C	179	THR
1	C	282	GLU
1	C	294	ASN
1	C	328	LEU
1	C	544	LEU
1	C	550	LEU
1	C	587	LEU
1	C	612	LEU
1	C	614	SER
1	C	625	HIS
2	D	19	LEU
2	D	36	TYR
2	D	68	ILE
2	D	83	ILE
2	D	189	THR
2	D	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	143	HIS
1	A	242	HIS
1	A	267	HIS
1	A	509	ASN
1	A	510	GLN
1	A	563	HIS
1	A	585	GLN
2	B	25	GLN
2	B	128	GLN
1	C	174	ASN
1	C	185	ASN
1	C	242	HIS
1	C	267	HIS
1	C	299	GLN
1	C	578	ASN
2	D	106	GLN
2	D	128	GLN
2	D	177	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 2 ligands modelled in this entry, 1 is 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	GOL	C	701	-	5,5,5	0.89	0	5,5,5	1.05	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
3	GOL	C	701	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	701	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	442/595 (74%)	-0.01	5 (1%) 78 60	67, 95, 124, 142	0
1	C	442/595 (74%)	0.06	4 (0%) 81 64	72, 101, 139, 158	0
2	B	223/228 (97%)	0.05	5 (2%) 62 41	73, 97, 115, 130	0
2	D	223/228 (97%)	0.01	4 (1%) 67 47	74, 93, 119, 146	0
All	All	1330/1646 (80%)	0.03	18 (1%) 73 53	67, 97, 129, 158	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ALA	3.6
1	A	337	PHE	3.2
2	B	132	GLN	3.0
2	B	136	SER	2.8
2	B	106	GLN	2.6
2	B	56	GLU	2.5
2	B	150	LEU	2.5
2	D	214	PRO	2.5
2	D	106	GLN	2.4
1	A	93	THR	2.4
1	A	206	LEU	2.3
2	D	41	GLY	2.2
1	C	313	THR	2.2
2	D	15	TRP	2.1
1	C	264	TYR	2.1
1	C	140	TYR	2.1
1	C	551	LEU	2.0
1	A	329	LEU	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(\AA^2)	Q<0.9
3	GOL	C	701	6/6	0.69	0.12	51,51,51,51	6
4	CO	D	301	1/1	0.99	0.01	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.