



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:12 AM UTC

PDB ID : 6WNX / pdb_00006wnx
Title : FBXW11-SKP1 in complex with a pSer33/pSer37 Beta-Catenin peptide
Authors : Ivanochko, D.; Edwards, A.M.; Bountra, C.; Arrowsmith, C.H.; Boettcher, J.;
Structural Genomics Consortium (SGC)
Deposited on : 2020-04-23
Resolution : 2.50 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

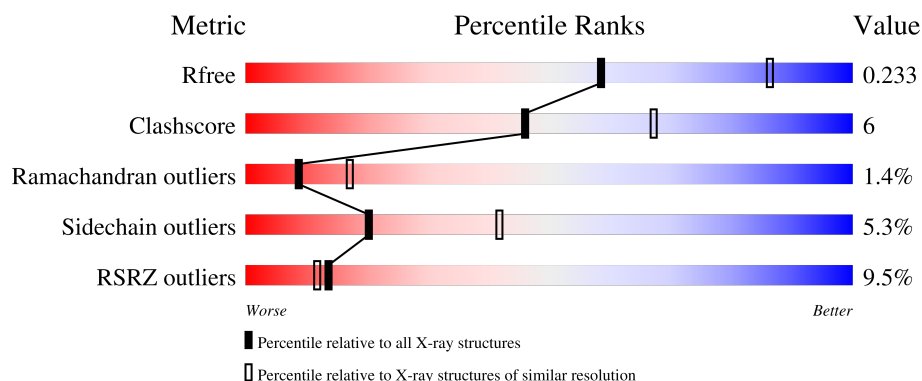
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	429	2% 80% 15% • •
1	D	429	9% 77% 15% • 6%
1	G	429	6% 77% 16% • 6%
2	B	145	8% 81% 14% • • •
2	E	145	43% 68% 19% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	145	6% 83% 11% ..
3	C	9	67% 22% 11%
3	F	9	11% 78% 22%
3	I	9	22% 67% 22% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13651 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 F-box/WD repeat-containing protein 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	1	0
			3305	2076	596	614	19			
1	D	402	Total	C	N	O	S	0	0	0
			3239	2037	584	600	18			
1	G	404	Total	C	N	O	S	0	0	0
			3252	2046	585	602	19			

- Molecule 2 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	1	0
			1145	728	186	225	6			
2	E	130	Total	C	N	O	S	0	0	0
			1038	662	169	202	5			
2	H	144	Total	C	N	O	S	0	0	0
			1153	733	186	228	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
B	?	-	GLU	deletion	UNP P63208
B	?	-	GLY	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
B	?	-	PRO	deletion	UNP P63208
B	?	-	PRO	deletion	UNP P63208
B	?	-	GLU	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
B	?	-	GLU	deletion	UNP P63208

Continued on next page...

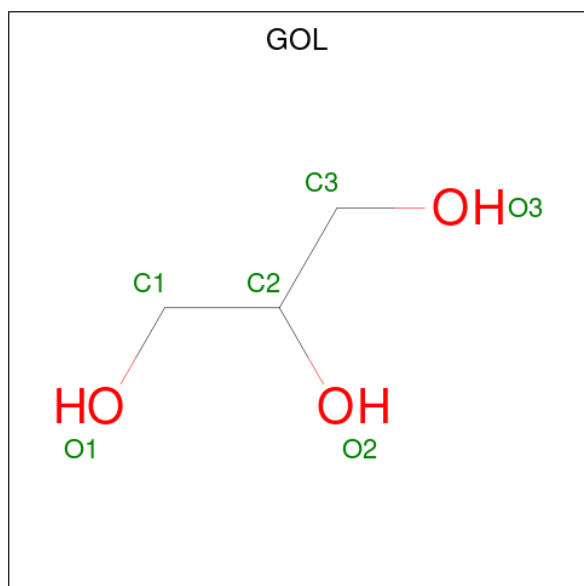
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P63208
B	?	-	LYS	deletion	UNP P63208
B	?	-	GLU	deletion	UNP P63208
B	?	-	LYS	deletion	UNP P63208
B	?	-	ARG	deletion	UNP P63208
B	?	-	THR	deletion	UNP P63208
E	?	-	ASP	deletion	UNP P63208
E	?	-	ASP	deletion	UNP P63208
E	?	-	GLU	deletion	UNP P63208
E	?	-	GLY	deletion	UNP P63208
E	?	-	ASP	deletion	UNP P63208
E	?	-	ASP	deletion	UNP P63208
E	?	-	PRO	deletion	UNP P63208
E	?	-	PRO	deletion	UNP P63208
E	?	-	GLU	deletion	UNP P63208
E	?	-	ASP	deletion	UNP P63208
E	?	-	ASP	deletion	UNP P63208
E	?	-	GLU	deletion	UNP P63208
E	?	-	ASN	deletion	UNP P63208
E	?	-	LYS	deletion	UNP P63208
E	?	-	GLU	deletion	UNP P63208
E	?	-	LYS	deletion	UNP P63208
E	?	-	ARG	deletion	UNP P63208
E	?	-	THR	deletion	UNP P63208
H	?	-	ASP	deletion	UNP P63208
H	?	-	ASP	deletion	UNP P63208
H	?	-	GLU	deletion	UNP P63208
H	?	-	GLY	deletion	UNP P63208
H	?	-	ASP	deletion	UNP P63208
H	?	-	ASP	deletion	UNP P63208
H	?	-	PRO	deletion	UNP P63208
H	?	-	PRO	deletion	UNP P63208
H	?	-	GLU	deletion	UNP P63208
H	?	-	ASP	deletion	UNP P63208
H	?	-	ASP	deletion	UNP P63208
H	?	-	GLU	deletion	UNP P63208
H	?	-	ASN	deletion	UNP P63208
H	?	-	LYS	deletion	UNP P63208
H	?	-	GLU	deletion	UNP P63208
H	?	-	LYS	deletion	UNP P63208
H	?	-	ARG	deletion	UNP P63208
H	?	-	THR	deletion	UNP P63208

- Molecule 3 is a protein called Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			68	35	11	20	2			
3	F	9	Total	C	N	O	P	0	0	0
			68	35	11	20	2			
3	I	9	Total	C	N	O	P	0	0	0
			68	35	11	20	2			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

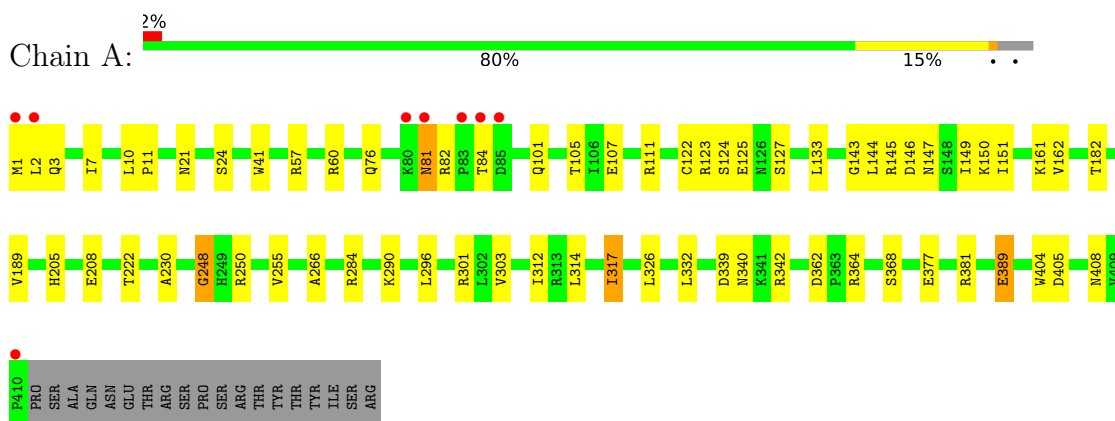
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	114	Total	O	0	0
			114	114		
6	B	20	Total	O	0	0
			20	20		
6	C	1	Total	O	0	0
			1	1		
6	D	65	Total	O	0	0
			65	65		
6	F	1	Total	O	0	0
			1	1		
6	G	36	Total	O	0	0
			36	36		
6	H	38	Total	O	0	0
			38	38		
6	I	2	Total	O	0	0
			2	2		

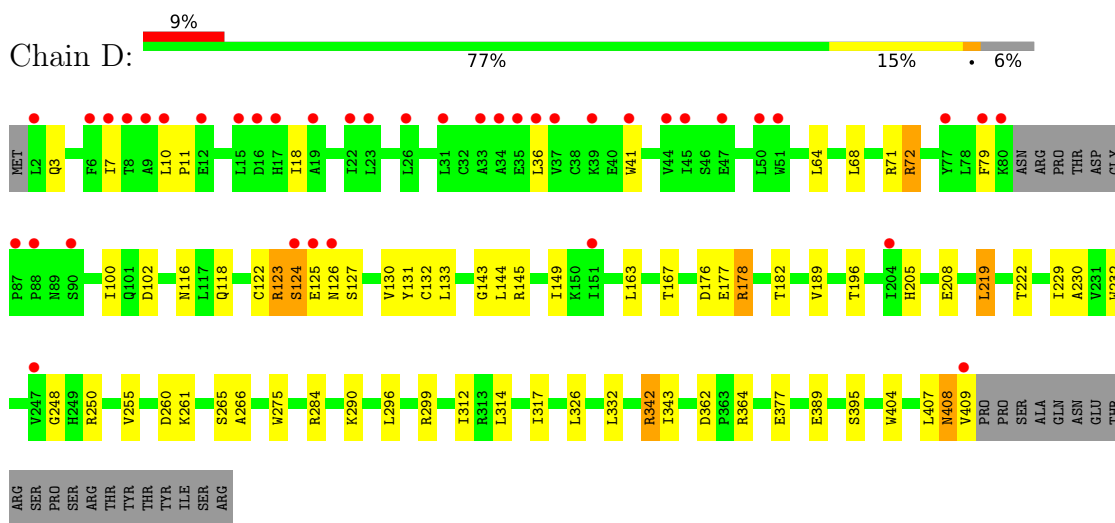
3 Residue-property plots [i](#)

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.

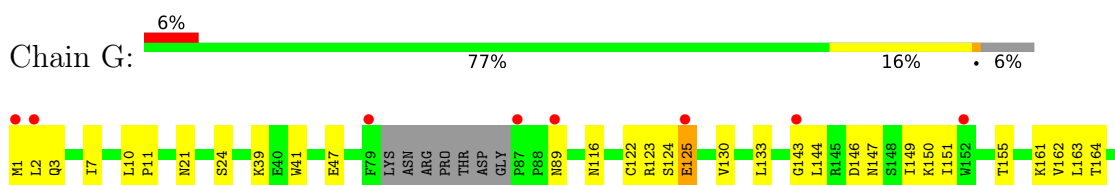
- Molecule 1: F-box/WD repeat-containing protein 11

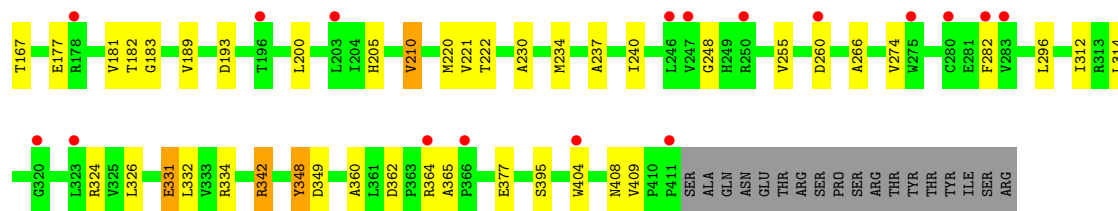


- Molecule 1: F-box/WD repeat-containing protein 11

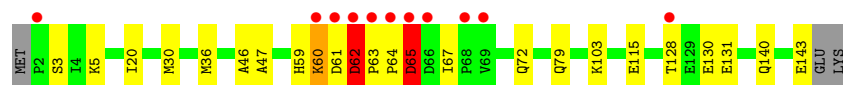
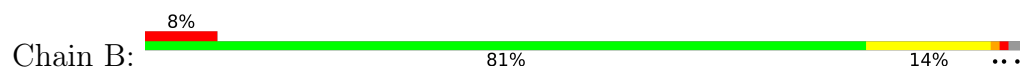


- Molecule 1: F-box/WD repeat-containing protein 11

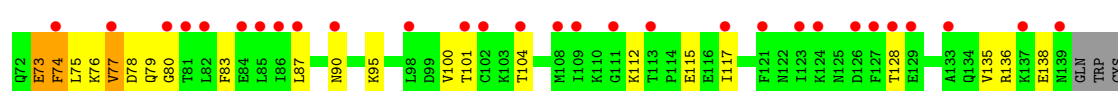
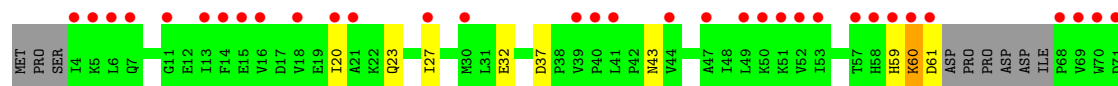
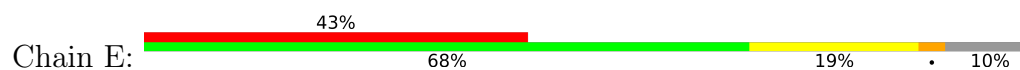




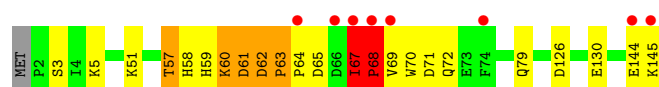
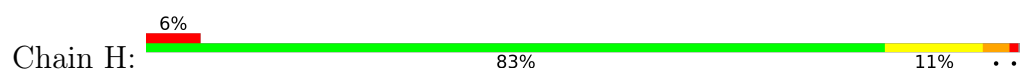
• Molecule 2: S-phase kinase-associated protein 1



• Molecule 2: S-phase kinase-associated protein 1



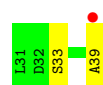
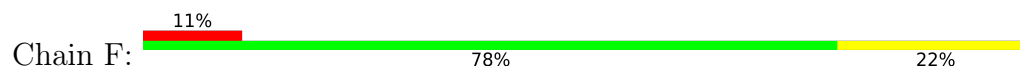
• Molecule 2: S-phase kinase-associated protein 1



• Molecule 3: Catenin beta-1



• Molecule 3: Catenin beta-1



• Molecule 3: Catenin beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.73Å 81.87Å 133.20Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	133.02 – 2.50 133.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	61.9 (133.02-2.50) 61.9 (133.02-2.50)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.251 (Not available) , 0.233	Depositor DCC
R_{free} test set	2632 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13651	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

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

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	1.01	0/3372	1.36	0/4567
1	D	0.97	0/3300	1.34	2/4466 (0.0%)
1	G	0.97	0/3315	1.34	5/4489 (0.1%)
2	B	1.03	0/1167	1.50	2/1582 (0.1%)
2	E	1.04	0/1053	1.44	0/1421
2	H	1.03	0/1174	1.58	11/1590 (0.7%)
3	C	1.27	0/46	1.49	1/56 (1.8%)
3	F	1.13	0/46	1.30	0/56
3	I	1.22	0/46	1.57	1/56 (1.8%)
All	All	1.00	0/13519	1.39	22/18283 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	ASP	CA-CB-CG	7.14	119.74	112.60
2	H	59	HIS	CA-C-N	7.09	132.32	121.83
2	H	59	HIS	C-N-CA	7.09	132.32	121.83
2	H	63	PRO	N-CA-C	6.68	118.85	110.70
2	H	70	TRP	N-CA-C	-6.19	104.46	111.14
3	I	32	ASP	CA-CB-CG	6.15	118.75	112.60
2	H	65	ASP	N-CA-C	-5.65	106.52	113.41
2	B	131	GLU	CB-CA-C	-5.26	101.74	110.68
1	G	210	VAL	CB-CA-C	5.24	117.90	111.25
2	H	60	LYS	CA-C-N	5.17	131.43	121.54
2	H	60	LYS	C-N-CA	5.17	131.43	121.54
2	H	68	PRO	CA-N-CD	-5.14	104.80	112.00
2	H	68	PRO	N-CA-CB	-5.14	97.86	103.25
3	C	36	HIS	CA-CB-CG	-5.10	108.70	113.80
1	D	342	ARG	CA-C-N	5.08	129.48	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	ARG	C-N-CA	5.08	129.48	123.19
1	G	342	ARG	CA-C-N	5.07	129.32	122.93
1	G	342	ARG	C-N-CA	5.07	129.32	122.93
1	G	89	ASN	N-CA-CB	5.07	117.36	110.01
1	G	125	GLU	CB-CG-CD	5.05	121.19	112.60
2	H	68	PRO	CB-CA-C	5.05	119.89	111.56
2	H	59	HIS	CB-CA-C	5.02	117.40	111.22

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	3305	0	3295	40	0
1	D	3239	0	3230	43	0
1	G	3252	0	3243	40	0
2	B	1145	0	1140	12	0
2	E	1038	0	1055	18	0
2	H	1153	0	1153	9	0
3	C	68	0	51	2	0
3	F	68	0	51	1	0
3	I	68	0	51	3	0
4	A	18	0	24	4	0
4	B	6	0	8	0	0
4	D	6	0	8	1	0
4	G	6	0	8	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	114	0	0	2	0
6	B	20	0	0	1	0
6	C	1	0	0	0	0
6	D	65	0	0	2	0
6	F	1	0	0	0	0
6	G	36	0	0	1	0
6	H	38	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	2	0	0	0	0
All	All	13651	0	13317	156	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 6.

All (156) 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)
2:E:73:GLU:O	2:E:76:LYS:HG3	1.72	0.88
1:D:116:ASN:HD21	1:D:408:ASN:HA	1.48	0.79
2:H:62:ASP:N	2:H:62:ASP:OD1	2.21	0.74
1:G:181:VAL:HG11	1:G:220:MET:CE	2.20	0.69
1:D:116:ASN:ND2	1:D:408:ASN:HA	2.08	0.68
1:A:127:SER:HB3	1:A:145:ARG:HG2	1.78	0.65
1:G:181:VAL:HG11	1:G:220:MET:HE2	1.80	0.63
1:A:408:ASN:HB3	1:D:196:THR:HB	1.81	0.63
1:G:116:ASN:ND2	1:G:408:ASN:O	2.32	0.61
2:H:57:THR:O	2:H:60:LYS:HB2	2.00	0.61
1:A:381:ARG:HH12	3:C:31:LEU:HD13	1.65	0.59
2:E:73:GLU:C	2:E:75:LEU:H	2.08	0.59
1:D:176:ASP:OD2	1:D:178:ARG:NH2	2.36	0.58
1:A:76:GLN:OE1	1:D:167:THR:CG2	2.52	0.58
1:A:248:GLY:O	4:A:502:GOL:H11	2.04	0.58
1:A:389[B]:GLU:H	1:A:389[B]:GLU:CD	2.11	0.57
1:D:219:LEU:HD23	1:D:232:TRP:O	2.06	0.56
1:G:324:ARG:NH1	1:G:365:ALA:O	2.39	0.56
1:D:290:LYS:HA	1:D:290:LYS:HE2	1.87	0.56
2:H:63:PRO:HB2	2:H:64:PRO:HD3	1.87	0.56
2:B:59:HIS:O	2:B:60:LYS:C	2.51	0.54
1:A:312:ILE:HB	1:A:326:LEU:HB2	1.90	0.54
2:E:101:THR:O	2:E:104:THR:OG1	2.22	0.54
1:A:250:ARG:CG	4:A:502:GOL:H12	2.38	0.54
2:E:78:ASP:O	2:E:80:GLY:N	2.41	0.54
1:G:324:ARG:NH2	1:G:360:ALA:O	2.41	0.54
1:G:181:VAL:HG11	1:G:220:MET:HE1	1.91	0.53
2:B:67:ILE:HG22	2:B:72:GLN:HG2	1.89	0.53
1:G:167:THR:HG22	1:G:167:THR:O	2.09	0.53
1:D:10:LEU:HB2	1:D:11:PRO:HD3	1.91	0.53
2:B:128:THR:HG22	2:B:130:GLU:H	1.74	0.52
1:D:250:ARG:O	3:F:39:ALA:HB2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:MET:HG3	1:G:240:ILE:HG12	1.92	0.52
1:G:312:ILE:HB	1:G:326:LEU:HB2	1.92	0.52
2:B:67:ILE:HD11	2:B:103:LYS:CG	2.40	0.52
1:D:296:LEU:C	1:D:296:LEU:HD23	2.35	0.51
1:A:101:GLN:HA	1:A:101:GLN:OE1	2.09	0.51
1:G:183:GLY:CA	1:G:210:VAL:HG13	2.41	0.51
1:D:255:VAL:HG13	1:D:266:ALA:HB3	1.93	0.51
1:D:312:ILE:HB	1:D:326:LEU:HB2	1.93	0.51
1:A:24:SER:O	1:A:57:ARG:NH1	2.44	0.51
1:D:132:CYS:HB2	6:D:740:HOH:O	2.10	0.51
1:G:10:LEU:HB2	1:G:11:PRO:HD3	1.93	0.50
2:H:71:ASP:OD1	2:H:71:ASP:N	2.44	0.50
1:A:3:GLN:HA	2:B:79:GLN:OE1	2.11	0.50
1:D:68:LEU:HD22	1:D:102:ASP:OD2	2.12	0.50
1:D:36:LEU:HD21	2:E:135:VAL:HG11	1.92	0.50
1:G:296:LEU:C	1:G:296:LEU:HD23	2.36	0.50
1:D:362:ASP:OD1	1:D:364:ARG:HB2	2.12	0.50
2:H:58:HIS:O	2:H:61:ASP:HB2	2.12	0.50
1:A:222:THR:OG1	1:A:230:ALA:HB3	2.11	0.50
1:A:296:LEU:C	1:A:296:LEU:HD23	2.37	0.50
1:G:222:THR:OG1	1:G:230:ALA:HB3	2.12	0.50
1:A:381:ARG:NH1	3:C:31:LEU:HD13	2.27	0.50
1:A:151:ILE:HD12	1:A:161:LYS:HB2	1.93	0.49
2:E:73:GLU:O	2:E:75:LEU:N	2.44	0.49
2:B:115:GLU:HB3	6:B:320:HOH:O	2.12	0.49
1:D:407:LEU:O	1:D:408:ASN:HB2	2.12	0.49
1:A:377:GLU:HB2	1:A:404:TRP:CH2	2.47	0.49
1:D:332:LEU:C	1:D:332:LEU:HD23	2.38	0.49
1:G:255:VAL:HG13	1:G:266:ALA:HB3	1.95	0.49
1:D:299:ARG:HG2	1:D:299:ARG:HH11	1.78	0.49
1:D:124:SER:OG	1:D:127:SER:O	2.31	0.48
2:E:73:GLU:O	2:E:76:LYS:CG	2.55	0.48
1:A:133:LEU:C	1:A:133:LEU:HD12	2.38	0.48
1:A:368:SER:OG	2:H:126:ASP:O	2.31	0.48
1:G:149:ILE:HD11	1:G:182:THR:HG21	1.96	0.48
2:B:67:ILE:HD11	2:B:103:LYS:HG2	1.95	0.48
1:D:222:THR:OG1	1:D:230:ALA:HB3	2.14	0.48
1:A:10:LEU:HB2	1:A:11:PRO:HD3	1.95	0.47
1:G:332:LEU:C	1:G:332:LEU:HD23	2.39	0.47
1:A:255:VAL:HG13	1:A:266:ALA:HB3	1.95	0.47
1:A:332:LEU:C	1:A:332:LEU:HD23	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ARG:NH1	6:D:703:HOH:O	2.47	0.47
2:E:73:GLU:C	2:E:75:LEU:N	2.73	0.47
1:G:362:ASP:OD1	1:G:364:ARG:HB2	2.15	0.47
1:A:21:ASN:O	1:A:24:SER:OG	2.21	0.47
1:G:193:ASP:OD1	6:G:601:HOH:O	2.20	0.47
1:D:18:ILE:HD11	2:E:90:ASN:CG	2.40	0.47
1:G:151:ILE:HD12	1:G:161:LYS:HB2	1.97	0.46
1:G:377:GLU:HB2	1:G:404:TRP:CH2	2.50	0.46
1:A:303:VAL:CG2	1:A:317:ILE:HG23	2.45	0.46
1:D:149:ILE:HD11	1:D:182:THR:HG21	1.97	0.46
1:G:133:LEU:C	1:G:133:LEU:HD12	2.41	0.46
1:D:377:GLU:HB2	1:D:404:TRP:CH2	2.51	0.46
1:D:64:LEU:HB2	1:D:389:GLU:HG3	1.98	0.46
2:E:60:LYS:O	2:E:60:LYS:CD	2.63	0.46
2:E:100:VAL:O	2:E:104:THR:HG23	2.16	0.46
1:D:133:LEU:C	1:D:133:LEU:HD12	2.41	0.46
1:A:290:LYS:HD3	4:A:503:GOL:H32	1.98	0.45
1:A:405:ASP:OD2	1:A:408:ASN:HB2	2.16	0.45
1:A:301:ARG:HA	1:A:317:ILE:HD11	1.98	0.45
1:G:167:THR:O	1:G:167:THR:CG2	2.64	0.45
1:A:122:CYS:O	1:A:123:ARG:C	2.60	0.45
1:D:260:ASP:HB2	4:D:601:GOL:H12	1.98	0.45
1:G:348:TYR:OH	3:I:32:ASP:OD2	2.30	0.45
1:D:143:GLY:C	1:D:144:LEU:HD12	2.42	0.45
1:D:149:ILE:HB	1:D:163:LEU:HB2	1.98	0.45
1:G:21:ASN:O	1:G:24:SER:OG	2.27	0.45
1:G:182:THR:O	1:G:189:VAL:HA	2.17	0.45
1:G:282:PHE:CD1	1:G:282:PHE:C	2.95	0.45
3:I:31:LEU:HA	3:I:31:LEU:HD12	1.80	0.45
1:A:143:GLY:C	1:A:144:LEU:HD12	2.42	0.45
2:E:74:PHE:O	2:E:74:PHE:CG	2.70	0.45
1:G:193:ASP:HB2	1:G:200:LEU:HD21	1.98	0.45
1:A:362:ASP:OD1	1:A:364:ARG:HB2	2.17	0.45
1:D:71:ARG:HD3	1:D:407:LEU:HD21	1.98	0.45
1:D:182:THR:O	1:D:189:VAL:HA	2.17	0.45
1:A:303:VAL:HG23	1:A:317:ILE:HG23	1.98	0.44
1:G:143:GLY:C	1:G:144:LEU:HD12	2.42	0.44
1:A:182:THR:O	1:A:189:VAL:HA	2.17	0.44
2:B:59:HIS:O	2:B:61:ASP:N	2.50	0.44
1:D:163:LEU:HD12	1:D:163:LEU:N	2.33	0.44
1:G:7:ILE:HB	1:G:41:TRP:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:PRO:HA	2:H:67:ILE:HG12	2.01	0.43
1:D:314:LEU:HD12	1:D:314:LEU:N	2.33	0.43
1:D:68:LEU:O	1:D:72:ARG:HB2	2.19	0.43
1:G:3:GLN:HA	2:H:79:GLN:OE1	2.19	0.43
1:D:284:ARG:NH1	1:D:317:ILE:O	2.50	0.43
2:E:73:GLU:OE1	2:E:74:PHE:N	2.51	0.43
1:G:122:CYS:O	1:G:123:ARG:C	2.62	0.43
2:E:75:LEU:HG	2:E:75:LEU:O	2.18	0.43
1:A:339:ASP:HB2	6:A:668:HOH:O	2.19	0.43
2:B:62:ASP:C	2:B:64:PRO:HD3	2.44	0.43
1:A:250:ARG:HG3	4:A:502:GOL:H12	1.99	0.43
2:E:23:GLN:HE22	2:E:59:HIS:CB	2.32	0.43
2:B:30:MET:HE2	2:B:36:MET:HG3	2.01	0.42
2:H:64:PRO:C	2:H:67:ILE:HG12	2.44	0.42
1:A:7:ILE:HB	1:A:41:TRP:CE2	2.54	0.42
2:E:135:VAL:HA	2:E:138:GLU:OE1	2.19	0.42
1:A:146:ASP:O	1:A:147:ASN:HB2	2.20	0.42
1:A:149:ILE:HD11	1:A:182:THR:HG21	2.01	0.42
1:G:183:GLY:HA3	1:G:210:VAL:HG13	2.01	0.42
1:G:237:ALA:O	1:G:240:ILE:CD1	2.68	0.42
2:E:83:PHE:CE2	2:E:87:LEU:HD11	2.55	0.42
1:A:284:ARG:NH1	1:A:317:ILE:O	2.53	0.41
1:A:150:LYS:HG2	1:A:162:VAL:HG22	2.01	0.41
1:G:150:LYS:HG2	1:G:162:VAL:HG22	2.02	0.41
1:A:314:LEU:HD12	1:A:314:LEU:N	2.35	0.41
1:D:163:LEU:N	1:D:163:LEU:CD1	2.83	0.41
1:D:229:ILE:HD11	1:D:265:SER:CB	2.50	0.41
2:B:59:HIS:HB3	2:B:62:ASP:HA	2.02	0.41
1:D:130:VAL:HB	1:D:395:SER:HB2	2.03	0.41
1:G:331:GLU:HG3	1:G:349:ASP:HB3	2.03	0.41
1:D:7:ILE:HB	1:D:41:TRP:CE2	2.55	0.41
2:E:112:LYS:HB2	2:E:117:ILE:HD11	2.03	0.41
1:G:314:LEU:HD12	1:G:314:LEU:N	2.36	0.41
1:G:146:ASP:O	1:G:147:ASN:HB2	2.20	0.40
1:A:105:THR:HG21	6:A:709:HOH:O	2.21	0.40
1:G:130:VAL:HB	1:G:395:SER:HB2	2.03	0.40
1:D:64:LEU:HD22	1:D:389:GLU:CD	2.47	0.40
2:B:46:ALA:O	2:B:47:ALA:C	2.64	0.40
1:D:122:CYS:O	1:D:123:ARG:C	2.64	0.40
1:D:131:TYR:OH	1:D:145:ARG:NH1	2.54	0.40
1:G:149:ILE:HB	1:G:163:LEU:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:ARG:NH2	3:I:34:GLY:HA3	2.36	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	409/429 (95%)	373 (91%)	31 (8%)	5 (1%)	10	20
1	D	398/429 (93%)	365 (92%)	29 (7%)	4 (1%)	12	24
1	G	400/429 (93%)	368 (92%)	29 (7%)	3 (1%)	16	31
2	B	141/145 (97%)	126 (89%)	12 (8%)	3 (2%)	5	9
2	E	126/145 (87%)	113 (90%)	10 (8%)	3 (2%)	4	8
2	H	142/145 (98%)	126 (89%)	13 (9%)	3 (2%)	5	9
3	C	5/9 (56%)	4 (80%)	0	1 (20%)	0	0
3	F	5/9 (56%)	5 (100%)	0	0	100	100
3	I	5/9 (56%)	5 (100%)	0	0	100	100
All	All	1631/1749 (93%)	1485 (91%)	124 (8%)	22 (1%)	9	18

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
2	E	74	PHE
2	H	68	PRO
1	A	84	THR
1	A	125	GLU
1	A	205	HIS
2	B	65	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	125	GLU
1	D	205	HIS
2	E	79	GLN
1	G	205	HIS
2	H	144	GLU
1	A	248	GLY
2	B	62	ASP
3	C	32	ASP
1	D	79	PHE
1	G	125	GLU
2	B	63	PRO
1	D	248	GLY
1	G	248	GLY
2	H	67	ILE
2	E	77	VAL

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	369/386 (96%)	355 (96%)	14 (4%)	29	56
1	D	361/386 (94%)	344 (95%)	17 (5%)	23	47
1	G	363/386 (94%)	348 (96%)	15 (4%)	27	53
2	B	131/133 (98%)	123 (94%)	8 (6%)	17	35
2	E	118/133 (89%)	105 (89%)	13 (11%)	6	13
2	H	132/133 (99%)	120 (91%)	12 (9%)	9	19
3	C	4/4 (100%)	3 (75%)	1 (25%)	0	1
3	F	4/4 (100%)	4 (100%)	0	100	100
3	I	4/4 (100%)	4 (100%)	0	100	100
All	All	1486/1569 (95%)	1406 (95%)	80 (5%)	20	41

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LEU
1	A	60	ARG
1	A	81	ASN
1	A	82	ARG
1	A	107	GLU
1	A	111	ARG
1	A	124	SER
1	A	208	GLU
1	A	317	ILE
1	A	340	ASN
1	A	342	ARG
1	A	389[A]	GLU
1	A	389[B]	GLU
2	B	3	SER
2	B	5	LYS
2	B	20	ILE
2	B	60	LYS
2	B	62	ASP
2	B	65	ASP
2	B	140	GLN
2	B	143	GLU
3	C	31	LEU
1	D	3	GLN
1	D	72	ARG
1	D	100	ILE
1	D	118	GLN
1	D	123	ARG
1	D	124	SER
1	D	126	ASN
1	D	177	GLU
1	D	178	ARG
1	D	208	GLU
1	D	219	LEU
1	D	261	LYS
1	D	275	TRP
1	D	342	ARG
1	D	343	ILE
1	D	408	ASN
1	D	409	VAL
2	E	20	ILE
2	E	27	ILE
2	E	32	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	37	ASP
2	E	43	ASN
2	E	60	LYS
2	E	61	ASP
2	E	73	GLU
2	E	77	VAL
2	E	95	LYS
2	E	115	GLU
2	E	128	THR
2	E	136	ARG
1	G	1	MET
1	G	2	LEU
1	G	39	LYS
1	G	47	GLU
1	G	124	SER
1	G	155	THR
1	G	164	THR
1	G	177	GLU
1	G	221	VAL
1	G	260	ASP
1	G	274	VAL
1	G	331	GLU
1	G	342	ARG
1	G	348	TYR
1	G	409	VAL
2	H	3	SER
2	H	5	LYS
2	H	51	LYS
2	H	57	THR
2	H	61	ASP
2	H	62	ASP
2	H	67	ILE
2	H	68	PRO
2	H	69	VAL
2	H	72	GLN
2	H	130	GLU
2	H	145	LYS

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

Mol	Chain	Res	Type
1	A	13	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	89	ASN
1	A	340	ASN
1	D	42	GLN
1	D	116	ASN
2	E	58	HIS
1	G	101	GLN
1	G	126	ASN
1	G	195	ASN
1	G	408	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SEP	C	37	3	8,9,10	1.03	0	7,12,14	1.08	0
3	SEP	C	33	3	8,9,10	0.64	0	7,12,14	1.05	0
3	SEP	F	33	3	8,9,10	0.72	0	7,12,14	1.23	1 (14%)
3	SEP	I	37	3	8,9,10	0.63	0	7,12,14	1.06	0
3	SEP	F	37	3	8,9,10	0.57	0	7,12,14	0.95	0
3	SEP	I	33	3	8,9,10	0.72	0	7,12,14	1.00	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	SEP	C	37	3	-	2/6/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	C	33	3	-	0/6/8/10	-
3	SEP	F	33	3	-	0/6/8/10	-
3	SEP	I	37	3	-	2/6/8/10	-
3	SEP	F	37	3	-	2/6/8/10	-
3	SEP	I	33	3	-	5/6/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	33	SEP	O3P-P-O2P	2.32	116.50	107.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	37	SEP	N-CA-CB-OG
3	C	37	SEP	C-CA-CB-OG
3	I	33	SEP	N-CA-CB-OG
3	I	33	SEP	C-CA-CB-OG
3	I	33	SEP	CB-OG-P-O2P
3	I	33	SEP	CB-OG-P-O3P
3	I	33	SEP	CB-OG-P-O1P
3	I	37	SEP	CB-OG-P-O1P
3	F	37	SEP	CA-CB-OG-P
3	F	37	SEP	N-CA-CB-OG
3	I	37	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
4	GOL	D	601	-	5,5,5	0.19	0	5,5,5	0.43	0
4	GOL	A	502	-	5,5,5	0.19	0	5,5,5	0.57	0
4	GOL	G	501	-	5,5,5	0.24	0	5,5,5	0.52	0
4	GOL	A	503	-	5,5,5	0.17	0	5,5,5	0.35	0
4	GOL	B	201	-	5,5,5	0.28	0	5,5,5	0.53	0
4	GOL	A	501	-	5,5,5	0.21	0	5,5,5	0.34	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
4	GOL	D	601	-	-	0/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	G	501	-	-	4/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	B	201	-	-	4/4/4/4	-
4	GOL	A	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GOL	C1-C2-C3-O3
4	A	502	GOL	C1-C2-C3-O3
4	A	503	GOL	C1-C2-C3-O3
4	G	501	GOL	O1-C1-C2-C3
4	G	501	GOL	C1-C2-C3-O3
4	A	503	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	501	GOL	O2-C2-C3-O3
4	B	201	GOL	O1-C1-C2-C3
4	B	201	GOL	C1-C2-C3-O3
4	A	501	GOL	O2-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
4	B	201	GOL	O1-C1-C2-O2
4	B	201	GOL	O2-C2-C3-O3
4	G	501	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	GOL	1	0
4	A	502	GOL	3	0
4	A	503	GOL	1	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	410/429 (95%)	0.01	8 (1%) 65 61	16, 36, 61, 132	1 (0%)
1	D	402/429 (93%)	0.55	40 (9%) 12 10	29, 54, 127, 157	0
1	G	404/429 (94%)	0.74	25 (6%) 26 23	32, 65, 96, 118	0
2	B	142/145 (97%)	0.38	11 (7%) 19 17	27, 46, 89, 121	1 (0%)
2	E	130/145 (89%)	2.05	62 (47%) 0 0	99, 124, 151, 156	0
2	H	144/145 (99%)	0.18	8 (5%) 30 26	21, 38, 89, 114	0
3	C	7/9 (77%)	0.32	0 100 100	23, 27, 39, 49	0
3	F	7/9 (77%)	0.57	1 (14%) 6 5	43, 46, 59, 74	0
3	I	7/9 (77%)	0.91	2 (28%) 1 1	39, 49, 64, 74	0
All	All	1653/1749 (94%)	0.53	157 (9%) 14 12	16, 52, 125, 157	2 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	LEU	7.6
2	H	67	ILE	6.2
2	H	68	PRO	5.6
2	E	68	PRO	4.9
1	D	7	ILE	4.9
1	D	37	VAL	4.7
1	A	83	PRO	4.7
2	E	85	LEU	4.7
1	D	6	PHE	4.7
1	D	409	VAL	4.6
2	E	14	PHE	4.4
2	B	63	PRO	4.4
1	D	45	ILE	4.3
2	E	81	THR	4.3
2	E	98	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	4	ILE	4.2
1	G	411	PRO	4.1
2	H	145	LYS	4.1
1	D	23	LEU	4.0
2	H	64	PRO	4.0
1	D	36	LEU	4.0
2	E	69	VAL	4.0
2	E	87	LEU	3.7
1	D	26	LEU	3.7
2	E	126	ASP	3.7
2	B	60	LYS	3.7
1	G	275	TRP	3.6
1	A	1	MET	3.6
2	E	41	LEU	3.5
2	E	121	PHE	3.5
1	G	323	LEU	3.5
1	D	204	ILE	3.5
1	D	87	PRO	3.4
2	E	13	ILE	3.4
2	E	44	VAL	3.4
2	E	6	LEU	3.4
2	E	11	GLY	3.4
2	B	128	THR	3.4
2	E	61	ASP	3.3
1	D	33	ALA	3.3
1	D	41	TRP	3.2
1	D	15	LEU	3.2
1	G	89	ASN	3.2
2	E	77	VAL	3.2
2	E	109	ILE	3.2
2	E	123	ILE	3.1
1	D	34	ALA	3.1
1	A	84	THR	3.1
1	A	80	LYS	3.1
2	E	133	ALA	3.1
1	G	1	MET	3.1
2	E	71	ASP	3.1
2	E	111	GLY	3.0
2	E	53	ILE	3.0
2	E	80	GLY	3.0
2	E	49	LEU	3.0
2	B	69	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	117	ILE	2.9
2	E	50	LYS	2.9
2	E	30	MET	2.8
1	G	282	PHE	2.8
1	G	247	VAL	2.8
2	B	62	ASP	2.8
1	D	80	LYS	2.8
3	I	39	ALA	2.8
2	E	27	ILE	2.8
1	D	39	LYS	2.8
1	D	77	TYR	2.7
2	E	59	HIS	2.7
2	E	52	VAL	2.7
1	D	22	ILE	2.7
1	G	87	PRO	2.7
1	D	8	THR	2.7
2	E	113	THR	2.7
2	E	84	GLU	2.7
1	G	79	PHE	2.7
1	D	88	PRO	2.7
2	E	139	ASN	2.6
2	E	18	VAL	2.6
2	E	70	TRP	2.6
2	B	68	PRO	2.6
1	G	250	ARG	2.6
2	H	69	VAL	2.6
2	B	65	ASP	2.6
2	E	102	CYS	2.6
1	G	283	VAL	2.6
1	D	17	HIS	2.6
1	A	81	ASN	2.6
2	B	66	ASP	2.5
1	D	125	GLU	2.5
1	D	50	LEU	2.5
1	D	151	ILE	2.5
2	E	101	THR	2.5
2	E	129	GLU	2.5
1	G	2	LEU	2.5
1	G	246	LEU	2.5
2	E	58	HIS	2.5
1	A	85	ASP	2.5
2	E	124	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	74	PHE	2.5
2	E	21	ALA	2.5
1	D	90	SER	2.5
2	E	57	THR	2.5
1	A	410	PRO	2.4
1	G	366	PRO	2.4
1	D	9	ALA	2.4
2	E	20	ILE	2.4
2	E	108	MET	2.4
3	F	39	ALA	2.4
2	E	7	GLN	2.4
1	D	51	TRP	2.4
1	D	79	PHE	2.3
1	D	19	ALA	2.3
1	D	10	LEU	2.3
2	E	82	LEU	2.3
1	D	247	VAL	2.3
1	G	320	GLY	2.3
2	E	137	LYS	2.3
2	E	128	THR	2.3
1	A	2	LEU	2.3
1	D	31	LEU	2.3
1	D	126	ASN	2.2
1	D	47	GLU	2.2
1	G	125	GLU	2.2
2	E	16	VAL	2.2
2	E	90	ASN	2.2
2	E	104	THR	2.2
1	D	124	SER	2.2
1	G	404	TRP	2.2
2	B	64	PRO	2.2
2	E	74	PHE	2.2
2	E	60	LYS	2.2
2	B	61	ASP	2.2
1	G	152	TRP	2.2
1	D	44	VAL	2.1
1	D	12	GLU	2.1
2	H	144	GLU	2.1
2	E	5	LYS	2.1
1	G	260	ASP	2.1
2	E	127	PHE	2.1
1	G	203	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	31	LEU	2.1
1	G	196	THR	2.1
2	E	86	ILE	2.1
1	G	280	CYS	2.1
1	G	178	ARG	2.1
1	G	364	ARG	2.1
1	D	35	GLU	2.1
2	E	51	LYS	2.1
2	E	47	ALA	2.0
1	G	143	GLY	2.0
1	D	16	ASP	2.0
2	H	66	ASP	2.0
2	E	40	PRO	2.0
2	E	39	VAL	2.0
2	E	15	GLU	2.0
2	B	2	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
3	SEP	F	33	10/11	0.97	0.06	42,45,46,46	0
3	SEP	I	33	10/11	0.97	0.06	43,46,47,47	0
3	SEP	I	37	10/11	0.97	0.06	45,51,57,58	0
3	SEP	C	33	10/11	0.98	0.06	22,23,25,26	0
3	SEP	F	37	10/11	0.98	0.06	45,47,49,49	0
3	SEP	C	37	10/11	0.99	0.05	26,27,32,32	0

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(Å ²)	Q<0.9
4	GOL	D	601	6/6	0.70	0.15	55,59,61,63	0
4	GOL	B	201	6/6	0.77	0.21	53,60,64,66	0
4	GOL	A	502	6/6	0.85	0.17	63,67,68,68	0
5	NA	D	602	1/1	0.85	0.25	41,41,41,41	0
4	GOL	G	501	6/6	0.86	0.20	74,76,78,81	0
4	GOL	A	501	6/6	0.87	0.14	54,62,64,66	0
4	GOL	A	503	6/6	0.93	0.14	61,68,70,71	0
5	NA	A	504	1/1	0.98	0.11	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.