



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:15 am BST

PDB ID : 6WNX  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

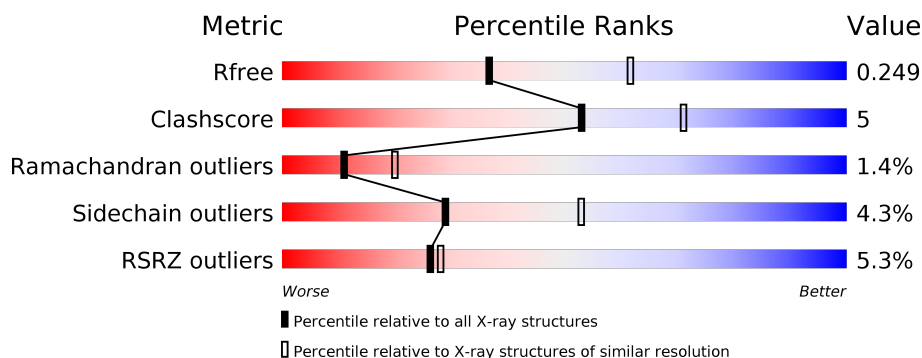
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	D	429	<div> <div>5%</div> <div>77%</div> <div>16%</div> <div>• 6%</div> </div>
1	G	429	<div> <div>%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
2	B	145	<div> <div>3%</div> <div>86%</div> <div>10%</div> <div>• • •</div> </div>
2	E	145	<div> <div>37%</div> <div>70%</div> <div>17%</div> <div>• 10%</div> </div>
2	H	145	<div> <div>%</div> <div>85%</div> <div>11%</div> <div>• • •</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	9	 78% 22%
3	F	9	 89% 11%
3	I	9	 78% 22%

## 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

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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 (three-letter code: 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 (three-letter code: NA) (formula: Na).

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

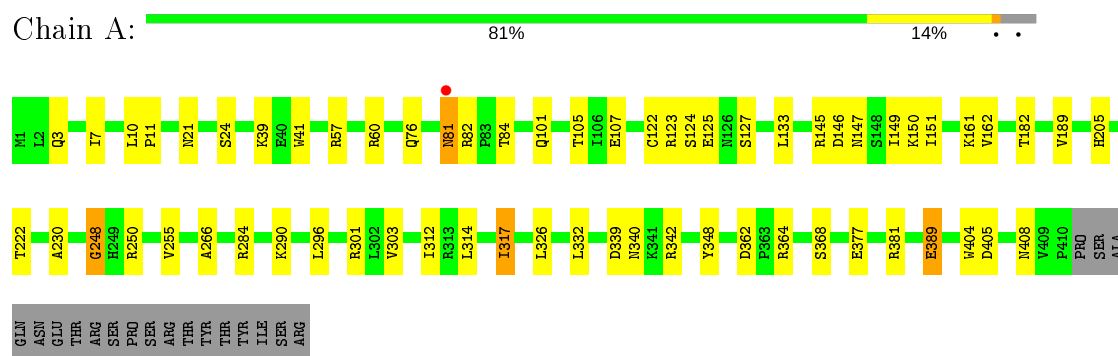
- Molecule 6 is water.

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

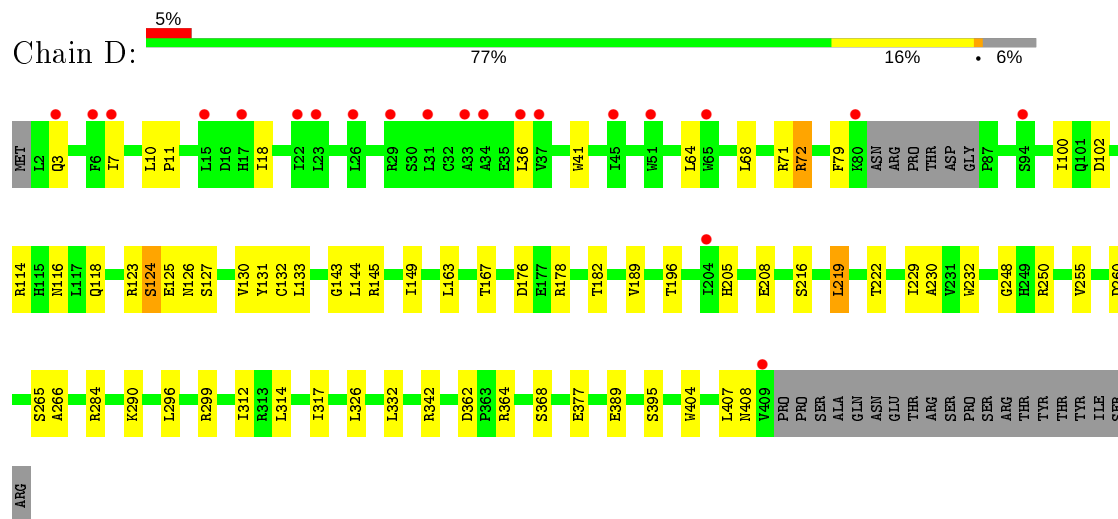
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

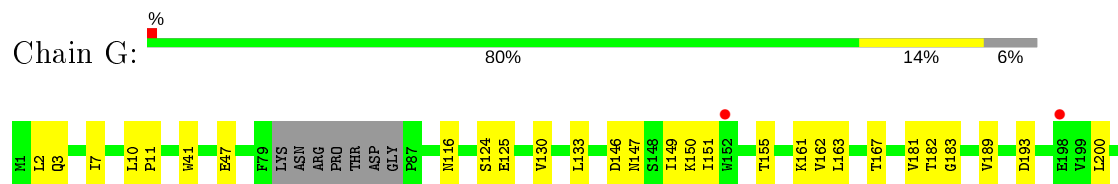
- Molecule 1: F-box/WD repeat-containing protein 11



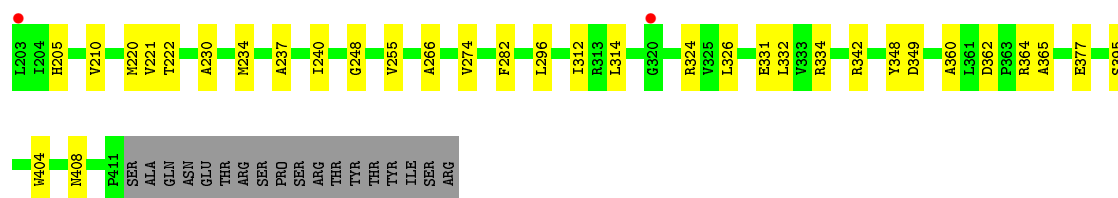
- Molecule 1: F-box/WD repeat-containing protein 11



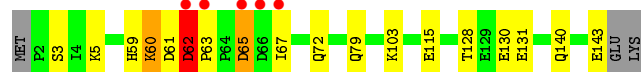
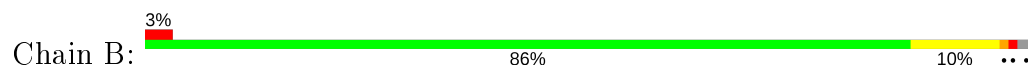
- Molecule 1: F-box/WD repeat-containing protein 11



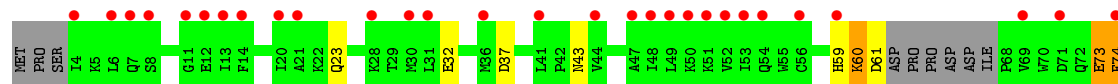




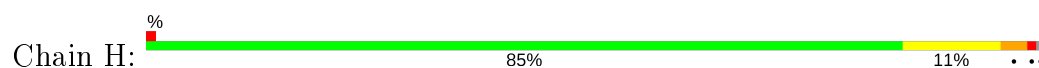
- Molecule 2: S-phase kinase-associated protein 1



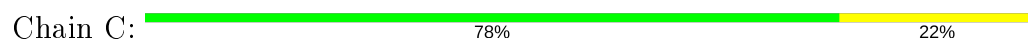
- Molecule 2: S-phase kinase-associated protein 1



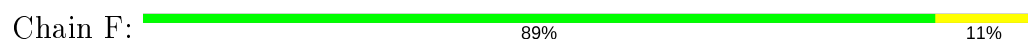
- Molecule 2: S-phase kinase-associated protein 1



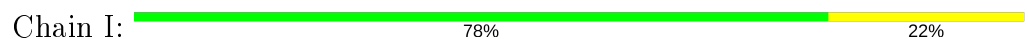
- Molecule 3: Catenin beta-1



- 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, $\alpha$ , $\beta$ , $\gamma$	119.73Å 81.87Å 133.20Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	133.02 – 2.50 133.03 – 2.50	Depositor EDS
% Data completeness (in resolution range)	61.9 (133.02-2.50) 61.9 (133.03-2.50)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.206 , 0.251 0.210 , 0.249	Depositor DCC
$R_{free}$ test set	2632 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NA, SEP

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	0.72	0/3372	0.91	0/4567
1	D	0.67	0/3300	0.87	0/4466
1	G	0.68	0/3315	0.86	0/4489
2	B	0.72	0/1167	0.83	0/1582
2	E	0.70	0/1053	0.79	0/1421
2	H	0.72	0/1174	0.89	0/1590
3	C	1.01	0/46	1.17	0/56
3	F	0.79	0/46	0.93	0/56
3	I	0.88	0/46	1.15	0/56
All	All	0.70	0/13519	0.87	0/18283

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3305	0	3295	39	0
1	D	3239	0	3230	41	0
1	G	3252	0	3243	36	0
2	B	1145	0	1140	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1038	0	1055	18	0
2	H	1153	0	1153	8	0
3	C	68	0	50	2	0
3	F	68	0	50	1	0
3	I	68	0	50	2	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
6	I	2	0	0	0	0
All	All	13651	0	13314	145	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 5.

All (145) 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:OD1	2:H:62:ASP:N	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: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
1:G:181:VAL:HG11	1:G:220:MET:HE1	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:181:VAL:HG11	1:G:220:MET:HE2	1.86	0.56
1:D:290:LYS:HE2	1:D:290:LYS:HA	1.87	0.56
2:H:63:PRO:HB2	2:H:64:PRO:HD3	1.87	0.56
2:E:73:GLU:C	2:E:75:LEU:H	2.08	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:A:389[B]:GLU:H	1:A:389[B]:GLU:CD	2.11	0.53
2:B:67:ILE:HG22	2:B:72:GLN:HG2	1.89	0.53
1:G:167:THR:O	1:G:167:THR:HG22	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
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: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: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: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:B:59:HIS:O	2:B:60:LYS:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:HB2	1:A:404:TRP:CH2	2.47	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:21:ASN:O	1:A:24:SER:OG	2.21	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:A:255:VAL:HG13	1:A:266:ALA:HB3	1.95	0.47
1:D:145:ARG:NH1	6:D:703:HOH:O	2.47	0.47
1:G:362:ASP:OD1	1:G:364:ARG:HB2	2.15	0.47
1:D:296:LEU:C	1:D:296:LEU:HD23	2.35	0.47
1:G:193:ASP:OD1	6:G:601:HOH:O	2.20	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: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:100:VAL:O	2:E:104:THR:HG23	2.16	0.46
2:E:60:LYS:O	2:E:60:LYS:CD	2.63	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:G:296:LEU:HD23	1:G:296:LEU:C	2.36	0.45
1:A:296:LEU:HD23	1:A:296:LEU:C	2.37	0.45
1:A:301:ARG:HA	1:A:317:ILE:HD11	1.98	0.45
1:G:167:THR:CG2	1:G:167:THR:O	2.64	0.45
1:D:260:ASP:HB2	4:D:601:GOL:H12	1.98	0.45
1:D:149:ILE:HB	1:D:163:LEU:HB2	1.98	0.45
1:G:182:THR:O	1:G:189:VAL:HA	2.17	0.45
3:I:31:LEU:HD12	3:I:31:LEU:HA	1.80	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:182:THR:O	1:D:189:VAL:HA	2.17	0.45
1:D:71:ARG:HD3	1:D:407:LEU:HD21	1.98	0.45
1:A:303:VAL:HG23	1:A:317:ILE:HG23	1.98	0.44
1:D:332:LEU:HD23	1:D:332:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:133:LEU:HD12	1:A:133:LEU:C	2.38	0.43
1:G:332:LEU:C	1:G:332:LEU:HD23	2.39	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
2:E:75:LEU:O	2:E:75:LEU:HG	2.18	0.43
1:A:339:ASP:HB2	6:A:668:HOH:O	2.19	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
1:A:332:LEU:C	1:A:332:LEU:HD23	2.39	0.42
1:A:7:ILE:HB	1:A:41:TRP:CE2	2.54	0.42
2:E:73:GLU:C	2:E:75:LEU:N	2.73	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
1:D:18:ILE:HD11	2:E:90:ASN:CG	2.40	0.42
2:E:83:PHE:CE2	2:E:87:LEU:HD11	2.55	0.42
1:G:133:LEU:C	1:G:133:LEU:HD12	2.41	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:CD1	1:D:163:LEU:N	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:133:LEU:C	1:D:133:LEU:HD12	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:122:CYS:O	1:A:123:ARG:C	2.60	0.40
1:D:143:GLY:C	1:D:144:LEU:HD12	2.42	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
1:G:282:PHE:CD1	1:G:282:PHE:C	2.95	0.40
1:G:334:ARG:NH2	3:I:34:GLY:HA3	2.36	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	409/429 (95%)	373 (91%)	31 (8%)	5 (1%)	13	24
1	D	398/429 (93%)	365 (92%)	29 (7%)	4 (1%)	15	28
1	G	400/429 (93%)	368 (92%)	29 (7%)	3 (1%)	19	35
2	B	141/145 (97%)	126 (89%)	12 (8%)	3 (2%)	7	11
2	E	126/145 (87%)	113 (90%)	10 (8%)	3 (2%)	6	9
2	H	142/145 (98%)	126 (89%)	13 (9%)	3 (2%)	7	11
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%)	11	21

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
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%)	357 (97%)	12 (3%)	38	64
1	D	361/386 (94%)	348 (96%)	13 (4%)	35	61
1	G	363/386 (94%)	355 (98%)	8 (2%)	52	77
2	B	131/133 (98%)	123 (94%)	8 (6%)	18	36
2	E	118/133 (89%)	107 (91%)	11 (9%)	9	17
2	H	132/133 (99%)	119 (90%)	13 (10%)	8	15
3	C	4/4 (100%)	4 (100%)	0	100	100
3	F	4/4 (100%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	4/4 (100%)	4 (100%)	0	100	100
All	All	1486/1569 (95%)	1421 (96%)	65 (4%)	29	52

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	60	ARG
1	A	81	ASN
1	A	82	ARG
1	A	107	GLU
1	A	124	SER
1	A	317	ILE
1	A	340	ASN
1	A	342	ARG
1	A	348	TYR
1	A	389[A]	GLU
1	A	389[B]	GLU
2	B	3	SER
2	B	5	LYS
2	B	60	LYS
2	B	62	ASP
2	B	65	ASP
2	B	131	GLU
2	B	140	GLN
2	B	143	GLU
1	D	3	GLN
1	D	72	ARG
1	D	100	ILE
1	D	114	ARG
1	D	118	GLN
1	D	123	ARG
1	D	124	SER
1	D	126	ASN
1	D	208	GLU
1	D	216	SER
1	D	219	LEU
1	D	342	ARG
1	D	368	SER
2	E	32	GLU
2	E	37	ASP
2	E	43	ASN

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Mol	Chain	Res	Type
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	2	LEU
1	G	47	GLU
1	G	124	SER
1	G	155	THR
1	G	221	VAL
1	G	274	VAL
1	G	342	ARG
1	G	348	TYR
2	H	3	SER
2	H	5	LYS
2	H	61	ASP
2	H	62	ASP
2	H	65	ASP
2	H	67	ILE
2	H	68	PRO
2	H	69	VAL
2	H	71	ASP
2	H	72	GLN
2	H	130	GLU
2	H	136	ARG
2	H	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	D	116	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	F	37	3	8,9,10	0.56	0	8,12,14	0.89	0
3	SEP	I	37	3	8,9,10	0.61	0	8,12,14	1.02	0
3	SEP	I	33	3	8,9,10	0.70	0	8,12,14	0.99	0
3	SEP	C	37	3	8,9,10	1.00	0	8,12,14	1.01	0
3	SEP	C	33	3	8,9,10	0.62	0	8,12,14	1.01	0
3	SEP	F	33	3	8,9,10	0.69	0	8,12,14	1.18	1 (12%)

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	F	37	3	-	2/5/8/10	-
3	SEP	I	37	3	-	2/5/8/10	-
3	SEP	I	33	3	-	4/5/8/10	-
3	SEP	C	37	3	-	1/5/8/10	-
3	SEP	C	33	3	-	0/5/8/10	-
3	SEP	F	33	3	-	0/5/8/10	-

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	107.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	33	SEP	N-CA-CB-OG
3	I	33	SEP	CB-OG-P-O2P
3	I	33	SEP	CB-OG-P-O3P
3	C	37	SEP	N-CA-CB-OG
3	I	37	SEP	CB-OG-P-O1P
3	I	33	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 carbohydrates 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	B	201	-	5,5,5	0.27	0	5,5,5	0.51	0
4	GOL	G	501	-	5,5,5	0.24	0	5,5,5	0.51	0
4	GOL	A	501	-	5,5,5	0.20	0	5,5,5	0.35	0
4	GOL	A	502	-	5,5,5	0.19	0	5,5,5	0.56	0
4	GOL	A	503	-	5,5,5	0.17	0	5,5,5	0.35	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	B	201	-	-	4/4/4/4	-
4	GOL	G	501	-	-	4/4/4/4	-
4	GOL	A	501	-	-	2/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	A	503	-	-	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	G	501	GOL	O1-C1-C2-C3
4	G	501	GOL	C1-C2-C3-O3
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	O2-C2-C3-O3
4	A	503	GOL	O2-C2-C3-O3
4	B	201	GOL	O1-C1-C2-C3
4	B	201	GOL	C1-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
4	A	501	GOL	O2-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	410/429 (95%)	-0.17	1 (0%) 95 95	19, 36, 61, 132	0
1	D	402/429 (93%)	0.11	21 (5%) 27 29	29, 54, 127, 157	0
1	G	404/429 (94%)	-0.02	4 (0%) 82 84	32, 65, 96, 118	0
2	B	142/145 (97%)	0.01	5 (3%) 44 47	27, 47, 89, 121	0
2	E	130/145 (89%)	1.97	54 (41%) 0 0	99, 124, 151, 156	0
2	H	144/145 (99%)	-0.14	2 (1%) 75 77	21, 38, 89, 114	0
3	C	7/9 (77%)	0.01	0 100 100	23, 27, 39, 49	0
3	F	7/9 (77%)	-0.28	0 100 100	43, 46, 59, 74	0
3	I	7/9 (77%)	0.06	0 100 100	39, 49, 64, 74	0
All	All	1653/1749 (94%)	0.12	87 (5%) 26 28	19, 52, 125, 157	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	85	LEU	6.8
2	E	13	ILE	6.7
2	E	14	PHE	6.7
2	E	98	LEU	6.2
2	B	65	ASP	5.9
2	E	117	ILE	5.3
2	E	54	GLN	5.3
2	E	133	ALA	5.2
2	E	81	THR	5.1
1	D	33	ALA	4.9
2	E	4	ILE	4.9
2	E	41	LEU	4.7
2	E	6	LEU	4.7
2	E	44	VAL	4.5
2	E	11	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	6	PHE	4.4
2	E	121	PHE	4.3
2	E	77	VAL	4.2
1	D	7	ILE	4.1
1	D	23	LEU	4.0
2	H	67	ILE	3.9
1	D	37	VAL	3.9
2	E	123	ILE	3.8
2	E	69	VAL	3.6
1	D	36	LEU	3.6
2	E	20	ILE	3.6
2	E	53	ILE	3.6
2	E	12	GLU	3.5
1	D	26	LEU	3.5
2	E	84	GLU	3.5
2	E	51	LYS	3.5
1	A	81	ASN	3.5
2	E	52	VAL	3.5
2	E	103	LYS	3.4
1	D	45	ILE	3.3
2	B	62	ASP	3.3
2	E	87	LEU	3.2
2	E	111	GLY	3.2
1	D	31	LEU	3.2
2	B	67	ILE	3.2
2	E	7	GLN	3.2
1	D	29	ARG	3.2
2	B	66	ASP	3.1
1	D	204	ILE	3.1
2	B	63	PRO	3.1
2	E	74	PHE	3.0
2	E	21	ALA	3.0
2	E	101	THR	3.0
2	E	113	THR	3.0
2	E	108	MET	2.9
2	E	36	MET	2.9
1	G	152	TRP	2.8
1	D	34	ALA	2.8
2	E	49	LEU	2.8
1	D	3	GLN	2.8
2	E	130	GLU	2.8
2	E	109	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	68	PRO	2.7
2	E	129	GLU	2.7
1	G	203	LEU	2.7
1	D	409	VAL	2.6
1	D	15	LEU	2.6
1	G	320	GLY	2.5
2	E	30	MET	2.5
2	E	8	SER	2.5
2	E	56	CYS	2.4
2	E	48	ILE	2.4
1	D	17	HIS	2.4
2	E	105	VAL	2.4
2	E	102	CYS	2.4
1	D	80	LYS	2.3
2	E	136	ARG	2.3
2	E	110	LYS	2.3
1	D	51	TRP	2.2
2	E	71	ASP	2.2
2	E	28	LYS	2.1
1	D	94	SER	2.1
2	E	47	ALA	2.1
1	D	22	ILE	2.1
2	E	59	HIS	2.1
1	D	65	TRP	2.1
1	G	198	GLU	2.1
2	E	115	GLU	2.1
2	E	128	THR	2.0
2	E	31	LEU	2.0
2	E	83	PHE	2.0
2	E	50	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SEP	F	37	10/11	0.97	0.12	45,47,49,49	0
3	SEP	F	33	10/11	0.97	0.12	42,45,46,46	0
3	SEP	I	33	10/11	0.98	0.10	43,46,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SEP	I	37	10/11	0.98	0.11	45,51,57,58	0
3	SEP	C	33	10/11	0.99	0.13	22,23,25,26	0
3	SEP	C	37	10/11	0.99	0.14	26,27,32,32	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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
4	GOL	B	201	6/6	0.77	0.28	53,60,64,66	0
4	GOL	G	501	6/6	0.81	0.16	74,76,78,81	0
4	GOL	D	601	6/6	0.82	0.14	55,59,61,63	0
4	GOL	A	502	6/6	0.82	0.16	63,67,68,68	0
4	GOL	A	503	6/6	0.86	0.21	61,68,70,71	0
4	GOL	A	501	6/6	0.87	0.20	54,62,64,66	0
5	NA	D	602	1/1	0.91	0.23	41,41,41,41	0
5	NA	A	504	1/1	0.97	0.15	30,30,30,30	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.