



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:24 am BST

PDB ID : 5HJ2  
Title : Integrin alpha2beta1 I-domain  
Authors : Brown, K.L.; Banerjee, S.  
Deposited on : 2016-01-12  
Resolution : 2.15 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

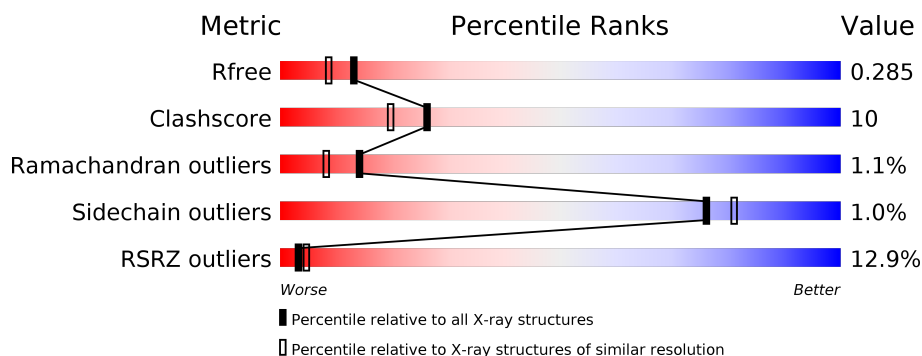
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	197	
1	B	197	
1	C	197	
1	D	197	
1	E	197	
1	F	197	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9501 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 Integrin alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	197	Total	C	N	O	S	0	0	0
			1520	962	256	297	5			
1	A	196	Total	C	N	O	S	0	0	0
			1515	959	255	296	5			
1	B	196	Total	C	N	O	S	0	0	0
			1515	959	255	296	5			
1	D	197	Total	C	N	O	S	0	0	0
			1520	962	256	297	5			
1	E	196	Total	C	N	O	S	0	0	0
			1515	959	255	296	5			
1	F	195	Total	C	N	O	S	0	0	0
			1509	956	254	294	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

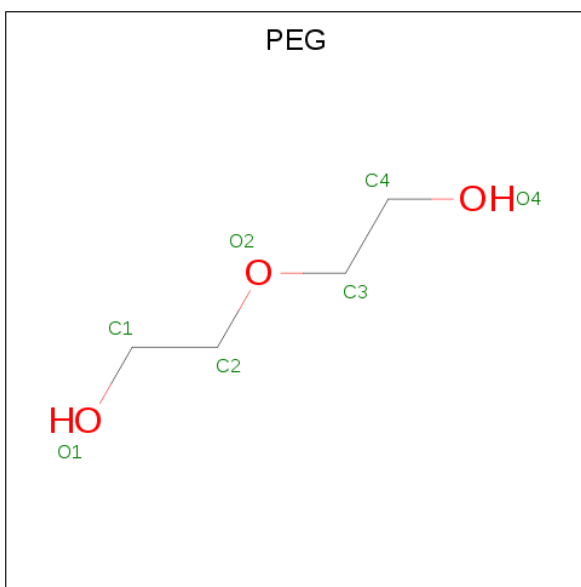
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	73	Total	O	0	0
			73	73		
7	A	82	Total	O	0	0
			82	82		
7	B	73	Total	O	0	0
			73	73		
7	D	76	Total	O	0	0
			76	76		
7	E	15	Total	O	0	0
			15	15		
7	F	45	Total	O	0	0
			45	45		

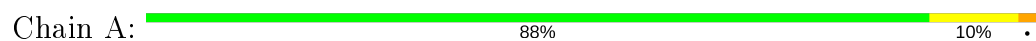
### 3 Residue-property plots [i](#)

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.

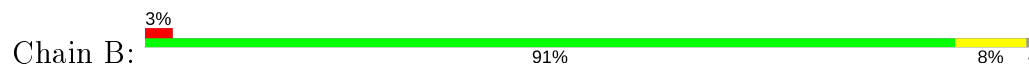
- Molecule 1: Integrin alpha-2



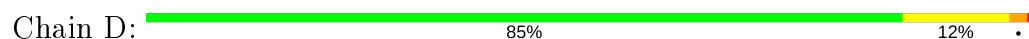
- Molecule 1: Integrin alpha-2



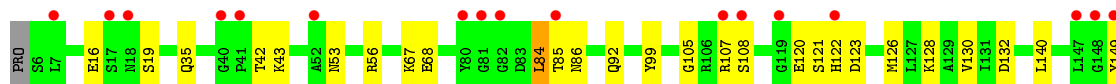
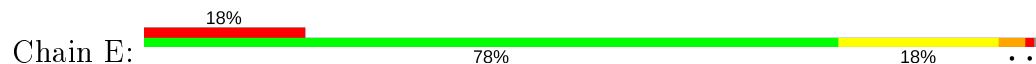
- Molecule 1: Integrin alpha-2

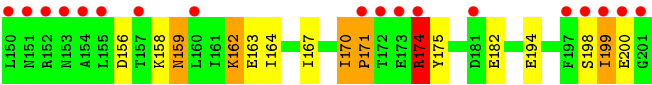


- Molecule 1: Integrin alpha-2

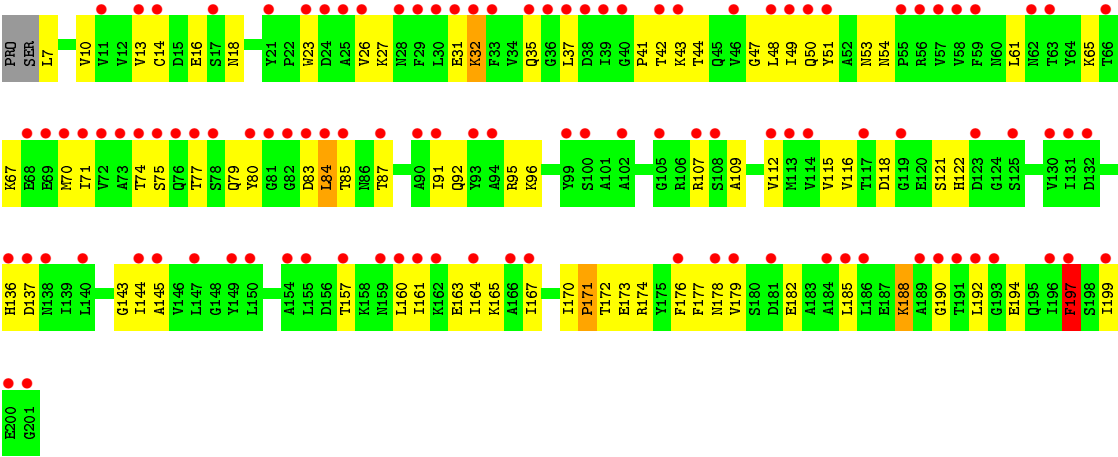


- Molecule 1: Integrin alpha-2





● Molecule 1: Integrin alpha-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.07Å 144.07Å 130.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.87 – 2.15 101.87 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (101.87-2.15) 91.7 (101.87-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.10 _2155)	Depositor
R, $R_{free}$	0.234 , 0.283 0.234 , 0.285	Depositor DCC
$R_{free}$ test set	2000 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, CA, PEG, SO4, CL

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	0.44	0/1539	0.63	1/2084 (0.0%)
1	B	0.46	0/1539	0.68	0/2084
1	C	0.48	0/1544	0.70	3/2091 (0.1%)
1	D	0.46	0/1544	0.70	2/2091 (0.1%)
1	E	0.58	4/1539 (0.3%)	0.70	4/2084 (0.2%)
1	F	0.49	1/1533 (0.1%)	0.84	9/2076 (0.4%)
All	All	0.49	5/9238 (0.1%)	0.71	19/12510 (0.2%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	174	ARG	CZ-NH2	-8.41	1.22	1.33
1	E	174	ARG	NE-CZ	-8.39	1.22	1.33
1	F	32	LYS	CD-CE	7.55	1.70	1.51
1	E	174	ARG	CZ-NH1	-7.34	1.23	1.33
1	E	174	ARG	CD-NE	-6.77	1.34	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	84	LEU	CB-CG-CD2	-9.69	94.52	111.00
1	F	32	LYS	CD-CE-NZ	8.48	131.20	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	84	LEU	CB-CG-CD1	7.48	123.71	111.00
1	E	174	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	E	174	ARG	CD-NE-CZ	-6.47	114.54	123.60
1	E	170	ILE	C-N-CD	-6.43	106.45	120.60
1	F	84	LEU	CA-CB-CG	6.39	130.00	115.30
1	C	15	ASP	CB-CG-OD1	6.01	123.71	118.30
1	F	43	LYS	CB-CA-C	5.89	122.17	110.40
1	F	188	LYS	CD-CE-NZ	-5.63	98.75	111.70
1	D	5	PRO	N-CA-CB	5.59	110.01	103.30
1	F	32	LYS	CA-CB-CG	-5.53	101.23	113.40
1	F	197	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	D	7	LEU	CA-CB-CG	-5.32	103.06	115.30
1	F	43	LYS	N-CA-CB	-5.19	101.25	110.60
1	C	5	PRO	N-CA-CB	5.10	109.42	103.30
1	C	15	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	15	ASP	CB-CG-OD1	5.04	122.83	118.30
1	E	84	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	159	ASN	Sidechain

## 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	1515	0	1508	22	0
1	B	1515	0	1508	9	0
1	C	1520	0	1510	11	0
1	D	1520	0	1510	24	0
1	E	1515	0	1508	51	1
1	F	1509	0	1504	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	2	0	0	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	7	0	10	3	0
5	A	5	0	0	0	0
5	D	10	0	0	0	0
6	D	6	0	8	0	0
6	F	6	0	8	0	1
7	A	82	0	0	6	0
7	B	73	0	0	2	0
7	C	73	0	0	4	0
7	D	76	0	0	5	0
7	E	15	0	0	2	1
7	F	45	0	0	19	1
All	All	9501	0	9074	189	4

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 10.

All (189) 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:E:174:ARG:HD3	1:E:174:ARG:H	1.25	1.01
1:E:174:ARG:NH1	1:E:175:TYR:H	1.59	1.01
1:C:171:PRO:O	7:C:401:HOH:O	1.80	0.99
1:E:174:ARG:NH1	1:E:175:TYR:N	2.16	0.93
1:F:31:GLU:HG3	1:F:71:ILE:HD11	1.51	0.92
1:A:28:ASN:ND2	3:A:303:CL:CL	2.40	0.91
1:E:174:ARG:NH2	1:E:175:TYR:HD2	1.69	0.90
1:A:171:PRO:O	7:A:401:HOH:O	1.90	0.88
1:D:128:LYS:NZ	7:D:402:HOH:O	1.95	0.88
1:D:16:GLU:OE1	7:D:401:HOH:O	1.92	0.87
1:E:174:ARG:CZ	1:E:175:TYR:HD2	1.88	0.86
1:B:107:ARG:O	7:B:401:HOH:O	1.95	0.85
1:E:171:PRO:HD2	1:E:174:ARG:HE	1.40	0.85
1:D:124:GLY:O	7:D:402:HOH:O	1.96	0.83
1:F:177:PHE:HB3	1:F:188:LYS:HE2	1.63	0.81
1:E:170:ILE:C	1:E:174:ARG:HH21	1.83	0.81
1:B:195:GLN:OE1	1:F:136:HIS:NE2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLN:HE21	1:E:130:VAL:HG22	1.47	0.79
1:E:174:ARG:HD3	1:E:174:ARG:N	1.88	0.79
1:E:174:ARG:HH12	1:E:175:TYR:H	1.28	0.78
1:E:120:GLU:OE2	1:E:159:ASN:HB3	1.83	0.78
1:C:107:ARG:O	7:C:403:HOH:O	2.02	0.78
1:E:171:PRO:CD	1:E:174:ARG:HE	1.98	0.76
1:F:84:LEU:HD22	1:F:122:HIS:CG	2.20	0.76
1:E:84:LEU:HB2	7:E:401:HOH:O	1.87	0.74
1:C:5:PRO:O	7:C:404:HOH:O	2.04	0.74
1:F:23:TRP:HH2	1:F:77:THR:HG23	1.53	0.72
1:D:35:GLN:HA	1:D:67:LYS:HE2	1.72	0.71
1:E:199:ILE:HG23	1:E:200:GLU:H	1.54	0.71
1:E:174:ARG:CZ	1:E:175:TYR:CD2	2.74	0.71
1:A:177:PHE:HD2	1:A:188:LYS:HD2	1.57	0.70
1:F:13:VAL:O	7:F:401:HOH:O	2.09	0.69
1:F:16:GLU:OE1	7:F:403:HOH:O	2.10	0.69
1:F:54:ASN:ND2	7:F:407:HOH:O	2.25	0.69
1:F:77:THR:OG1	7:F:402:HOH:O	2.10	0.69
1:E:19:SER:HB2	1:E:149:TYR:CD2	2.28	0.69
1:F:118:ASP:OD2	7:F:404:HOH:O	2.12	0.68
1:F:91:ILE:HD11	7:F:442:HOH:O	1.95	0.67
1:F:144:ILE:HD12	1:F:177:PHE:HB2	1.77	0.67
1:E:42:THR:HG23	1:E:43:LYS:HG3	1.77	0.66
1:D:7:LEU:HD23	1:F:107:ARG:HG2	1.76	0.66
1:F:115:VAL:HG11	7:F:442:HOH:O	1.96	0.65
1:E:68:GLU:N	1:E:68:GLU:OE2	2.30	0.64
1:E:174:ARG:HH11	1:E:175:TYR:N	1.94	0.63
1:E:121:SER:OG	1:E:163:GLU:OE2	2.16	0.62
1:B:8:ILE:HD13	1:B:196:ILE:HG22	1.82	0.62
1:D:5:PRO:HA	1:D:6:SER:C	2.20	0.62
1:B:127:LEU:HD22	1:D:171:PRO:HG3	1.81	0.62
1:E:182:GLU:N	1:E:182:GLU:OE2	2.28	0.61
1:F:23:TRP:CH2	1:F:77:THR:HG23	2.33	0.61
1:F:10:VAL:HA	1:F:112:VAL:HG13	1.83	0.60
1:E:174:ARG:NH2	1:E:175:TYR:CD2	2.60	0.60
1:E:19:SER:HB2	1:E:149:TYR:HD2	1.67	0.60
1:F:31:GLU:O	1:F:35:GLN:HG2	2.00	0.60
1:A:174:ARG:NH1	7:A:403:HOH:O	2.11	0.60
1:F:144:ILE:N	1:F:164:ILE:HD11	2.17	0.60
1:B:200:GLU:OE2	7:B:404:HOH:O	2.17	0.59
1:F:87:THR:HB	1:F:121:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:GLU:HG3	1:F:71:ILE:CD1	2.29	0.59
1:D:7:LEU:CD2	1:F:107:ARG:HG2	2.32	0.59
1:F:54:ASN:HB2	7:F:430:HOH:O	2.01	0.59
1:F:16:GLU:OE1	1:F:50:GLN:NE2	2.34	0.59
1:E:84:LEU:HB3	1:E:122:HIS:ND1	2.18	0.58
1:F:182:GLU:OE1	7:F:404:HOH:O	2.17	0.58
1:E:198:SER:OG	1:E:198:SER:O	2.20	0.58
1:A:23:TRP:CD2	1:A:79:GLN:HB2	2.39	0.58
1:B:32:LYS:HG2	1:B:189:ALA:HB3	1.84	0.58
1:F:167:ILE:HD13	7:F:442:HOH:O	2.03	0.58
1:E:174:ARG:N	1:E:174:ARG:HH11	2.02	0.57
1:E:53:ASN:O	1:E:86:ASN:ND2	2.35	0.57
1:B:6:SER:OG	1:B:200:GLU:OE1	2.14	0.57
1:E:174:ARG:H	1:E:174:ARG:HH11	1.51	0.57
1:F:167:ILE:HG21	7:F:442:HOH:O	2.04	0.57
1:A:177:PHE:CD2	1:A:188:LYS:HD2	2.40	0.56
1:C:128:LYS:HD3	1:A:173:GLU:HB2	1.86	0.56
1:C:174:ARG:O	1:C:195:GLN:NE2	2.39	0.56
1:A:62:ASN:OD1	7:A:404:HOH:O	2.18	0.55
1:C:38:ASP:OD1	1:C:43:LYS:NZ	2.30	0.54
1:F:31:GLU:CG	1:F:71:ILE:HD11	2.32	0.54
1:F:160:LEU:O	1:F:164:ILE:HG22	2.08	0.54
1:F:143:GLY:C	1:F:164:ILE:HD11	2.28	0.53
1:E:162:LYS:HD2	1:E:163:GLU:N	2.23	0.53
1:E:199:ILE:HG23	1:E:200:GLU:N	2.22	0.53
1:F:35:GLN:O	1:F:67:LYS:NZ	2.25	0.53
1:A:35:GLN:HG2	1:A:71:ILE:HD11	1.90	0.53
1:F:157:THR:O	1:F:161:ILE:HG22	2.09	0.53
1:E:140:LEU:HD22	1:E:199:ILE:HD11	1.91	0.52
1:E:107:ARG:NH2	1:E:108:SER:HB3	2.24	0.52
1:A:172:THR:N	7:A:402:HOH:O	1.96	0.51
1:C:179:VAL:HG22	1:C:188:LYS:HG3	1.91	0.51
1:F:179:VAL:CG2	1:F:188:LYS:HZ3	2.24	0.51
1:D:6:SER:O	7:D:404:HOH:O	2.19	0.51
1:E:85:THR:O	1:E:85:THR:HG23	2.11	0.51
1:D:50:GLN:NE2	7:D:401:HOH:O	2.44	0.51
1:F:41:PRO:HG3	1:F:65:LYS:HD3	1.93	0.51
1:F:37:LEU:HD23	1:F:44:THR:HG21	1.93	0.50
1:A:35:GLN:HA	1:A:67:LYS:HE2	1.93	0.50
1:F:42:THR:OG1	1:F:42:THR:O	2.27	0.50
1:F:53:ASN:ND2	7:F:413:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:THR:HG23	1:E:121:SER:HA	1.93	0.50
1:F:170:ILE:HG23	1:F:171:PRO:HA	1.94	0.50
1:D:6:SER:HB2	1:D:8:ILE:HG13	1.92	0.50
1:F:185:LEU:HD23	1:F:188:LYS:NZ	2.26	0.50
1:D:171:PRO:O	1:D:172:THR:HB	2.11	0.49
1:E:128:LYS:HD3	1:E:132:ASP:OD2	2.12	0.49
1:F:49:ILE:HG13	7:F:436:HOH:O	2.12	0.49
1:F:177:PHE:CD1	1:F:188:LYS:HD3	2.48	0.49
1:F:92:GLN:NE2	7:F:408:HOH:O	2.32	0.49
1:D:108:SER:OG	1:F:107:ARG:HG3	2.12	0.49
1:C:10:VAL:O	1:C:46:VAL:HA	2.14	0.48
1:D:6:SER:HB3	1:D:200:GLU:CD	2.34	0.48
1:E:99:TYR:O	1:E:105:GLY:HA3	2.14	0.48
1:F:116:VAL:O	7:F:401:HOH:O	2.20	0.48
1:D:74:THR:O	1:D:77:THR:HG22	2.12	0.48
1:E:156:ASP:OD2	1:E:158:LYS:HD3	2.14	0.48
1:F:145:ALA:HB2	1:F:164:ILE:HG21	1.96	0.48
1:F:23:TRP:CD1	1:F:79:GLN:HB2	2.49	0.47
1:E:107:ARG:CZ	1:E:108:SER:HB3	2.44	0.47
1:D:191:THR:O	1:D:195:GLN:HG3	2.14	0.47
1:E:174:ARG:HH11	1:E:174:ARG:CA	2.27	0.47
1:D:33:PHE:CE1	1:D:196:ILE:HD12	2.50	0.47
1:E:35:GLN:HA	1:E:67:LYS:HE2	1.97	0.47
1:E:123:ASP:O	1:E:126:MET:HG2	2.15	0.47
1:D:5:PRO:HA	1:D:6:SER:O	2.15	0.47
1:F:165:LYS:NZ	7:F:406:HOH:O	2.21	0.47
1:F:23:TRP:O	1:F:26:VAL:HG12	2.14	0.46
1:F:23:TRP:CG	1:F:79:GLN:HB2	2.50	0.46
1:F:174:ARG:HB3	7:F:405:HOH:O	2.15	0.46
1:F:121:SER:OG	1:F:163:GLU:OE2	2.24	0.46
1:F:194:GLU:O	1:F:197:PHE:HB3	2.16	0.46
1:F:145:ALA:O	1:F:179:VAL:HG23	2.15	0.46
1:F:14:CYS:HB3	7:F:437:HOH:O	2.15	0.46
1:A:6:SER:HA	7:A:454:HOH:O	2.16	0.45
1:E:164:ILE:HA	1:E:164:ILE:HD13	1.71	0.45
1:E:164:ILE:HD13	1:E:167:ILE:HD12	1.99	0.45
1:D:176:PHE:C	1:D:177:PHE:HD1	2.20	0.45
1:E:174:ARG:HH12	1:E:175:TYR:N	1.95	0.45
1:D:38:ASP:OD2	1:D:43:LYS:HD3	2.16	0.45
1:F:179:VAL:CG2	1:F:188:LYS:NZ	2.80	0.45
1:F:27:LYS:HD2	1:F:75:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ASN:HA	7:E:401:HOH:O	2.17	0.44
1:A:159:ASN:O	1:A:162:LYS:HE3	2.18	0.44
1:D:170:ILE:HG23	1:D:171:PRO:HA	1.99	0.44
1:E:170:ILE:C	1:E:174:ARG:NH2	2.62	0.44
1:F:179:VAL:HG22	1:F:188:LYS:NZ	2.33	0.44
1:F:170:ILE:HA	1:F:171:PRO:C	2.38	0.43
1:F:174:ARG:HH11	1:F:199:ILE:HD12	1.83	0.43
1:F:144:ILE:HG23	1:F:188:LYS:HZ3	1.84	0.43
1:A:54:ASN:HB3	4:A:304:PEG:H11	2.00	0.43
1:A:162:LYS:HD2	1:A:163:GLU:N	2.34	0.43
1:F:95:ARG:HD3	1:F:137:ASP:OD1	2.19	0.43
1:F:53:ASN:N	1:F:53:ASN:OD1	2.52	0.43
1:D:182:GLU:OE1	1:D:182:GLU:N	2.48	0.43
1:F:145:ALA:HB2	1:F:164:ILE:HD13	2.01	0.42
1:F:70:MET:O	1:F:74:THR:HG23	2.19	0.42
1:A:159:ASN:O	1:A:162:LYS:HG3	2.20	0.42
1:F:185:LEU:HD23	1:F:188:LYS:HZ1	1.83	0.42
1:F:48:LEU:HD11	7:F:437:HOH:O	2.19	0.42
1:D:23:TRP:CD2	1:D:79:GLN:HB2	2.54	0.42
1:E:194:GLU:O	1:E:198:SER:HB3	2.20	0.42
1:C:88:PHE:CE2	1:C:124:GLY:HA2	2.54	0.42
1:E:171:PRO:N	1:E:174:ARG:HH21	2.16	0.42
1:F:7:LEU:HB3	1:F:109:ALA:HA	2.01	0.42
1:C:128:LYS:CD	1:A:173:GLU:HB2	2.49	0.42
1:F:173:GLU:O	1:F:173:GLU:HG2	2.19	0.42
1:E:16:GLU:OE1	1:E:56:ARG:NH2	2.43	0.42
1:F:194:GLU:HA	1:F:197:PHE:CB	2.50	0.42
1:A:79:GLN:HB3	7:A:466:HOH:O	2.19	0.41
1:B:23:TRP:CD2	1:B:79:GLN:HB2	2.55	0.41
1:F:95:ARG:NH1	1:F:96:LYS:HG2	2.35	0.41
1:F:190:GLY:O	1:F:194:GLU:HG3	2.20	0.41
1:F:18:ASN:ND2	1:F:83:ASP:OD1	2.53	0.41
1:A:99:TYR:O	1:A:105:GLY:HA3	2.21	0.41
1:F:161:ILE:HD13	1:F:161:ILE:HG21	1.88	0.41
1:D:6:SER:HA	1:D:7:LEU:HB2	2.01	0.41
1:F:177:PHE:CD1	1:F:192:LEU:HD12	2.56	0.41
1:E:170:ILE:HA	1:E:171:PRO:O	2.21	0.41
1:F:23:TRP:HB2	1:F:79:GLN:OE1	2.21	0.41
1:C:172:THR:N	7:C:402:HOH:O	1.92	0.41
1:F:176:PHE:CE2	1:F:178:ASN:HB2	2.56	0.41
1:F:51:TYR:CE2	1:F:85:THR:HG23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:CG	4:A:304:PEG:H11	2.42	0.41
1:F:116:VAL:HA	1:F:144:ILE:HB	2.03	0.40
1:A:170:ILE:HA	1:A:171:PRO:C	2.41	0.40
1:A:93:TYR:CE2	4:A:304:PEG:H41	2.56	0.40
1:B:10:VAL:O	1:B:46:VAL:HA	2.21	0.40
1:E:174:ARG:HD3	1:E:174:ARG:HH11	1.36	0.40
1:F:143:GLY:C	1:F:144:ILE:HD13	2.41	0.40
1:F:47:GLY:N	1:F:61:LEU:HD23	2.36	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ASN:CG	1:E:159:ASN:ND2[7_555]	1.35	0.85
6:F:301:GOL:C3	6:F:301:GOL:O3[7_554]	1.41	0.79
7:E:415:HOH:O	7:E:415:HOH:O[7_555]	2.06	0.14
7:F:435:HOH:O	7:F:435:HOH:O[7_554]	2.11	0.09

## 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	194/197 (98%)	189 (97%)	3 (2%)	2 (1%)	15	9
1	B	194/197 (98%)	189 (97%)	3 (2%)	2 (1%)	15	9
1	C	195/197 (99%)	191 (98%)	2 (1%)	2 (1%)	15	9
1	D	195/197 (99%)	190 (97%)	2 (1%)	3 (2%)	10	5
1	E	194/197 (98%)	189 (97%)	3 (2%)	2 (1%)	15	9
1	F	193/197 (98%)	188 (97%)	3 (2%)	2 (1%)	15	9
All	All	1165/1182 (99%)	1136 (98%)	16 (1%)	13 (1%)	14	8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	PRO
1	D	6	SER
1	E	171	PRO
1	C	172	THR
1	A	172	THR
1	B	172	THR
1	D	172	THR
1	E	199	ILE
1	F	172	THR
1	B	171	PRO
1	F	171	PRO
1	C	171	PRO
1	D	171	PRO

### 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	164/165 (99%)	162 (99%)	2 (1%)	71	76
1	B	164/165 (99%)	163 (99%)	1 (1%)	86	90
1	C	164/165 (99%)	164 (100%)	0	100	100
1	D	164/165 (99%)	162 (99%)	2 (1%)	71	76
1	E	164/165 (99%)	162 (99%)	2 (1%)	71	76
1	F	163/165 (99%)	160 (98%)	3 (2%)	59	63
All	All	983/990 (99%)	973 (99%)	10 (1%)	76	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	162	LYS
1	B	7	LEU
1	D	53	ASN

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Mol	Chain	Res	Type
1	D	172	THR
1	E	162	LYS
1	E	174	ARG
1	F	32	LYS
1	F	80	TYR
1	F	197	PHE

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	195	GLN
1	D	50	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 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	$\# Z  > 2$
5	SO4	D	305	-	4,4,4	0.13	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	F	301	-	5,5,5	0.45	0	5,5,5	2.21	1 (20%)
5	SO4	D	304	-	4,4,4	0.18	0	6,6,6	0.54	0
6	GOL	D	303	-	5,5,5	0.35	0	5,5,5	0.54	0
4	PEG	A	304	-	6,6,6	0.49	0	5,5,5	0.37	0
5	SO4	A	305	-	4,4,4	0.18	0	6,6,6	0.12	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
6	GOL	F	301	-	-	2/4/4/4	-
6	GOL	D	303	-	-	0/4/4/4	-
4	PEG	A	304	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	GOL	O3-C3-C2	4.90	133.69	110.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	301	GOL	O1-C1-C2-C3
6	F	301	GOL	O1-C1-C2-O2
4	A	304	PEG	O1-C1-C2-O2
4	A	304	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	301	GOL	0	1
4	A	304	PEG	3	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	196/197 (99%)	-0.09	0	100	100	14, 23, 33, 42	0
1	B	196/197 (99%)	-0.04	5 (2%)	56	64	14, 23, 39, 74	0
1	C	197/197 (100%)	-0.05	2 (1%)	82	86	14, 20, 35, 73	0
1	D	197/197 (100%)	-0.03	0	100	100	14, 23, 38, 48	0
1	E	196/197 (99%)	1.09	35 (17%)	1	1	25, 45, 71, 89	0
1	F	195/197 (98%)	2.47	110 (56%)	0	0	39, 59, 79, 87	0
All	All	1177/1182 (99%)	0.56	152 (12%)	3	5	14, 27, 69, 89	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	23	TRP	8.6
1	E	150	LEU	8.6
1	E	197	PHE	8.5
1	E	199	ILE	8.2
1	F	201	GLY	6.7
1	E	201	GLY	6.5
1	F	42	THR	6.3
1	F	154	ALA	6.2
1	F	161	ILE	5.9
1	F	196	ILE	5.8
1	F	197	PHE	5.7
1	E	80	TYR	5.7
1	E	154	ALA	5.6
1	F	59	PHE	5.5
1	E	174	ARG	5.3
1	F	25	ALA	5.3
1	F	49	ILE	5.2
1	F	91	ILE	5.0
1	F	166	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	32	LYS	4.9
1	E	171	PRO	4.9
1	C	201	GLY	4.9
1	F	189	ALA	4.8
1	F	58	VAL	4.8
1	B	201	GLY	4.7
1	E	172	THR	4.6
1	F	69	GLU	4.6
1	F	138	ASN	4.6
1	F	149	TYR	4.6
1	F	80	TYR	4.5
1	E	152	ARG	4.5
1	F	56	ARG	4.5
1	F	63	THR	4.4
1	F	77	THR	4.4
1	E	148	GLY	4.4
1	F	17	SER	4.4
1	F	200	GLU	4.4
1	F	66	THR	4.3
1	F	40	GLY	4.2
1	F	33	PHE	4.2
1	F	83	ASP	4.0
1	F	73	ALA	3.9
1	F	31	GLU	3.9
1	B	200	GLU	3.9
1	F	21	TYR	3.9
1	F	130	VAL	3.9
1	F	26	VAL	3.9
1	F	36	GLY	3.8
1	F	147	LEU	3.8
1	F	76	GLN	3.8
1	F	155	LEU	3.8
1	F	38	ASP	3.8
1	F	181	ASP	3.7
1	F	14	CYS	3.7
1	E	160	LEU	3.7
1	F	185	LEU	3.7
1	F	39	ILE	3.6
1	F	119	GLY	3.6
1	F	136	HIS	3.6
1	E	119	GLY	3.5
1	F	84	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	140	LEU	3.5
1	F	43	LYS	3.5
1	F	112	VAL	3.5
1	F	13	VAL	3.5
1	F	70	MET	3.5
1	F	87	THR	3.4
1	F	150	LEU	3.4
1	E	149	TYR	3.4
1	F	46	VAL	3.4
1	F	71	ILE	3.3
1	F	178	ASN	3.3
1	F	144	ILE	3.3
1	F	192	LEU	3.3
1	E	173	GLU	3.3
1	E	198	SER	3.2
1	E	108	SER	3.2
1	E	155	LEU	3.1
1	B	197	PHE	3.1
1	F	93	TYR	3.1
1	F	199	ILE	3.1
1	F	186	LEU	3.1
1	F	167	ILE	3.1
1	F	105	GLY	3.0
1	F	160	LEU	3.0
1	F	37	LEU	3.0
1	F	82	GLY	3.0
1	F	72	VAL	2.9
1	F	164	ILE	2.9
1	F	85	THR	2.9
1	F	55	PRO	2.9
1	F	113	MET	2.9
1	C	200	GLU	2.9
1	F	48	LEU	2.9
1	E	18	ASN	2.8
1	F	90	ALA	2.8
1	E	107	ARG	2.8
1	E	7	LEU	2.8
1	E	122	HIS	2.8
1	F	191	THR	2.8
1	F	50	GLN	2.8
1	F	102	ALA	2.8
1	F	68	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	40	GLY	2.8
1	F	132	ASP	2.7
1	E	157	THR	2.7
1	F	145	ALA	2.7
1	E	200	GLU	2.7
1	F	162	LYS	2.6
1	B	6	SER	2.6
1	F	24	ASP	2.6
1	E	52	ALA	2.6
1	F	62	ASN	2.6
1	F	193	GLY	2.5
1	F	35	GLN	2.4
1	F	57	VAL	2.4
1	F	75	SER	2.4
1	F	176	PHE	2.4
1	F	114	VAL	2.4
1	E	82	GLY	2.4
1	F	190	GLY	2.4
1	B	171	PRO	2.4
1	F	137	ASP	2.3
1	F	11	VAL	2.3
1	F	131	ILE	2.3
1	F	123	ASP	2.3
1	F	108	SER	2.3
1	E	147	LEU	2.2
1	F	30	LEU	2.2
1	F	28	ASN	2.2
1	E	17	SER	2.2
1	E	85	THR	2.2
1	E	41	PRO	2.2
1	F	157	THR	2.2
1	F	81	GLY	2.2
1	F	179	VAL	2.2
1	E	151	ASN	2.2
1	F	159	ASN	2.2
1	F	74	THR	2.2
1	F	78	SER	2.2
1	F	29	PHE	2.1
1	E	181	ASP	2.1
1	F	99	TYR	2.1
1	F	100	SER	2.1
1	F	94	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	107	ARG	2.0
1	E	153	ASN	2.0
1	F	125	SER	2.0
1	F	117	THR	2.0
1	F	184	ALA	2.0
1	E	81	GLY	2.0
1	F	51	TYR	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 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(Å <sup>2</sup> )	Q<0.9
5	SO4	D	305	5/5	0.60	0.23	83,85,95,95	0
5	SO4	A	305	5/5	0.82	0.25	51,52,56,71	0
6	GOL	F	301	6/6	0.83	0.18	51,52,60,60	1
3	CL	D	302	1/1	0.84	0.09	62,62,62,62	0
3	CL	B	302	1/1	0.86	0.14	40,40,40,40	0
6	GOL	D	303	6/6	0.87	0.12	28,32,35,35	0
4	PEG	A	304	7/7	0.89	0.13	24,26,30,31	0
2	CA	E	301	1/1	0.90	0.06	52,52,52,52	0
3	CL	A	303	1/1	0.91	0.08	52,52,52,52	0
2	CA	D	301	1/1	0.95	0.10	37,37,37,37	0
2	CA	C	301	1/1	0.96	0.05	40,40,40,40	0
3	CL	A	302	1/1	0.96	0.06	27,27,27,27	1
2	CA	A	301	1/1	0.97	0.07	35,35,35,35	0
5	SO4	D	304	5/5	0.98	0.10	22,22,28,36	0
2	CA	B	301	1/1	0.99	0.08	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.