



# Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2022 – 02:19 PM EDT

PDB ID : 7TUS  
Title : Sculpting a uniquely reactive cysteine residue for site-specific antibody conjugation  
Authors : Park, H.; Rader, C.  
Deposited on : 2022-02-03  
Resolution : 2.40 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 : 2.28.1  
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) : 2.28.1

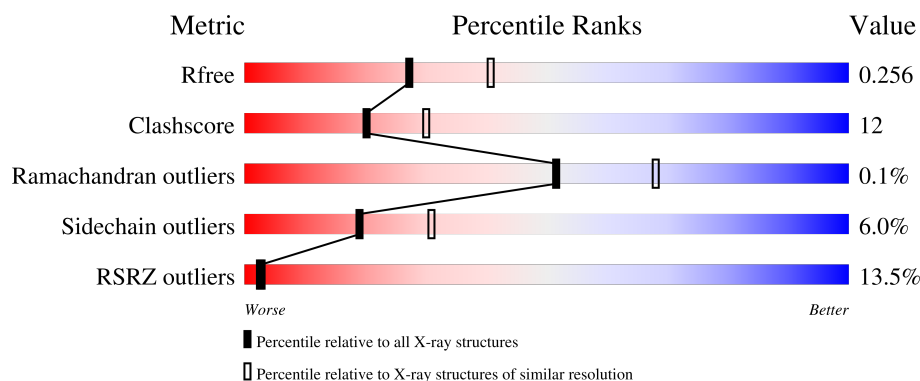
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	221	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	C	221	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	E	221	<div> <div>21%</div> <div>76%</div> <div>19%</div> <div>5%</div> </div>
1	G	221	<div> <div>11%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
2	B	219	<div> <div>8%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	219	<div><div>5%</div><div><div></div><div>69%</div><div>29%</div><div>..</div></div></div>
2	F	219	<div><div>36%</div><div><div></div><div>76%</div><div>20%</div><div>..</div></div></div>
2	H	219	<div><div>18%</div><div><div></div><div>77%</div><div>20%</div><div>..</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13140 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 Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1631	1032	272	320	7			
1	C	215	Total	C	N	O	S	0	0	0
			1627	1031	271	318	7			
1	E	209	Total	C	N	O	S	0	0	0
			1519	956	258	298	7			
1	G	219	Total	C	N	O	S	0	0	0
			1641	1036	274	324	7			

- Molecule 2 is a protein called Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1649	1037	275	332	5			
2	D	216	Total	C	N	O	S	0	0	0
			1642	1029	276	332	5			
2	F	216	Total	C	N	O	S	0	0	0
			1532	967	255	305	5			
2	H	217	Total	C	N	O	S	0	0	0
			1590	1002	264	319	5			

- Molecule 3 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
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total	O	0	0
			50	50		
6	B	17	Total	O	0	0
			17	17		

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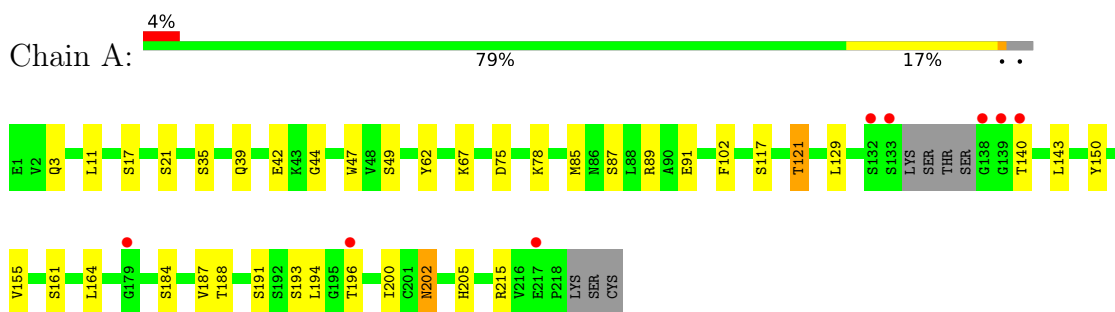
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	66	Total 66	O 66	0	0
6	D	47	Total 47	O 47	0	0
6	E	12	Total 12	O 12	0	0
6	F	2	Total 2	O 2	0	0
6	G	27	Total 27	O 27	0	0
6	H	15	Total 15	O 15	0	0

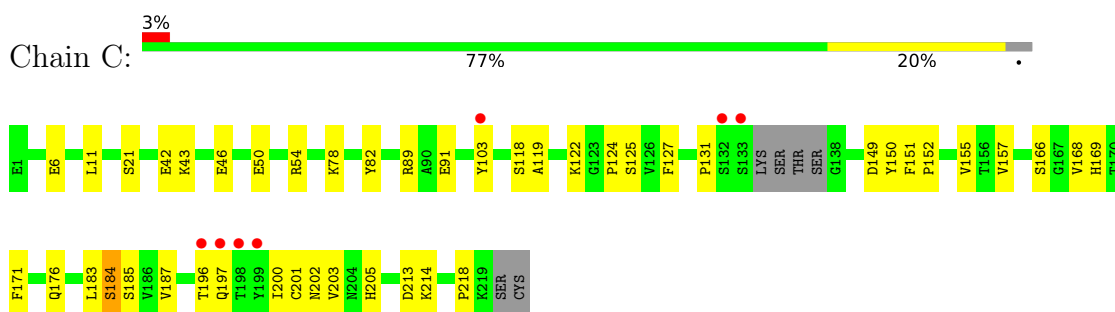
### 3 Residue-property plots [i](#)

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.

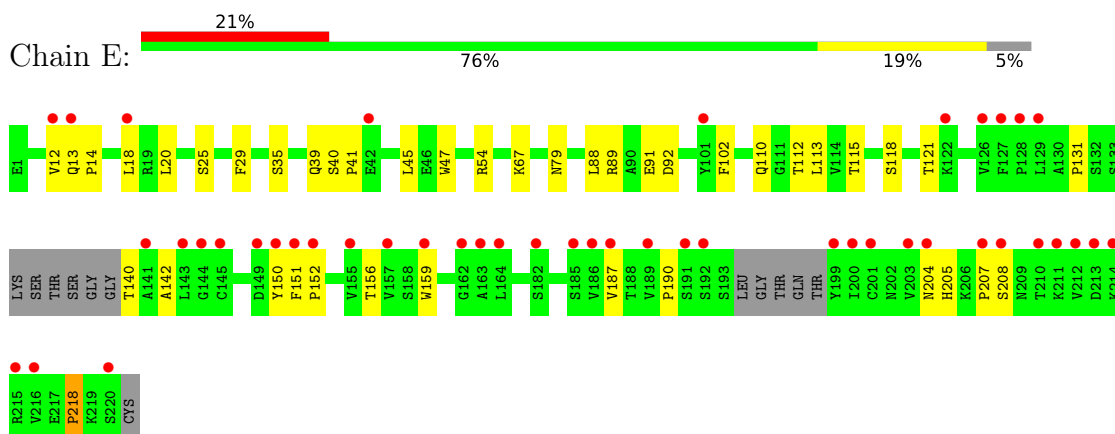
- Molecule 1: Antibody Heavy Chain



- Molecule 1: Antibody Heavy Chain



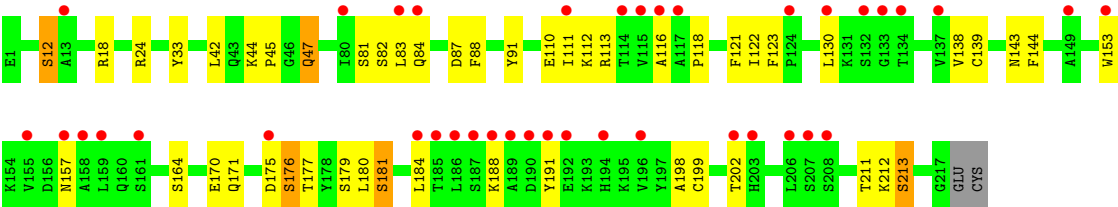
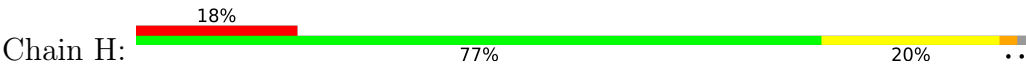
- Molecule 1: Antibody Heavy Chain



- Molecule 1: Antibody Heavy Chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.47Å 73.57Å 127.58Å 90.00° 110.06° 90.00°	Depositor
Resolution (Å)	39.95 – 2.40 39.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.8 (39.95-2.40) 97.8 (39.95-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, $R_{free}$	0.218 , 0.257 0.217 , 0.256	Depositor DCC
$R_{free}$ test set	3774 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.89% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PEG, MG

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	0.57	0/1673	0.71	0/2280
1	C	0.61	0/1669	0.73	0/2275
1	E	0.52	1/1556 (0.1%)	0.69	1/2126 (0.0%)
1	G	0.55	1/1684 (0.1%)	0.66	0/2297
2	B	0.51	0/1687	0.66	0/2292
2	D	0.56	1/1679 (0.1%)	0.68	2/2282 (0.1%)
2	F	0.46	0/1567	0.60	0/2144
2	H	0.44	0/1627	0.60	0/2218
All	All	0.53	3/13142 (0.0%)	0.67	3/17914 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	218	PRO	N-CD	11.30	1.63	1.47
2	D	209	PRO	N-CD	6.04	1.56	1.47
1	G	98	CYS	CB-SG	-5.55	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	218	PRO	CA-N-CD	-13.80	92.19	111.50
2	D	209	PRO	CA-N-CD	-7.38	101.17	111.50
2	D	209	PRO	N-CD-CG	-6.42	93.57	103.20

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	1631	0	1567	26	0
1	C	1627	0	1555	40	1
1	E	1519	0	1361	35	0
1	G	1641	0	1551	41	1
2	B	1649	0	1590	61	0
2	D	1642	0	1584	55	0
2	F	1532	0	1390	25	0
2	H	1590	0	1477	40	0
3	A	7	0	10	1	0
3	C	7	0	10	2	0
3	D	7	0	10	0	0
3	E	7	0	10	1	0
3	G	14	0	20	6	0
4	A	15	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
5	B	1	0	0	0	0
6	A	50	0	0	1	0
6	B	17	0	0	1	0
6	C	66	0	0	3	0
6	D	47	0	0	1	0
6	E	12	0	0	1	0
6	F	2	0	0	0	0
6	G	27	0	0	2	0
6	H	15	0	0	0	0
All	All	13140	0	12135	312	1

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 12.

All (312) 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:G:203:VAL:CG1	1:G:212:VAL:HG22	1.57	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:SER:OG	1:G:210:THR:HG23	1.43	1.18
1:G:203:VAL:HG12	1:G:212:VAL:HG22	1.28	1.15
1:C:127:PHE:CE2	2:D:129:GLN:HG3	1.85	1.11
2:B:129:GLN:HE22	2:B:136:SER:CB	1.67	1.06
2:B:129:GLN:HE22	2:B:136:SER:HB2	1.17	1.05
1:C:127:PHE:HE2	2:D:129:GLN:HG3	1.18	1.03
1:G:203:VAL:HG12	1:G:212:VAL:CG2	1.93	0.99
2:B:128:GLU:HA	2:B:131:LYS:HD3	1.43	0.99
1:G:203:VAL:CG1	1:G:212:VAL:CG2	2.40	0.98
2:B:128:GLU:OE1	2:B:128:GLU:N	1.98	0.95
2:D:160:GLN:HB3	2:D:163:ASN:HD21	1.33	0.94
2:F:108:LYS:HE3	2:F:110:GLU:HB2	1.50	0.91
2:B:5:THR:HB	2:B:24:ARG:HG2	1.55	0.89
2:H:88:PHE:HB2	2:H:111:ILE:HD11	1.56	0.88
2:H:171:GLN:HE21	2:H:176:SER:HB3	1.36	0.87
2:B:20:THR:HG22	2:B:79:THR:OG1	1.75	0.86
2:F:2:LEU:HD12	2:F:29:LEU:HD21	1.58	0.85
2:D:137:VAL:HG13	2:D:153:TRP:CH2	2.11	0.85
1:G:204:ASN:HD22	1:G:205:HIS:N	1.74	0.85
2:B:66:ARG:NH2	2:B:87:ASP:OD1	2.08	0.85
1:A:42:GLU:N	1:A:42:GLU:OE1	2.10	0.85
2:D:148:GLU:OE1	2:D:148:GLU:N	2.09	0.84
2:B:150:LYS:HD3	2:B:152:GLN:NE2	1.93	0.84
1:G:208:SER:OG	1:G:210:THR:CG2	2.26	0.84
1:A:161:SER:H	1:A:202:ASN:HD21	1.23	0.83
1:E:218:PRO:HD2	1:E:218:PRO:O	1.79	0.83
1:C:42:GLU:N	1:C:42:GLU:OE1	2.12	0.82
2:B:128:GLU:HA	2:B:131:LYS:CD	2.11	0.80
2:D:152:GLN:NE2	2:D:159:LEU:CD1	2.45	0.79
1:E:18:LEU:HD12	1:E:88:LEU:CD1	2.13	0.78
2:D:124:PRO:HA	2:D:137:VAL:HG23	1.65	0.78
2:D:152:GLN:NE2	2:D:159:LEU:HD11	1.99	0.78
2:B:127:ASP:O	2:B:131:LYS:HG3	1.84	0.78
2:B:129:GLN:NE2	2:B:136:SER:HB2	1.98	0.77
2:D:166:GLU:HG2	2:D:180:LEU:HD21	1.65	0.76
2:H:164:SER:HB3	2:H:184:LEU:HD23	1.68	0.76
2:H:130:LEU:HD22	2:H:188:LYS:HG3	1.67	0.74
2:H:175:ASP:OD1	2:H:177:THR:HG23	1.88	0.73
1:G:126:VAL:HG21	1:G:203:VAL:HG11	1.70	0.72
1:G:203:VAL:HG13	1:G:212:VAL:HG22	1.67	0.72
2:D:120:VAL:O	2:D:212:LYS:HE2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:HG11	1:E:18:LEU:HD11	1.73	0.71
2:H:122:ILE:HD13	2:H:199:CYS:SG	2.30	0.71
2:B:129:GLN:O	2:B:132:SER:OG	2.04	0.70
2:D:42:LEU:HD21	2:D:44:LYS:HE3	1.75	0.69
2:B:155:VAL:HG23	2:B:197:TYR:CE1	2.27	0.69
1:C:127:PHE:CE2	2:D:129:GLN:CG	2.70	0.69
1:C:196:THR:HG23	1:C:197:GLN:HG2	1.73	0.69
2:D:155:VAL:HG12	2:D:194:HIS:CD2	2.27	0.69
1:A:200:ILE:HG22	1:A:215:ARG:HG3	1.76	0.67
1:G:123:GLY:HA3	1:G:210:THR:HG21	1.75	0.67
2:H:42:LEU:HD12	2:H:91:TYR:CE2	2.30	0.67
1:C:125:SER:HB3	1:C:127:PHE:CE1	2.30	0.67
2:H:122:ILE:CD1	2:H:199:CYS:SG	2.83	0.67
2:B:127:ASP:HA	2:B:130:LEU:HD12	1.78	0.66
2:D:137:VAL:HG13	2:D:153:TRP:CZ3	2.30	0.66
1:C:118:SER:HB2	2:H:24:ARG:HH12	1.59	0.66
1:C:155:VAL:CG2	1:C:183:LEU:HD13	2.25	0.66
1:C:155:VAL:HG23	1:C:183:LEU:HD13	1.78	0.66
1:E:18:LEU:HD12	1:E:88:LEU:HD11	1.78	0.65
1:G:203:VAL:HG11	1:G:212:VAL:HG22	1.68	0.65
1:G:126:VAL:HG21	1:G:212:VAL:HG21	1.77	0.65
2:F:108:LYS:CE	2:F:110:GLU:HB2	2.26	0.65
1:A:200:ILE:HD12	1:A:202:ASN:OD1	1.97	0.64
2:B:25:SER:OG	2:B:74:THR:HA	1.99	0.63
2:H:157:ASN:OD1	2:H:157:ASN:O	2.17	0.63
1:G:204:ASN:HD22	1:G:204:ASN:C	1.99	0.63
1:E:18:LEU:CD1	1:E:88:LEU:CD1	2.76	0.63
2:D:152:GLN:HE21	2:D:159:LEU:CD1	2.11	0.63
2:F:40:TRP:HB2	2:F:53:ILE:HB	1.79	0.62
1:E:20:LEU:HD22	1:E:112:THR:HG21	1.81	0.62
1:A:161:SER:N	1:A:202:ASN:HD21	1.96	0.62
2:B:129:GLN:NE2	2:B:136:SER:CB	2.51	0.62
1:E:218:PRO:O	1:E:218:PRO:CD	2.49	0.61
2:D:153:TRP:CD1	2:D:184:LEU:HD13	2.36	0.61
1:C:127:PHE:CD2	2:D:129:GLN:HB2	2.35	0.61
1:E:159:TRP:CE2	1:E:187:VAL:CG2	2.84	0.61
1:C:183:LEU:HD23	1:C:184:SER:N	2.15	0.61
2:H:180:LEU:HD23	2:H:181:SER:N	2.16	0.61
2:B:85:PRO:HA	2:B:111:ILE:HG12	1.81	0.61
2:B:40:TRP:HB2	2:B:53:ILE:HB	1.82	0.60
2:F:41:TYR:HE1	2:F:94:SER:HB3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:GLN:NE2	2:D:159:LEU:HD13	2.15	0.60
2:D:155:VAL:HG12	2:D:194:HIS:HD2	1.63	0.60
2:D:188:LYS:HD2	2:D:189:ALA:N	2.17	0.60
2:B:71:GLY:HA3	2:B:76:PHE:HA	1.82	0.60
1:G:203:VAL:HG11	1:G:212:VAL:CG2	2.28	0.59
2:H:143:ASN:N	2:H:143:ASN:HD22	1.99	0.59
2:B:88:PHE:HB3	2:B:111:ILE:HD13	1.84	0.59
1:G:135:SER:HA	2:H:121:PHE:HD2	1.68	0.59
2:B:84:GLN:HB3	2:B:86:GLU:OE1	2.03	0.59
1:C:91:GLU:N	1:C:91:GLU:OE1	2.35	0.58
1:G:42:GLU:HG2	1:G:43:LYS:HG3	1.84	0.58
1:A:193:SER:HA	1:A:196:THR:HG22	1.85	0.58
2:D:160:GLN:HB3	2:D:163:ASN:ND2	2.11	0.58
1:E:39:GLN:HB2	1:E:45:LEU:CD2	2.34	0.58
1:A:129:LEU:HD22	2:B:138:VAL:CG2	2.34	0.57
2:H:88:PHE:HB2	2:H:111:ILE:CD1	2.33	0.57
1:E:39:GLN:HB2	1:E:45:LEU:HD23	1.86	0.57
2:B:150:LYS:HD3	2:B:152:GLN:HE22	1.68	0.56
2:D:153:TRP:CG	2:D:184:LEU:HD13	2.40	0.56
1:C:124:PRO:HB3	1:C:150:TYR:HB3	1.88	0.56
2:B:27:GLN:NE2	6:B:401:HOH:O	2.38	0.56
1:E:13:GLN:HG2	1:E:14:PRO:HD2	1.88	0.56
1:G:202:ASN:ND2	1:G:213:ASP:OD2	2.40	0.55
1:A:89:ARG:NH2	6:A:402:HOH:O	2.20	0.55
2:B:172:ASP:OD1	2:B:173:SER:N	2.39	0.55
1:A:164:LEU:HD21	1:A:187:VAL:HG21	1.89	0.55
1:E:12:VAL:CG1	1:E:18:LEU:HD11	2.36	0.55
2:H:12:SER:OG	2:H:110:GLU:HB2	2.07	0.55
2:D:170:GLU:OE1	6:D:401:HOH:O	2.18	0.55
2:B:5:THR:HB	2:B:24:ARG:CG	2.34	0.54
2:H:113:ARG:HH21	2:H:116:ALA:HB2	1.72	0.54
2:D:152:GLN:HE22	2:D:159:LEU:CD1	2.19	0.54
1:G:11:LEU:HB2	1:G:152:PRO:HG3	1.88	0.54
2:F:10:SER:HB2	2:F:108:LYS:HD2	1.89	0.54
2:B:91:TYR:O	2:B:106:GLY:HA2	2.09	0.54
1:A:102:PHE:HB3	3:A:301:PEG:H31	1.90	0.53
2:D:84:GLN:HB3	2:D:86:GLU:OE1	2.08	0.53
2:B:145:TYR:CD1	2:B:146:PRO:HA	2.43	0.53
1:C:89:ARG:HG3	1:C:89:ARG:HH11	1.73	0.53
1:E:159:TRP:CZ2	1:E:187:VAL:HG23	2.44	0.53
2:D:164:SER:HA	2:D:183:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:ARG:HG3	2:H:81:SER:HA	1.90	0.52
1:A:191:SER:HA	1:A:194:LEU:HG	1.92	0.52
1:C:183:LEU:HD23	1:C:183:LEU:C	2.30	0.52
2:D:152:GLN:HE22	2:D:159:LEU:HD11	1.69	0.52
2:F:21:ILE:HG12	2:F:107:THR:HG21	1.92	0.52
2:F:123:PHE:HB2	2:F:138:VAL:HG23	1.92	0.52
1:C:11:LEU:HB2	1:C:152:PRO:HG3	1.91	0.51
1:E:113:LEU:HD13	1:E:113:LEU:C	2.30	0.51
1:A:91:GLU:OE1	1:A:91:GLU:N	2.34	0.51
1:C:54:ARG:HD2	6:C:415:HOH:O	2.10	0.51
1:C:42:GLU:HG2	1:C:43:LYS:H	1.75	0.51
2:B:45:PRO:HB3	2:B:170:GLU:HG3	1.91	0.51
1:A:150:TYR:CE2	1:A:155:VAL:HG13	2.46	0.51
2:D:125:PRO:HD3	2:D:137:VAL:HG23	1.91	0.51
2:D:138:VAL:HG12	2:D:183:THR:HG23	1.92	0.51
2:H:83:LEU:HD12	2:H:84:GLN:N	2.25	0.51
1:C:171:PHE:CE1	2:D:169:THR:HG23	2.46	0.51
2:H:130:LEU:HD11	2:H:191:TYR:HE2	1.76	0.51
2:D:40:TRP:HB2	2:D:53:ILE:HB	1.92	0.50
2:D:156:ASP:HB2	2:D:194:HIS:CD2	2.46	0.50
1:G:204:ASN:C	1:G:204:ASN:ND2	2.65	0.50
2:B:21:ILE:HG12	2:B:107:THR:HG21	1.92	0.50
1:E:39:GLN:CG	1:E:45:LEU:HD23	2.42	0.50
2:H:118:PRO:HB3	2:H:144:PHE:HB3	1.92	0.50
1:A:194:LEU:N	1:A:194:LEU:HD23	2.25	0.50
2:B:145:TYR:CD1	2:B:146:PRO:CA	2.95	0.50
2:D:156:ASP:OD2	2:D:194:HIS:CD2	2.65	0.50
1:E:102:PHE:HB3	3:E:301:PEG:H12	1.94	0.50
2:B:155:VAL:CG2	2:B:197:TYR:CE1	2.94	0.50
2:H:130:LEU:HD11	2:H:191:TYR:CE2	2.47	0.50
2:H:153:TRP:CG	2:H:184:LEU:HG	2.47	0.49
2:F:183:THR:O	2:F:183:THR:HG22	2.12	0.49
2:D:206:LEU:HD13	2:D:210:VAL:HG23	1.94	0.49
2:F:36:PRO:HD2	2:F:56:VAL:HG21	1.93	0.49
1:G:203:VAL:HG13	1:G:203:VAL:O	2.11	0.49
2:D:163:ASN:OD1	2:D:184:LEU:HD11	2.13	0.49
1:E:159:TRP:CD2	1:E:187:VAL:HG21	2.47	0.49
2:F:110:GLU:OE2	2:F:171:GLN:NE2	2.45	0.49
1:G:103:TYR:H	3:G:302:PEG:H32	1.77	0.49
1:A:155:VAL:HG12	1:A:205:HIS:CD2	2.47	0.49
1:C:169:HIS:CD2	2:D:142:ASN:HD21	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ASN:O	2:D:184:LEU:HA	2.13	0.49
1:C:127:PHE:CD1	1:C:127:PHE:N	2.76	0.49
1:G:153:GLU:OE1	1:G:181:TYR:CZ	2.65	0.49
2:D:146:PRO:HB2	2:D:148:GLU:OE1	2.13	0.49
2:D:156:ASP:OD2	2:D:194:HIS:CG	2.66	0.49
2:B:66:ARG:HH21	2:B:87:ASP:CG	2.10	0.48
2:H:123:PHE:HB2	2:H:138:VAL:HG22	1.95	0.48
2:D:164:SER:HB3	2:D:184:LEU:HD12	1.95	0.48
1:G:89:ARG:HG2	1:G:92:ASP:OD2	2.13	0.48
2:D:85:PRO:HA	2:D:111:ILE:HG12	1.95	0.48
3:G:301:PEG:O4	6:G:401:HOH:O	2.20	0.48
1:G:159:TRP:CH2	1:G:201:CYS:HB3	2.48	0.48
1:G:176:GLN:OE1	1:G:180:LEU:O	2.32	0.48
2:B:88:PHE:HB2	2:B:109:VAL:O	2.14	0.48
1:C:78:LYS:NZ	1:C:82:TYR:OH	2.47	0.48
1:E:156:THR:OG1	1:E:204:ASN:HB3	2.14	0.48
1:G:73:SER:OG	1:G:82:TYR:HB2	2.14	0.48
1:C:201:CYS:O	1:C:213:ASP:HA	2.14	0.48
2:D:156:ASP:OD2	2:D:194:HIS:CB	2.62	0.47
2:D:137:VAL:CG1	2:D:153:TRP:CZ3	2.95	0.47
2:H:12:SER:HA	2:H:110:GLU:O	2.13	0.47
1:C:157:VAL:HG11	1:C:185:SER:HB3	1.96	0.47
2:H:143:ASN:HA	2:H:177:THR:OG1	2.15	0.47
2:B:19:VAL:CG2	2:B:80:ILE:HD12	2.44	0.47
2:B:20:THR:CG2	2:B:79:THR:OG1	2.57	0.47
2:D:152:GLN:HE21	2:D:152:GLN:HB3	1.52	0.47
1:E:91:GLU:HG3	1:E:91:GLU:O	2.13	0.47
1:C:103:TYR:CD1	3:C:301:PEG:H41	2.49	0.47
1:E:89:ARG:HG2	1:E:92:ASP:OD2	2.14	0.47
2:H:153:TRP:CD2	2:H:184:LEU:HG	2.49	0.47
2:F:41:TYR:CE1	2:F:94:SER:HB3	2.50	0.47
2:F:25:SER:OG	2:F:27:GLN:O	2.28	0.47
2:B:147:ARG:HB2	2:B:178:TYR:CE2	2.50	0.46
1:C:131:PRO:HG2	1:C:218:PRO:HA	1.95	0.46
1:E:39:GLN:CB	1:E:45:LEU:HD23	2.44	0.46
1:G:203:VAL:HG12	1:G:212:VAL:HG23	1.90	0.46
1:E:159:TRP:CE2	1:E:187:VAL:HG21	2.51	0.46
2:B:129:GLN:NE2	2:B:136:SER:N	2.64	0.45
1:G:126:VAL:HG21	1:G:212:VAL:CG2	2.45	0.45
1:G:203:VAL:HG12	1:G:212:VAL:O	2.16	0.45
1:A:11:LEU:HD23	1:A:121:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:LYS:O	2:H:47:GLN:HB2	2.16	0.45
1:A:35:SER:HB2	1:A:49:SER:O	2.17	0.45
1:A:62:TYR:HB2	1:A:67:LYS:HG3	1.99	0.45
1:C:91:GLU:H	1:C:91:GLU:CD	2.18	0.45
2:H:157:ASN:O	2:H:157:ASN:CG	2.54	0.45
2:B:45:PRO:CB	2:B:170:GLU:HG3	2.46	0.45
1:G:124:PRO:HB3	1:G:150:TYR:HB3	1.99	0.45
2:B:198:ALA:HB2	2:B:213:SER:HB3	1.99	0.45
1:C:122:LYS:CE	1:C:149:ASP:O	2.65	0.45
2:D:150:LYS:HB3	2:D:202:THR:HB	1.98	0.45
2:B:13:ALA:HB3	2:B:83:LEU:CD2	2.47	0.45
1:C:78:LYS:NZ	6:C:404:HOH:O	2.46	0.45
2:D:42:LEU:HD12	2:D:91:TYR:CE2	2.51	0.45
1:E:13:GLN:HG3	1:E:118:SER:HA	1.99	0.45
1:G:135:SER:HA	2:H:121:PHE:CD2	2.50	0.45
1:C:176:GLN:HG2	2:D:165:GLN:HE22	1.81	0.44
3:G:302:PEG:H42	3:G:302:PEG:H22	1.76	0.44
2:D:196:VAL:HA	2:D:214:PHE:O	2.17	0.44
2:D:188:LYS:HD2	2:D:188:LYS:C	2.38	0.44
1:G:176:GLN:NE2	1:G:182:SER:OG	2.50	0.44
2:H:122:ILE:HD12	2:H:139:CYS:HA	2.00	0.44
1:C:155:VAL:HG12	1:C:205:HIS:HB2	1.99	0.44
3:C:301:PEG:H21	6:C:412:HOH:O	2.17	0.44
1:E:140:THR:HA	1:E:190:PRO:HA	1.98	0.44
2:B:193:LYS:HD2	2:B:193:LYS:HA	1.58	0.44
2:F:112:LYS:HB3	2:F:112:LYS:HE2	1.70	0.44
2:F:98:HIS:ND1	2:F:99:LEU:O	2.50	0.44
1:G:102:PHE:HB2	3:G:301:PEG:H12	2.00	0.44
2:H:82:SER:O	2:H:84:GLN:OE1	2.36	0.44
2:F:110:GLU:HG2	2:F:171:GLN:OE1	2.18	0.43
1:G:210:THR:O	1:G:210:THR:OG1	2.28	0.43
2:B:59:ARG:NH1	2:B:63:VAL:O	2.50	0.43
2:D:164:SER:HB3	2:D:184:LEU:CD1	2.47	0.43
1:E:67:LYS:HB3	1:E:67:LYS:HE3	1.67	0.43
1:E:131:PRO:HB3	1:E:142:ALA:O	2.18	0.43
2:B:88:PHE:CB	2:B:111:ILE:HD13	2.47	0.43
2:B:145:TYR:CD1	2:B:146:PRO:N	2.86	0.43
1:C:200:ILE:O	1:C:200:ILE:HD12	2.18	0.43
1:A:200:ILE:CG2	1:A:215:ARG:HG3	2.45	0.43
2:B:184:LEU:HD21	2:B:186:LEU:HD11	2.01	0.43
1:C:43:LYS:HD2	1:C:46:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:PHE:HA	1:E:152:PRO:HA	1.71	0.43
2:H:144:PHE:HE1	2:H:179:SER:HA	1.82	0.43
2:B:56:VAL:HG12	2:B:57:SER:HB3	2.01	0.43
2:B:129:GLN:NE2	2:B:136:SER:OG	2.51	0.43
2:D:200:GLU:HA	2:D:210:VAL:O	2.18	0.43
2:B:155:VAL:HG23	2:B:197:TYR:CD1	2.54	0.43
1:C:157:VAL:HG22	1:C:203:VAL:HG22	1.99	0.43
1:E:29:PHE:HB3	1:E:79:ASN:OD1	2.19	0.43
2:F:11:LEU:CD2	2:F:19:VAL:HG23	2.49	0.43
2:H:45:PRO:HB3	2:H:170:GLU:HG3	2.00	0.43
2:F:144:PHE:HE1	2:F:179:SER:HA	1.84	0.42
1:A:75:ASP:OD2	1:A:78:LYS:HD2	2.18	0.42
1:C:119:ALA:HB3	1:C:151:PHE:CE2	2.53	0.42
2:H:12:SER:HB3	2:H:112:LYS:HG3	2.00	0.42
2:B:84:GLN:HB2	2:B:87:ASP:OD1	2.19	0.42
2:D:121:PHE:N	2:D:121:PHE:CD1	2.87	0.42
2:H:143:ASN:N	2:H:143:ASN:ND2	2.65	0.42
1:A:129:LEU:CD2	2:B:138:VAL:HG21	2.50	0.42
2:D:171:GLN:HG2	2:D:176:SER:HA	2.02	0.42
2:B:141:LEU:HB2	2:B:180:LEU:HB3	2.02	0.42
1:G:203:VAL:CG1	1:G:203:VAL:O	2.68	0.42
1:G:216:VAL:O	1:G:216:VAL:HG13	2.19	0.42
3:G:302:PEG:H12	6:G:415:HOH:O	2.18	0.42
2:H:144:PHE:CE1	2:H:179:SER:HA	2.54	0.42
1:A:129:LEU:CD2	2:B:138:VAL:CG2	2.97	0.42
2:B:155:VAL:HG22	2:B:194:HIS:HD2	1.85	0.42
1:E:40:SER:HB2	1:E:41:PRO:HD2	2.01	0.42
2:B:24:ARG:CG	2:B:24:ARG:O	2.67	0.42
1:C:6:GLU:HA	1:C:21:SER:O	2.19	0.42
2:B:172:ASP:HB3	2:B:175:ASP:OD1	2.19	0.41
1:E:18:LEU:HD12	1:E:88:LEU:HD12	1.97	0.41
1:G:129:LEU:HD23	1:G:129:LEU:HA	1.88	0.41
1:E:54:ARG:NH2	6:E:402:HOH:O	2.52	0.41
1:C:168:VAL:HG22	1:C:187:VAL:HB	2.02	0.41
1:C:214:LYS:HD2	1:C:214:LYS:HA	1.87	0.41
2:D:5:THR:OG1	2:D:24:ARG:HB2	2.19	0.41
2:H:198:ALA:HB2	2:H:213:SER:HB2	2.01	0.41
1:A:39:GLN:HA	1:A:44:GLY:O	2.21	0.41
2:B:195:LYS:HE2	2:B:195:LYS:HB2	1.87	0.41
2:F:161:SER:O	2:F:163:ASN:N	2.44	0.41
1:A:140:THR:CG2	1:A:188:THR:HB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:HIS:ND1	1:E:208:SER:HB2	2.36	0.41
2:F:6:GLN:HE21	2:F:104:GLY:HA3	1.86	0.41
1:G:136:THR:HA	1:G:141:ALA:HA	2.03	0.41
1:A:47:TRP:CH2	2:B:99:LEU:HD22	2.56	0.41
2:B:40:TRP:CE2	2:B:78:LEU:HB2	2.56	0.41
1:C:122:LYS:NZ	1:C:149:ASP:O	2.54	0.41
1:C:157:VAL:HG11	1:C:185:SER:CB	2.51	0.41
1:E:47:TRP:CH2	2:F:99:LEU:HD22	2.56	0.41
2:F:143:ASN:HA	2:F:177:THR:HB	2.02	0.41
1:A:17:SER:HA	1:A:85:MET:O	2.21	0.41
2:B:42:LEU:HD11	2:B:44:LYS:HE3	2.03	0.41
2:D:41:TYR:HE1	2:D:94:SER:HB3	1.86	0.41
2:F:144:PHE:CD1	2:F:144:PHE:N	2.88	0.41
1:G:39:GLN:HA	1:G:44:GLY:O	2.20	0.41
1:G:106:SER:OG	3:G:301:PEG:H21	2.21	0.41
1:E:113:LEU:HD11	1:E:115:THR:OG1	2.21	0.40
2:F:42:LEU:HD23	2:F:42:LEU:HA	1.91	0.40
2:F:71:GLY:HA3	2:F:76:PHE:HA	2.03	0.40
2:H:198:ALA:HB1	2:H:211:THR:HG22	2.03	0.40
2:B:19:VAL:HG21	2:B:80:ILE:HD12	2.04	0.40
1:G:66:VAL:HB	1:G:70:PHE:CG	2.57	0.40
1:E:205:HIS:CE1	1:E:207:PRO:HG2	2.56	0.40
2:H:83:LEU:CD1	2:H:87:ASP:HB2	2.52	0.40
2:H:184:LEU:HD23	2:H:184:LEU:HA	1.87	0.40

All (1) 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:C:103:TYR:OH	1:G:103:TYR:OH[2_455]	1.07	1.13

## 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	210/221 (95%)	205 (98%)	5 (2%)	0	100	100
1	C	211/221 (96%)	204 (97%)	7 (3%)	0	100	100
1	E	203/221 (92%)	191 (94%)	12 (6%)	0	100	100
1	G	217/221 (98%)	209 (96%)	8 (4%)	0	100	100
2	B	214/219 (98%)	211 (99%)	3 (1%)	0	100	100
2	D	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
2	F	214/219 (98%)	202 (94%)	10 (5%)	2 (1%)	17	25
2	H	215/219 (98%)	203 (94%)	12 (6%)	0	100	100
All	All	1698/1760 (96%)	1632 (96%)	64 (4%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	143	ASN
2	F	162	GLY

### 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	183/191 (96%)	175 (96%)	8 (4%)	28	45
1	C	180/191 (94%)	176 (98%)	4 (2%)	52	71
1	E	153/191 (80%)	148 (97%)	5 (3%)	38	57
1	G	180/191 (94%)	170 (94%)	10 (6%)	21	34
2	B	188/195 (96%)	172 (92%)	16 (8%)	10	16
2	D	188/195 (96%)	173 (92%)	15 (8%)	12	18
2	F	157/195 (80%)	139 (88%)	18 (12%)	5	7
2	H	170/195 (87%)	162 (95%)	8 (5%)	26	42
All	All	1399/1544 (91%)	1315 (94%)	84 (6%)	19	31

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	21	SER
1	A	87	SER
1	A	117	SER
1	A	121	THR
1	A	143	LEU
1	A	184	SER
1	A	202	ASN
2	B	24	ARG
2	B	26	SER
2	B	38	LEU
2	B	39	ASN
2	B	42	LEU
2	B	44	LYS
2	B	55	LYS
2	B	68	SER
2	B	70	SER
2	B	75	ASP
2	B	82	SER
2	B	88	PHE
2	B	94	SER
2	B	167	SER
2	B	190	ASP
2	B	194	HIS
1	C	50	GLU
1	C	166	SER
1	C	184	SER
1	C	202	ASN
2	D	3	GLN
2	D	12	SER
2	D	14	SER
2	D	18	ARG
2	D	31	HIS
2	D	126	SER
2	D	127	ASP
2	D	147	ARG
2	D	152	GLN
2	D	157	ASN
2	D	161	SER
2	D	182	SER
2	D	187	SER
2	D	188	LYS

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Mol	Chain	Res	Type
2	D	190	ASP
1	E	25	SER
1	E	35	SER
1	E	110	GLN
1	E	121	THR
1	E	150	TYR
2	F	2	LEU
2	F	5	THR
2	F	24	ARG
2	F	25	SER
2	F	27	GLN
2	F	35	SER
2	F	38	LEU
2	F	39	ASN
2	F	42	LEU
2	F	48	SER
2	F	70	SER
2	F	75	ASP
2	F	77	THR
2	F	83	LEU
2	F	90	VAL
2	F	108	LYS
2	F	136	SER
2	F	212	LYS
1	G	19	ARG
1	G	35	SER
1	G	40	SER
1	G	69	ARG
1	G	71	THR
1	G	85	MET
1	G	198	THR
1	G	200	ILE
1	G	204	ASN
1	G	209	ASN
2	H	12	SER
2	H	33	TYR
2	H	47	GLN
2	H	176	SER
2	H	181	SER
2	H	202	THR
2	H	212	LYS
2	H	213	SER



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	202	ASN
2	B	84	GLN
2	B	129	GLN
2	B	152	GLN
2	B	160	GLN
1	C	79	ASN
2	D	3	GLN
2	D	27	GLN
2	D	142	ASN
2	D	152	GLN
2	D	165	GLN
1	E	13	GLN
2	F	6	GLN
2	F	171	GLN
2	H	84	GLN
2	H	142	ASN
2	H	143	ASN
2	H	157	ASN
2	H	171	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PEG	A	301	-	6,6,6	0.34	0	5,5,5	0.24	0
3	PEG	D	301	-	6,6,6	0.43	0	5,5,5	0.34	0
4	SO4	C	302	-	4,4,4	0.36	0	6,6,6	0.27	0
3	PEG	C	301	-	6,6,6	0.37	0	5,5,5	0.15	0
3	PEG	G	302	-	6,6,6	0.39	0	5,5,5	0.19	0
4	SO4	E	302	-	4,4,4	0.21	0	6,6,6	0.17	0
4	SO4	A	302	-	4,4,4	0.39	0	6,6,6	0.28	0
4	SO4	A	304	-	4,4,4	0.30	0	6,6,6	0.30	0
4	SO4	A	303	-	4,4,4	0.18	0	6,6,6	0.22	0
3	PEG	E	301	-	6,6,6	0.23	0	5,5,5	0.11	0
3	PEG	G	301	-	6,6,6	0.22	0	5,5,5	0.20	0
4	SO4	G	303	-	4,4,4	0.30	0	6,6,6	0.29	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	PEG	A	301	-	-	2/4/4/4	-
3	PEG	D	301	-	-	3/4/4/4	-
3	PEG	C	301	-	-	3/4/4/4	-
3	PEG	G	302	-	-	3/4/4/4	-
3	PEG	E	301	-	-	2/4/4/4	-
3	PEG	G	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	302	PEG	C4-C3-O2-C2
3	A	301	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	D	301	PEG	O2-C3-C4-O4
3	C	301	PEG	O2-C3-C4-O4
3	D	301	PEG	O1-C1-C2-O2
3	E	301	PEG	O1-C1-C2-O2
3	G	301	PEG	O2-C3-C4-O4
3	G	302	PEG	O1-C1-C2-O2
3	A	301	PEG	O1-C1-C2-O2
3	E	301	PEG	O2-C3-C4-O4
3	G	302	PEG	O2-C3-C4-O4
3	C	301	PEG	C4-C3-O2-C2
3	G	301	PEG	C4-C3-O2-C2
3	D	301	PEG	C1-C2-O2-C3
3	C	301	PEG	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	PEG	1	0
3	C	301	PEG	2	0
3	G	302	PEG	3	0
3	E	301	PEG	1	0
3	G	301	PEG	3	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, 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	214/221 (96%)	0.29	8 (3%) 41 41	29, 48, 107, 139	0
1	C	215/221 (97%)	0.52	7 (3%) 46 45	27, 43, 121, 152	0
1	E	209/221 (94%)	1.25	46 (22%) 0 0	30, 82, 151, 167	0
1	G	219/221 (99%)	0.76	24 (10%) 5 5	29, 70, 145, 160	0
2	B	216/219 (98%)	0.50	18 (8%) 11 10	42, 71, 108, 133	0
2	D	216/219 (98%)	0.45	12 (5%) 24 23	28, 51, 119, 150	0
2	F	216/219 (98%)	1.86	79 (36%) 0 0	57, 127, 163, 184	0
2	H	217/219 (99%)	0.98	39 (17%) 1 1	37, 89, 136, 148	0
All	All	1722/1760 (97%)	0.83	233 (13%) 3 2	27, 71, 144, 184	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	173	SER	11.4
1	E	199	TYR	10.5
1	E	200	ILE	10.5
1	E	143	LEU	10.0
1	E	126	VAL	8.6
2	F	127	ASP	7.9
2	F	168	VAL	7.7
2	F	177	THR	7.0
1	G	200	ILE	7.0
2	F	187	SER	6.7
2	F	157	ASN	6.6
2	F	161	SER	6.6
1	E	216	VAL	6.4
2	F	186	LEU	6.1
1	E	220	SER	6.0
1	E	127	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
2	F	130	LEU	5.9
1	G	199	TYR	5.8
2	H	158	ALA	5.8
2	F	125	PRO	5.7
1	E	212	VAL	5.7
1	G	190	PRO	5.6
1	E	144	GLY	5.2
2	F	153	TRP	5.0
1	E	203	VAL	5.0
1	E	129	LEU	5.0
2	F	197	TYR	5.0
1	E	159	TRP	5.0
1	E	186	VAL	5.0
2	H	187	SER	5.0
2	F	83	LEU	5.0
2	B	130	LEU	4.8
1	E	128	PRO	4.8
2	F	174	LYS	4.7
1	E	189	VAL	4.7
2	F	156	ASP	4.6
1	G	141	ALA	4.6
2	H	186	LEU	4.6
2	H	124	PRO	4.6
2	H	161	SER	4.6
2	F	159	LEU	4.5
2	F	158	ALA	4.5
2	F	164	SER	4.5
2	H	189	ALA	4.5
1	C	133	SER	4.5
2	D	33	TYR	4.4
2	F	114	THR	4.4
2	F	139	CYS	4.3
1	G	193	SER	4.3
2	F	167	SER	4.3
2	F	81	SER	4.3
1	E	141	ALA	4.3
2	H	207	SER	4.3
2	H	137	VAL	4.2
1	E	163	ALA	4.2
2	F	140	LEU	4.1
2	F	191	TYR	4.1
2	F	196	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	130	LEU	4.1
2	B	134	THR	4.1
2	H	206	LEU	4.0
1	G	203	VAL	4.0
1	G	189	VAL	4.0
1	G	143	LEU	3.9
2	F	31	HIS	3.9
2	F	85	PRO	3.9
2	F	175	ASP	3.8
2	H	132	SER	3.8
1	E	187	VAL	3.8
1	C	199	TYR	3.8
2	H	188	LYS	3.8
2	H	184	LEU	3.8
1	E	191	SER	3.8
2	F	179	SER	3.8
1	G	180	LEU	3.8
2	F	8	PRO	3.8
1	G	179	GLY	3.7
2	F	123	PHE	3.7
1	E	164	LEU	3.7
2	D	196	VAL	3.7
2	F	155	VAL	3.7
2	F	198	ALA	3.6
2	B	214	PHE	3.6
2	F	189	ALA	3.6
2	H	192	GLU	3.5
2	H	83	LEU	3.5
2	F	160	GLN	3.5
2	F	172	ASP	3.5
2	H	133	GLY	3.5
2	H	203	HIS	3.5
1	E	204	ASN	3.5
1	E	12	VAL	3.4
1	E	149	ASP	3.4
2	F	184	LEU	3.4
1	E	122	LYS	3.4
2	F	183	THR	3.4
1	G	212	VAL	3.4
2	F	138	VAL	3.3
1	E	42	GLU	3.3
1	C	196	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	115	VAL	3.2
2	F	12	SER	3.2
2	H	191	TYR	3.2
2	H	208	SER	3.2
1	E	151	PHE	3.2
2	F	111	ILE	3.2
2	F	110	GLU	3.2
2	F	16	GLY	3.2
2	B	33	TYR	3.1
2	F	119	SER	3.1
1	G	187	VAL	3.1
1	E	145	CYS	3.1
1	E	192	SER	3.1
2	F	213	SER	3.1
2	F	87	ASP	3.1
2	H	117	ALA	3.1
2	F	170	GLU	3.1
2	H	134	THR	3.1
1	E	208	SER	3.1
2	F	13	ALA	3.1
2	H	185	THR	3.0
1	A	138	GLY	3.0
1	A	217	GLU	3.0
2	D	197	TYR	3.0
2	F	5	THR	3.0
1	A	139	GLY	3.0
2	D	160	GLN	3.0
2	H	116	ALA	3.0
1	E	152	PRO	3.0
1	G	196	THR	3.0
2	D	127	ASP	2.9
2	F	141	LEU	2.9
2	F	82	SER	2.9
2	F	121	PHE	2.9
1	C	103	TYR	2.9
2	F	135	ALA	2.9
1	E	182	SER	2.8
1	E	13	GLN	2.8
2	B	196	VAL	2.8
2	H	111	ILE	2.8
2	D	130	LEU	2.8
1	E	201	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	201	VAL	2.8
2	F	18	ARG	2.7
2	B	159	LEU	2.7
2	H	153	TRP	2.7
1	E	214	LYS	2.7
2	B	197	TYR	2.7
2	D	31	HIS	2.7
1	G	142	ALA	2.7
1	E	155	VAL	2.7
2	F	137	VAL	2.7
2	F	208	SER	2.7
2	B	185	THR	2.6
2	H	149	ALA	2.6
1	G	198	THR	2.6
1	C	132	SER	2.6
1	E	162	GLY	2.6
2	B	213	SER	2.6
2	D	215	ASN	2.6
1	A	140	THR	2.6
2	D	199	CYS	2.5
1	G	194	LEU	2.5
1	E	213	ASP	2.5
1	G	135	SER	2.5
1	G	130	ALA	2.5
2	F	67	PHE	2.5
2	H	157	ASN	2.5
2	F	178	TYR	2.5
1	G	129	LEU	2.5
2	F	212	LYS	2.5
2	F	199	CYS	2.5
2	B	186	LEU	2.5
2	H	114	THR	2.5
1	G	218	PRO	2.4
1	C	197	GLN	2.4
2	H	84	GLN	2.4
2	H	202	THR	2.4
2	H	196	VAL	2.4
2	D	191	TYR	2.4
1	E	185	SER	2.4
2	D	137	VAL	2.4
2	F	122	ILE	2.4
2	B	133	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	13	ALA	2.4
1	A	133	SER	2.4
1	E	215	ARG	2.3
2	H	175	ASP	2.3
2	B	12	SER	2.3
1	A	179	GLY	2.3
1	G	186	VAL	2.3
1	E	207	PRO	2.3
1	E	150	TYR	2.3
2	F	134	THR	2.3
2	D	131	LYS	2.3
2	B	189	ALA	2.3
1	E	18	LEU	2.3
2	B	193	LYS	2.3
2	F	88	PHE	2.3
2	F	214	PHE	2.3
2	H	194	HIS	2.2
2	F	113	ARG	2.2
2	F	21	ILE	2.2
1	C	198	THR	2.2
2	F	96	GLY	2.2
2	F	193	LYS	2.2
2	B	30	LEU	2.2
2	H	159	LEU	2.2
1	G	131	PRO	2.2
2	B	24	ARG	2.2
2	F	132	SER	2.2
2	F	149	ALA	2.2
1	A	196	THR	2.2
1	E	101	TYR	2.1
2	B	1	GLU	2.1
1	A	132	SER	2.1
2	H	155	VAL	2.1
2	F	128	GLU	2.1
1	G	146	LEU	2.1
2	F	29	LEU	2.1
1	G	140	THR	2.1
2	B	124	PRO	2.1
2	F	176	SER	2.1
2	F	37	TYR	2.1
2	H	190	ASP	2.1
2	F	84	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	147	ARG	2.1
1	E	157	VAL	2.0
2	F	22	THR	2.0
2	F	27	GLN	2.0
1	E	210	THR	2.0
1	E	211	LYS	2.0
2	H	80	ILE	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 monosaccharides 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
3	PEG	A	301	7/7	0.76	0.35	52,60,63,67	0
3	PEG	E	301	7/7	0.82	0.38	60,63,67,68	0
5	MG	B	301	1/1	0.84	0.19	67,67,67,67	0
3	PEG	D	301	7/7	0.86	0.25	40,44,48,50	0
3	PEG	G	302	7/7	0.88	0.20	42,45,49,51	0
3	PEG	C	301	7/7	0.88	0.19	38,40,45,46	0
4	SO4	A	303	5/5	0.89	0.15	60,66,72,79	0
3	PEG	G	301	7/7	0.93	0.21	47,53,59,60	0
4	SO4	A	302	5/5	0.95	0.16	47,53,58,62	0
4	SO4	E	302	5/5	0.96	0.13	50,53,56,61	0
4	SO4	C	302	5/5	0.96	0.18	43,46,51,56	0
4	SO4	G	303	5/5	0.97	0.14	39,43,46,48	0
4	SO4	A	304	5/5	0.97	0.11	45,45,54,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.