



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:18 pm GMT

PDB ID : 2RCE  
Title : DFP modified DegS delta PDZ  
Authors : Sohn, J.; Grant, R.A.; Sauer, R.T.  
Deposited on : 2007-09-19  
Resolution : 2.35 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

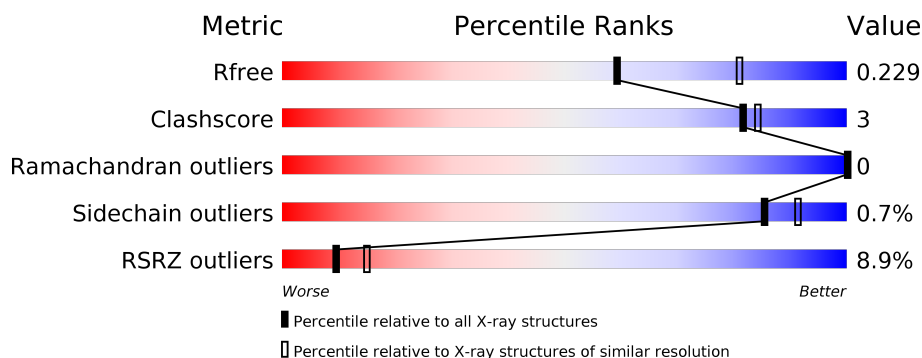
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	111664	1015 (2.36-2.36)
Clashscore	122126	1081 (2.36-2.36)
Ramachandran outliers	120053	1066 (2.36-2.36)
Sidechain outliers	120020	1067 (2.36-2.36)
RSRZ outliers	108989	1002 (2.36-2.36)

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. 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	243	<div> <div>7%</div> <div>79% 5% 16%</div> </div>
1	B	243	<div> <div>7%</div> <div>84% 12%</div> </div>
1	C	243	<div> <div>7%</div> <div>85% 12%</div> </div>
1	D	243	<div> <div>6%</div> <div>79% 7% 15%</div> </div>
1	E	243	<div> <div>7%</div> <div>77% 6% 16%</div> </div>
1	F	243	<div> <div>9%</div> <div>84% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	243	
1	H	243	
1	I	243	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14556 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 Protease degS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	P	S	0	0	0
			1535	954	274	303	1	3			
1	B	213	Total	C	N	O	P	S	0	0	0
			1599	996	286	313	1	3			
1	C	214	Total	C	N	O	P	S	0	0	0
			1611	1003	290	314	1	3			
1	D	207	Total	C	N	O	P	S	0	0	0
			1559	973	281	301	1	3			
1	E	203	Total	C	N	O	P	S	0	0	0
			1526	954	268	300	1	3			
1	F	211	Total	C	N	O	P	S	0	0	0
			1585	988	283	310	1	3			
1	G	205	Total	C	N	O	P	S	0	0	0
			1538	962	272	300	1	3			
1	H	192	Total	C	N	O	P	S	0	0	0
			1436	900	255	277	1	3			
1	I	198	Total	C	N	O	P	S	0	0	0
			1488	933	261	290	1	3			

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	expression tag	UNP P0AEE3
A	15	ARG	-	expression tag	UNP P0AEE3
A	16	GLY	-	expression tag	UNP P0AEE3
A	17	SER	-	expression tag	UNP P0AEE3
A	18	HIS	-	expression tag	UNP P0AEE3
A	19	HIS	-	expression tag	UNP P0AEE3
A	20	HIS	-	expression tag	UNP P0AEE3
A	21	HIS	-	expression tag	UNP P0AEE3
A	22	HIS	-	expression tag	UNP P0AEE3
A	23	HIS	-	expression tag	UNP P0AEE3
A	24	GLY	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	-	expression tag	UNP P0AEE3
A	26	SER	-	expression tag	UNP P0AEE3
B	14	MET	-	expression tag	UNP P0AEE3
B	15	ARG	-	expression tag	UNP P0AEE3
B	16	GLY	-	expression tag	UNP P0AEE3
B	17	SER	-	expression tag	UNP P0AEE3
B	18	HIS	-	expression tag	UNP P0AEE3
B	19	HIS	-	expression tag	UNP P0AEE3
B	20	HIS	-	expression tag	UNP P0AEE3
B	21	HIS	-	expression tag	UNP P0AEE3
B	22	HIS	-	expression tag	UNP P0AEE3
B	23	HIS	-	expression tag	UNP P0AEE3
B	24	GLY	-	expression tag	UNP P0AEE3
B	25	ARG	-	expression tag	UNP P0AEE3
B	26	SER	-	expression tag	UNP P0AEE3
C	14	MET	-	expression tag	UNP P0AEE3
C	15	ARG	-	expression tag	UNP P0AEE3
C	16	GLY	-	expression tag	UNP P0AEE3
C	17	SER	-	expression tag	UNP P0AEE3
C	18	HIS	-	expression tag	UNP P0AEE3
C	19	HIS	-	expression tag	UNP P0AEE3
C	20	HIS	-	expression tag	UNP P0AEE3
C	21	HIS	-	expression tag	UNP P0AEE3
C	22	HIS	-	expression tag	UNP P0AEE3
C	23	HIS	-	expression tag	UNP P0AEE3
C	24	GLY	-	expression tag	UNP P0AEE3
C	25	ARG	-	expression tag	UNP P0AEE3
C	26	SER	-	expression tag	UNP P0AEE3
D	14	MET	-	expression tag	UNP P0AEE3
D	15	ARG	-	expression tag	UNP P0AEE3
D	16	GLY	-	expression tag	UNP P0AEE3
D	17	SER	-	expression tag	UNP P0AEE3
D	18	HIS	-	expression tag	UNP P0AEE3
D	19	HIS	-	expression tag	UNP P0AEE3
D	20	HIS	-	expression tag	UNP P0AEE3
D	21	HIS	-	expression tag	UNP P0AEE3
D	22	HIS	-	expression tag	UNP P0AEE3
D	23	HIS	-	expression tag	UNP P0AEE3
D	24	GLY	-	expression tag	UNP P0AEE3
D	25	ARG	-	expression tag	UNP P0AEE3
D	26	SER	-	expression tag	UNP P0AEE3
E	14	MET	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	15	ARG	-	expression tag	UNP P0AEE3
E	16	GLY	-	expression tag	UNP P0AEE3
E	17	SER	-	expression tag	UNP P0AEE3
E	18	HIS	-	expression tag	UNP P0AEE3
E	19	HIS	-	expression tag	UNP P0AEE3
E	20	HIS	-	expression tag	UNP P0AEE3
E	21	HIS	-	expression tag	UNP P0AEE3
E	22	HIS	-	expression tag	UNP P0AEE3
E	23	HIS	-	expression tag	UNP P0AEE3
E	24	GLY	-	expression tag	UNP P0AEE3
E	25	ARG	-	expression tag	UNP P0AEE3
E	26	SER	-	expression tag	UNP P0AEE3
F	14	MET	-	expression tag	UNP P0AEE3
F	15	ARG	-	expression tag	UNP P0AEE3
F	16	GLY	-	expression tag	UNP P0AEE3
F	17	SER	-	expression tag	UNP P0AEE3
F	18	HIS	-	expression tag	UNP P0AEE3
F	19	HIS	-	expression tag	UNP P0AEE3
F	20	HIS	-	expression tag	UNP P0AEE3
F	21	HIS	-	expression tag	UNP P0AEE3
F	22	HIS	-	expression tag	UNP P0AEE3
F	23	HIS	-	expression tag	UNP P0AEE3
F	24	GLY	-	expression tag	UNP P0AEE3
F	25	ARG	-	expression tag	UNP P0AEE3
F	26	SER	-	expression tag	UNP P0AEE3
G	14	MET	-	expression tag	UNP P0AEE3
G	15	ARG	-	expression tag	UNP P0AEE3
G	16	GLY	-	expression tag	UNP P0AEE3
G	17	SER	-	expression tag	UNP P0AEE3
G	18	HIS	-	expression tag	UNP P0AEE3
G	19	HIS	-	expression tag	UNP P0AEE3
G	20	HIS	-	expression tag	UNP P0AEE3
G	21	HIS	-	expression tag	UNP P0AEE3
G	22	HIS	-	expression tag	UNP P0AEE3
G	23	HIS	-	expression tag	UNP P0AEE3
G	24	GLY	-	expression tag	UNP P0AEE3
G	25	ARG	-	expression tag	UNP P0AEE3
G	26	SER	-	expression tag	UNP P0AEE3
H	14	MET	-	expression tag	UNP P0AEE3
H	15	ARG	-	expression tag	UNP P0AEE3
H	16	GLY	-	expression tag	UNP P0AEE3
H	17	SER	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	18	HIS	-	expression tag	UNP P0AEE3
H	19	HIS	-	expression tag	UNP P0AEE3
H	20	HIS	-	expression tag	UNP P0AEE3
H	21	HIS	-	expression tag	UNP P0AEE3
H	22	HIS	-	expression tag	UNP P0AEE3
H	23	HIS	-	expression tag	UNP P0AEE3
H	24	GLY	-	expression tag	UNP P0AEE3
H	25	ARG	-	expression tag	UNP P0AEE3
H	26	SER	-	expression tag	UNP P0AEE3
I	14	MET	-	expression tag	UNP P0AEE3
I	15	ARG	-	expression tag	UNP P0AEE3
I	16	GLY	-	expression tag	UNP P0AEE3
I	17	SER	-	expression tag	UNP P0AEE3
I	18	HIS	-	expression tag	UNP P0AEE3
I	19	HIS	-	expression tag	UNP P0AEE3
I	20	HIS	-	expression tag	UNP P0AEE3
I	21	HIS	-	expression tag	UNP P0AEE3
I	22	HIS	-	expression tag	UNP P0AEE3
I	23	HIS	-	expression tag	UNP P0AEE3
I	24	GLY	-	expression tag	UNP P0AEE3
I	25	ARG	-	expression tag	UNP P0AEE3
I	26	SER	-	expression tag	UNP P0AEE3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	109	Total O 109 109	0	0
2	C	98	Total O 98 98	0	0
2	D	68	Total O 68 68	0	0
2	E	62	Total O 62 62	0	0
2	F	93	Total O 93 93	0	0
2	G	63	Total O 63 63	0	0
2	H	52	Total O 52 52	0	0

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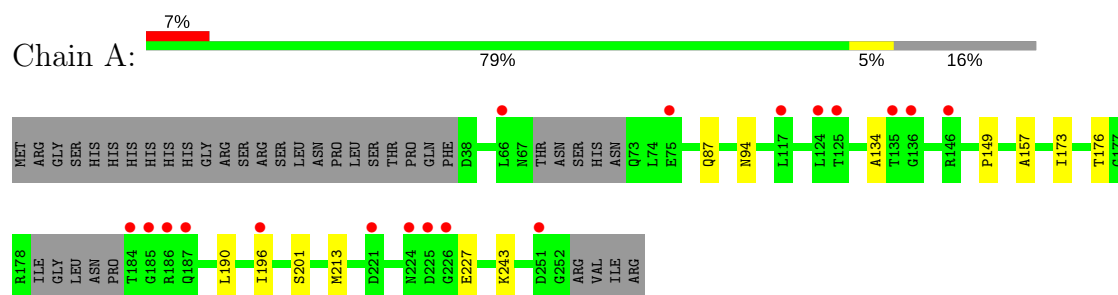
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	42	Total	O	0	0
			42	42		

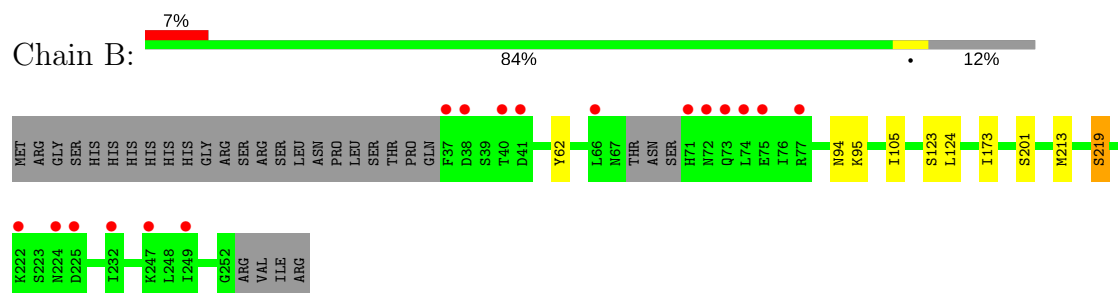
### 3 Residue-property plots [i](#)

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.

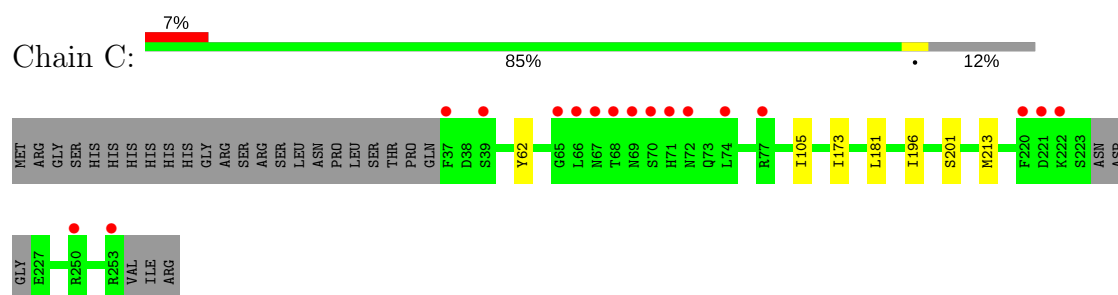
#### • Molecule 1: Protease degS



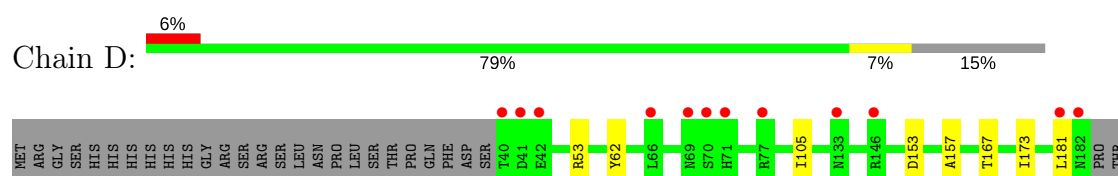
#### • Molecule 1: Protease degS

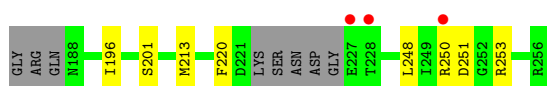


#### • Molecule 1: Protease degS

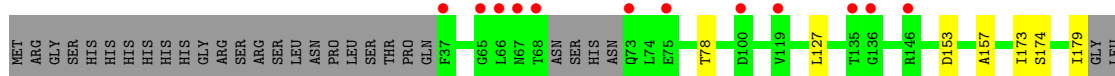
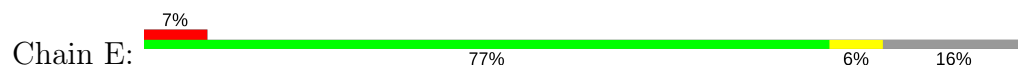


#### • Molecule 1: Protease degS

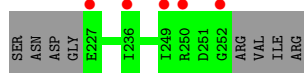
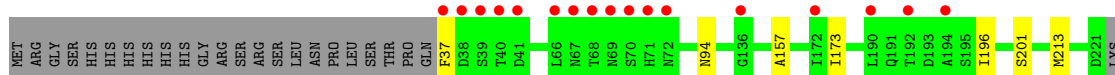
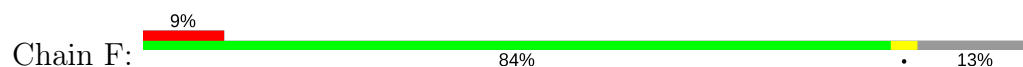




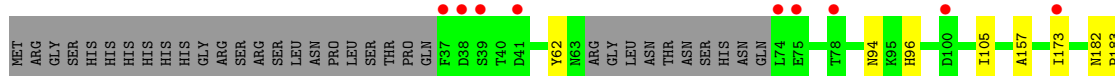
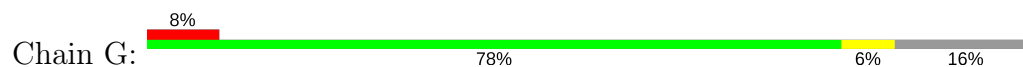
• Molecule 1: Protease degS



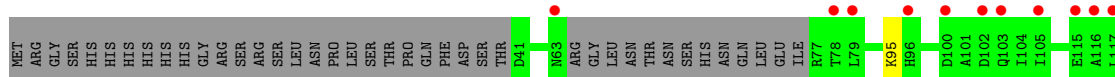
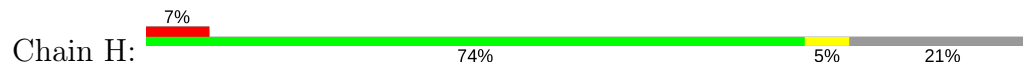
• Molecule 1: Protease degS



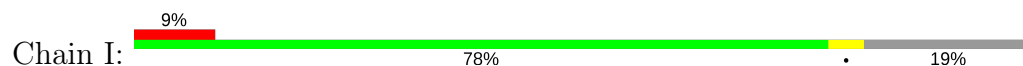
• Molecule 1: Protease degS

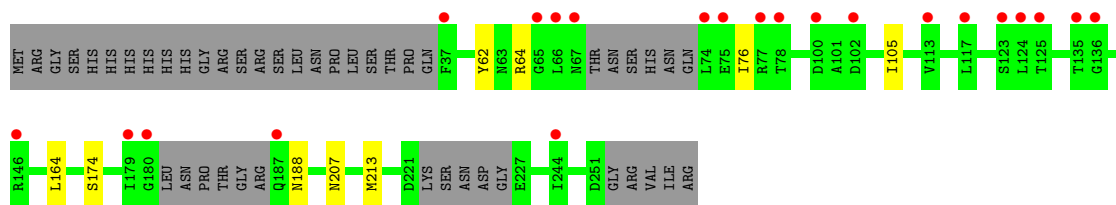


• Molecule 1: Protease degS



• Molecule 1: Protease degS





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.53Å 132.75Å 231.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.22 – 2.35 37.14 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.0 (37.22-2.35) 91.0 (37.14-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.236 0.190 , 0.229	Depositor DCC
$R_{free}$ test set	4127 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4661e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: MIS

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	0/1538	0.58	0/2085
1	B	0.40	0/1606	0.56	0/2180
1	C	0.40	0/1618	0.56	0/2196
1	D	0.41	0/1563	0.54	0/2121
1	E	0.37	0/1530	0.53	0/2076
1	F	0.41	0/1592	0.56	0/2163
1	G	0.38	0/1543	0.55	0/2093
1	H	0.36	0/1440	0.53	0/1956
1	I	0.36	0/1491	0.51	0/2022
All	All	0.39	0/13921	0.55	0/18892

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	1535	0	1547	11	0
1	B	1599	0	1608	7	0
1	C	1611	0	1626	9	0
1	D	1559	0	1584	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1526	0	1540	10	0
1	F	1585	0	1595	7	0
1	G	1538	0	1555	10	0
1	H	1436	0	1460	9	0
1	I	1488	0	1504	5	0
2	A	92	0	0	2	0
2	B	109	0	0	2	0
2	C	98	0	0	2	0
2	D	68	0	0	1	0
2	E	62	0	0	2	0
2	F	93	0	0	1	0
2	G	63	0	0	1	0
2	H	52	0	0	1	0
2	I	42	0	0	0	0
All	All	14556	0	14019	77	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 3.

All (77) 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:F:173:ILE:HD11	1:F:213:MET:HE3	1.49	0.93
1:H:173:ILE:HD11	1:H:213:MET:HE3	1.74	0.68
1:E:213:MET:HE1	2:E:273:HOH:O	1.95	0.66
1:F:173:ILE:CD1	1:F:213:MET:HE3	2.26	0.66
1:B:173:ILE:HD11	1:B:213:MET:HE3	1.78	0.65
1:B:213:MET:HE2	2:B:298:HOH:O	1.96	0.65
1:G:173:ILE:HD11	1:G:213:MET:HE3	1.78	0.64
1:E:213:MET:CE	2:E:273:HOH:O	2.48	0.62
1:A:213:MET:CE	2:A:292:HOH:O	2.46	0.61
1:A:213:MET:HE1	2:A:292:HOH:O	1.99	0.61
1:C:173:ILE:HD11	1:C:213:MET:HE3	1.81	0.60
1:I:207:ASN:HB3	1:I:213:MET:HE2	1.84	0.60
1:A:176:THR:HG22	1:A:190:LEU:HD22	1.82	0.60
1:C:213:MET:HE2	2:C:276:HOH:O	2.02	0.60
1:C:196:ILE:CG2	1:C:201:MIS:H31	2.32	0.59
1:D:173:ILE:HD11	1:D:213:MET:HE3	1.84	0.58
1:E:153:ASP:HB2	1:E:173:ILE:HD12	1.86	0.58
1:H:95:LYS:NZ	1:H:123:SER:HB3	2.21	0.56
1:G:62:TYR:HB2	1:G:105:ILE:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:HB3	1:A:213:MET:HE3	1.89	0.54
1:A:173:ILE:HD11	1:A:213:MET:HE3	1.88	0.54
1:B:201:MIS:H31	1:B:219:SER:HB2	1.91	0.53
1:H:213:MET:HE2	2:H:279:HOH:O	2.10	0.52
1:C:181:LEU:HD11	1:D:105:ILE:HD12	1.90	0.52
1:B:62:TYR:HB2	1:B:105:ILE:HB	1.92	0.52
1:F:196:ILE:HG22	1:F:201:MIS:H31	1.92	0.52
1:A:173:ILE:CD1	1:A:213:MET:HE3	2.41	0.51
1:D:153:ASP:HB2	1:D:173:ILE:HD12	1.93	0.51
1:D:181:LEU:HD21	1:D:220:PHE:HA	1.94	0.50
1:F:196:ILE:CG2	1:F:201:MIS:H31	2.43	0.49
1:D:157:ALA:HB1	1:D:196:ILE:HD11	1.93	0.49
1:G:173:ILE:CD1	1:G:213:MET:HE3	2.43	0.49
1:E:127:LEU:HD11	1:E:236:ILE:HG21	1.95	0.49
1:D:157:ALA:CB	1:D:196:ILE:HD11	2.42	0.48
1:G:213:MET:HE1	2:G:294:HOH:O	2.13	0.48
1:H:95:LYS:HZ3	1:H:123:SER:HB3	1.77	0.48
1:E:179:ILE:HB	1:E:189:PHE:HD2	1.79	0.48
1:E:173:ILE:HD11	1:E:213:MET:HE3	1.95	0.47
1:H:196:ILE:HG22	1:H:201:MIS:H31	1.97	0.47
1:A:149:PRO:HA	1:A:213:MET:HE1	1.97	0.47
1:D:167:THR:HG23	1:E:174:SER:HB3	1.96	0.47
1:C:181:LEU:CD1	1:D:105:ILE:HD12	2.44	0.47
1:H:196:ILE:CG2	1:H:201:MIS:H31	2.45	0.47
1:A:196:ILE:CG2	1:A:201:MIS:H31	2.45	0.46
1:D:248:LEU:HD23	1:D:253:ARG:HA	1.98	0.46
1:G:157:ALA:HB1	1:G:196:ILE:HD11	1.97	0.45
1:I:64:ARG:HG2	1:I:76:ILE:HD13	1.98	0.45
1:D:213:MET:HE2	2:D:292:HOH:O	2.15	0.45
1:D:62:TYR:HB2	1:D:105:ILE:HB	1.99	0.45
1:A:157:ALA:HB1	1:A:196:ILE:HD11	1.99	0.45
1:A:243:LYS:HB3	1:A:243:LYS:HE2	1.69	0.45
1:C:196:ILE:HG22	1:C:201:MIS:H31	1.98	0.44
1:H:173:ILE:HD11	1:H:213:MET:CE	2.47	0.44
1:G:220:PHE:HE2	1:I:164:LEU:HD21	1.83	0.44
1:E:196:ILE:CG2	1:E:201:MIS:H31	2.47	0.44
1:G:94:ASN:HB3	1:G:96:HIS:CE1	2.53	0.43
1:B:213:MET:CE	2:B:298:HOH:O	2.60	0.43
1:H:167:THR:HG23	1:I:174:SER:HB3	2.01	0.43
1:A:87:GLN:O	1:A:134:ALA:HB1	2.19	0.43
1:B:94:ASN:HD22	1:B:94:ASN:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ALA:HB1	1:E:196:ILE:HD11	2.01	0.42
1:H:236:ILE:CG2	1:H:240:LEU:HD22	2.49	0.42
1:C:62:TYR:HB2	1:C:105:ILE:HB	2.01	0.42
1:D:250:ARG:HG2	1:D:251:ASP:OD1	2.20	0.42
1:C:173:ILE:HD11	1:C:213:MET:CE	2.47	0.41
1:C:213:MET:CE	2:C:276:HOH:O	2.65	0.41
1:E:250:ARG:O	1:E:251:ASP:HB2	2.19	0.41
1:G:182:ASN:HB2	1:G:183:PRO:CD	2.49	0.41
1:D:53:ARG:HD3	1:F:37:PHE:CZ	2.55	0.41
1:I:62:TYR:HB2	1:I:105:ILE:HB	2.03	0.41
1:D:173:ILE:HD11	1:D:213:MET:CE	2.50	0.41
1:F:213:MET:CE	2:F:266:HOH:O	2.68	0.41
1:B:95:LYS:NZ	1:B:123:SER:HB3	2.36	0.41
1:G:228:THR:HA	1:G:229:PRO:HD3	1.82	0.41
1:F:157:ALA:HB1	1:F:196:ILE:HD11	2.03	0.40
1:D:196:ILE:CG2	1:D:201:MIS:H31	2.51	0.40
1:G:236:ILE:HG23	1:G:240:LEU:HD23	2.03	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	198/243 (82%)	192 (97%)	6 (3%)	0	100	100
1	B	208/243 (86%)	204 (98%)	4 (2%)	0	100	100
1	C	209/243 (86%)	205 (98%)	4 (2%)	0	100	100
1	D	200/243 (82%)	196 (98%)	4 (2%)	0	100	100
1	E	196/243 (81%)	186 (95%)	10 (5%)	0	100	100
1	F	206/243 (85%)	201 (98%)	5 (2%)	0	100	100
1	G	198/243 (82%)	192 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	185/243 (76%)	183 (99%)	2 (1%)	0	100	100
1	I	189/243 (78%)	187 (99%)	2 (1%)	0	100	100
All	All	1789/2187 (82%)	1746 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	164/199 (82%)	162 (99%)	2 (1%)	74	84
1	B	171/199 (86%)	169 (99%)	2 (1%)	74	84
1	C	173/199 (87%)	173 (100%)	0	100	100
1	D	167/199 (84%)	167 (100%)	0	100	100
1	E	164/199 (82%)	162 (99%)	2 (1%)	74	84
1	F	170/199 (85%)	169 (99%)	1 (1%)	87	93
1	G	164/199 (82%)	164 (100%)	0	100	100
1	H	153/199 (77%)	150 (98%)	3 (2%)	58	69
1	I	159/199 (80%)	158 (99%)	1 (1%)	87	93
All	All	1485/1791 (83%)	1474 (99%)	11 (1%)	85	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	227	GLU
1	B	124	LEU
1	B	219	SER
1	E	78	THR
1	E	221	ASP
1	F	94	ASN
1	H	189	PHE

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Mol	Chain	Res	Type
1	H	219	SER
1	H	228	THR
1	I	188	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	$\# Z  > 2$
1	MIS	A	201	1	12,12,13	0.61	0	11,16,18	0.95	0
1	MIS	B	201	1	12,12,13	0.63	0	11,16,18	1.10	1 (9%)
1	MIS	C	201	1	12,12,13	0.66	0	11,16,18	0.85	0
1	MIS	D	201	1	12,12,13	0.63	0	11,16,18	0.77	0
1	MIS	E	201	1	12,12,13	0.62	0	11,16,18	0.87	0
1	MIS	F	201	1	12,12,13	0.63	0	11,16,18	1.15	1 (9%)
1	MIS	G	201	1	12,12,13	0.67	0	11,16,18	1.30	1 (9%)
1	MIS	H	201	1	12,12,13	0.63	0	11,16,18	0.89	0
1	MIS	I	201	1	12,12,13	0.63	0	11,16,18	0.82	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
1	MIS	A	201	1	-	0/10/13/15	0/0/0/0
1	MIS	B	201	1	-	0/10/13/15	0/0/0/0
1	MIS	C	201	1	-	0/10/13/15	0/0/0/0
1	MIS	D	201	1	-	0/10/13/15	0/0/0/0
1	MIS	E	201	1	-	0/10/13/15	0/0/0/0
1	MIS	F	201	1	-	0/10/13/15	0/0/0/0
1	MIS	G	201	1	-	0/10/13/15	0/0/0/0
1	MIS	H	201	1	-	0/10/13/15	0/0/0/0
1	MIS	I	201	1	-	0/10/13/15	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	MIS	OG-CB-CA	2.32	110.46	108.17
1	F	201	MIS	OG-CB-CA	2.51	110.64	108.17
1	G	201	MIS	OG-CB-CA	3.69	111.80	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	201	MIS	1	0
1	B	201	MIS	1	0
1	C	201	MIS	2	0
1	D	201	MIS	1	0
1	E	201	MIS	1	0
1	F	201	MIS	2	0
1	H	201	MIS	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	204/243 (83%)	0.41	18 (8%) 10 15	20, 33, 68, 99	0
1	B	212/243 (87%)	0.49	17 (8%) 12 19	21, 33, 76, 113	0
1	C	213/243 (87%)	0.18	17 (7%) 12 19	20, 32, 69, 93	0
1	D	206/243 (84%)	-0.04	15 (7%) 15 23	21, 33, 71, 83	1 (0%)
1	E	202/243 (83%)	0.47	17 (8%) 11 17	20, 33, 62, 73	0
1	F	210/243 (86%)	0.54	22 (10%) 6 10	21, 32, 67, 92	0
1	G	204/243 (83%)	0.50	19 (9%) 8 14	23, 32, 72, 102	0
1	H	191/243 (78%)	0.28	16 (8%) 11 17	20, 31, 55, 69	0
1	I	197/243 (81%)	0.66	22 (11%) 5 8	21, 33, 62, 74	0
All	All	1839/2187 (84%)	0.39	163 (8%) 9 15	20, 33, 67, 113	1 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	68	THR	8.0
1	G	225	ASP	7.2
1	G	252	GLY	7.0
1	F	37	PHE	6.8
1	A	184	THR	6.8
1	B	66	LEU	6.3
1	B	37	PHE	6.2
1	I	37	PHE	5.4
1	A	225	ASP	5.3
1	F	69	ASN	5.3
1	B	74	LEU	5.3
1	D	181	LEU	5.3
1	I	66	LEU	5.2
1	B	72	ASN	5.1
1	B	71	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	100	ASP	4.9
1	C	68	THR	4.9
1	H	78	THR	4.7
1	G	253	ARG	4.7
1	C	66	LEU	4.6
1	E	225	ASP	4.5
1	B	225	ASP	4.5
1	E	226	GLY	4.3
1	H	100	ASP	4.3
1	G	37	PHE	4.2
1	I	67	ASN	4.2
1	I	117	LEU	4.2
1	G	78	THR	4.1
1	I	124	LEU	4.1
1	F	38	ASP	4.1
1	I	77	ARG	4.1
1	A	226	GLY	4.1
1	G	38	ASP	4.1
1	F	67	ASN	4.0
1	C	71	HIS	3.9
1	G	250	ARG	3.9
1	E	66	LEU	3.9
1	D	40	THR	3.9
1	I	65	GLY	3.9
1	F	39	SER	3.8
1	B	224	ASN	3.8
1	C	74	LEU	3.8
1	D	77	ARG	3.7
1	C	77	ARG	3.6
1	H	102	ASP	3.6
1	F	66	LEU	3.6
1	B	38	ASP	3.6
1	I	179	ILE	3.5
1	G	226	GLY	3.5
1	H	103	GLN	3.5
1	B	77	ARG	3.4
1	C	250	ARG	3.4
1	G	39	SER	3.4
1	G	227	GLU	3.4
1	H	134	ALA	3.4
1	D	41	ASP	3.3
1	H	123	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	135	THR	3.2
1	A	224	ASN	3.2
1	G	74	LEU	3.2
1	H	221	ASP	3.2
1	A	136	GLY	3.1
1	H	63	ASN	3.1
1	E	37	PHE	3.1
1	I	74	LEU	3.0
1	G	247	LYS	3.0
1	F	41	ASP	3.0
1	A	66	LEU	3.0
1	H	135	THR	3.0
1	C	70	SER	2.9
1	F	40	THR	2.9
1	I	75	GLU	2.9
1	A	186	ARG	2.9
1	C	72	ASN	2.9
1	C	39	SER	2.9
1	A	185	GLY	2.9
1	E	65	GLY	2.8
1	F	252	GLY	2.8
1	E	73	GLN	2.8
1	E	224	ASN	2.8
1	F	72	ASN	2.8
1	I	113	VAL	2.8
1	I	136	GLY	2.8
1	I	102	ASP	2.8
1	C	65	GLY	2.7
1	H	117	LEU	2.7
1	D	227	GLU	2.7
1	C	221	ASP	2.7
1	I	244	ILE	2.7
1	I	146	ARG	2.7
1	E	75	GLU	2.7
1	A	75	GLU	2.7
1	B	222	LYS	2.7
1	B	247	LYS	2.6
1	I	100	ASP	2.6
1	E	68	THR	2.6
1	G	228	THR	2.6
1	E	119	VAL	2.6
1	E	247	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	240	LEU	2.6
1	E	67	ASN	2.5
1	D	146	ARG	2.5
1	F	190	LEU	2.5
1	C	69	ASN	2.5
1	E	146	ARG	2.5
1	H	116	ALA	2.5
1	D	133	ASN	2.5
1	H	220	PHE	2.5
1	I	123	SER	2.5
1	B	249	ILE	2.5
1	C	37	PHE	2.5
1	G	192	THR	2.5
1	G	249	ILE	2.5
1	D	69	ASN	2.5
1	I	125	THR	2.5
1	D	42	GLU	2.5
1	D	70	SER	2.4
1	H	115	GLU	2.4
1	A	135	THR	2.4
1	I	78	THR	2.4
1	F	250	ARG	2.4
1	B	75	GLU	2.4
1	F	227	GLU	2.4
1	B	41	ASP	2.4
1	I	180	GLY	2.4
1	G	41	ASP	2.3
1	A	187	GLN	2.3
1	B	40	THR	2.3
1	D	228	THR	2.3
1	D	182	ASN	2.3
1	A	221	ASP	2.3
1	I	135	THR	2.3
1	D	250	ARG	2.3
1	B	73	GLN	2.2
1	I	187	GLN	2.2
1	B	232	ILE	2.2
1	G	173	ILE	2.2
1	F	192	THR	2.2
1	D	66	LEU	2.2
1	D	71	HIS	2.2
1	H	96	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	220	PHE	2.2
1	F	249	ILE	2.2
1	E	100	ASP	2.2
1	F	172	ILE	2.1
1	A	117	LEU	2.1
1	A	124	LEU	2.1
1	E	136	GLY	2.1
1	A	251	ASP	2.1
1	C	222	LYS	2.1
1	C	253	ARG	2.1
1	F	194	ALA	2.1
1	F	136	GLY	2.1
1	A	146	ARG	2.0
1	H	79	LEU	2.0
1	H	105	ILE	2.0
1	A	125	THR	2.0
1	G	75	GLU	2.0
1	C	67	ASN	2.0
1	F	70	SER	2.0
1	F	71	HIS	2.0
1	A	196	ILE	2.0
1	F	236	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	MIS	I	201	13/14	0.95	0.11	23,34,41,41	0
1	MIS	H	201	13/14	0.97	0.10	23,34,40,40	0
1	MIS	C	201	13/14	0.98	0.10	23,34,41,41	0
1	MIS	E	201	13/14	0.98	0.15	23,33,40,40	0
1	MIS	D	201	13/14	0.98	0.08	23,33,40,41	0
1	MIS	A	201	13/14	0.98	0.15	23,33,40,41	0
1	MIS	B	201	13/14	0.98	0.15	23,34,40,42	0
1	MIS	G	201	13/14	0.98	0.12	26,35,42,43	0
1	MIS	F	201	13/14	0.99	0.12	23,33,41,41	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.