



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:37 pm GMT

PDB ID : 3DHO  
Title : Structure of Streptogramin Acetyltransferase in Complex with an Inhibitor  
Authors : Roderick,S.L.; Pesaresi,A.; Wright,G.D.  
Deposited on : 2008-06-18  
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

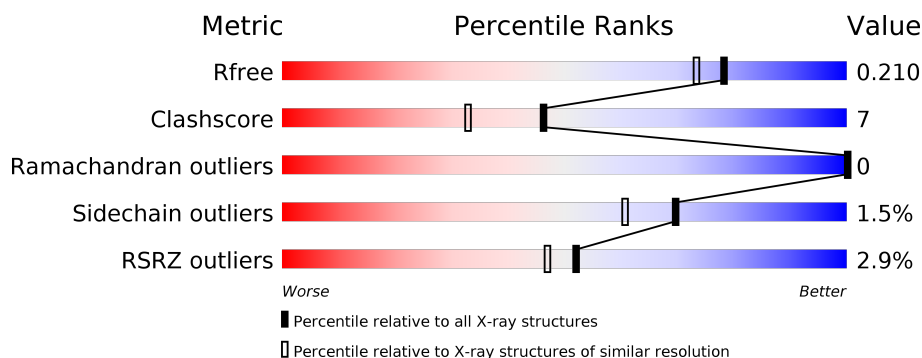
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	209	
1	B	209	
1	C	209	
1	D	209	
1	E	209	
1	F	209	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	A	403	-	-	X	X
2	DMS	C	400	-	-	-	X
2	DMS	D	405	-	-	X	X
3	B2M	D	305	-	-	-	X
3	B2M	E	303	-	-	-	X
3	B2M	E	304	-	-	X	X
4	FMT	B	501	-	-	-	X
4	FMT	B	502	-	-	X	-
4	FMT	C	504	-	-	-	X

## 2 Entry composition [i](#)

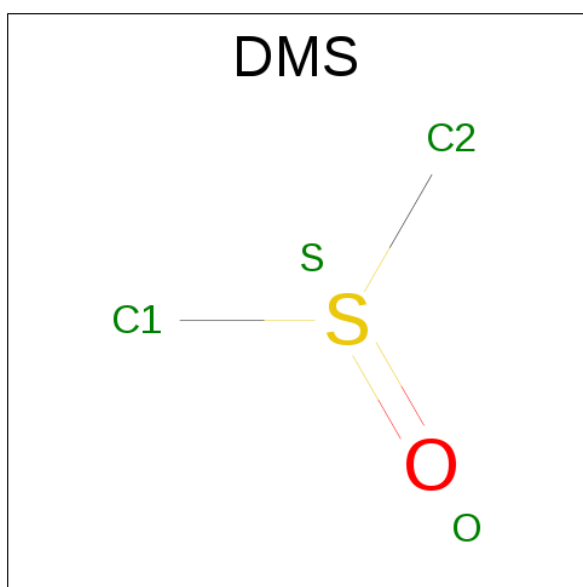
There are 5 unique types of molecules in this entry. The entry contains 11211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Streptogramin A acetyltransferase.

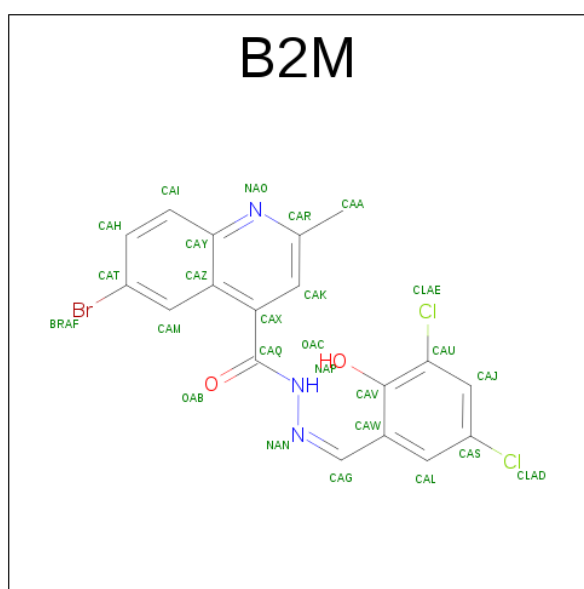
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1609	1038	265	297	9			
1	B	203	Total	C	N	O	S	0	0	0
			1609	1038	265	297	9			
1	C	203	Total	C	N	O	S	0	0	0
			1609	1038	265	297	9			
1	D	203	Total	C	N	O	S	0	0	0
			1609	1038	265	297	9			
1	E	203	Total	C	N	O	S	0	0	0
			1609	1038	265	297	9			
1	F	203	Total	C	N	O	S	0	0	0
			1609	1038	265	297	9			

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 4 2 1 1	0	0
2	A	1	Total C O S 4 2 1 1	0	0
2	B	1	Total C O S 4 2 1 1	0	0
2	B	1	Total C O S 4 2 1 1	0	0
2	C	1	Total C O S 4 2 1 1	0	0
2	D	1	Total C O S 4 2 1 1	0	0

- Molecule 3 is 6-BROMO-N'-[(1Z)-(3,5-DICHLORO-2-HYDROXYPHENYL)METHYLIDENE]-2-METHYLQUINOLINE-4-CARBOHYDRAZIDE (three-letter code: B2M) (formula:  $C_{18}H_{12}BrCl_2N_3O_2$ ).



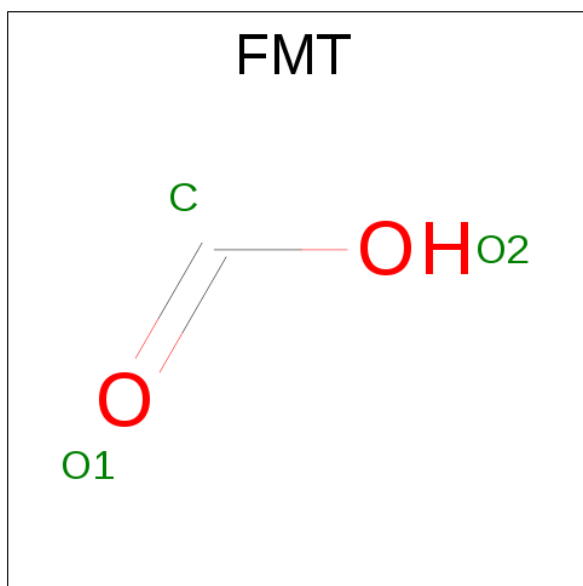
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Br C Cl N O 26 1 18 2 3 2	0	0
3	B	1	Total Br C Cl N O 26 1 18 2 3 2	0	0
3	C	1	Total Br C Cl N O 26 1 18 2 3 2	0	0
3	D	1	Total Br C Cl N O 26 1 18 2 3 2	0	0
3	E	1	Total Br C Cl N O 26 1 18 2 3 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total	Br	C	Cl	N	O	0	0
			26	1	18	2	3	2		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total 223	O 223	0	0
5	B	236	Total 236	O 236	0	0
5	C	250	Total 250	O 250	0	0
5	D	238	Total 238	O 238	0	0
5	E	199	Total 199	O 199	0	0
5	F	204	Total 204	O 204	0	0

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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

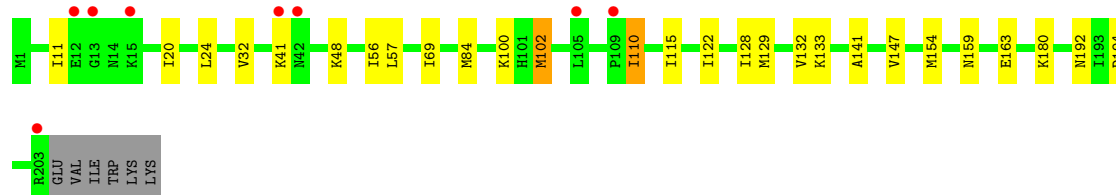
- Molecule 1: Streptogramin A acetyltransferase

Chain A: 




- Molecule 1: Streptogramin A acetyltransferase

Chain B: 




- Molecule 1: Streptogramin A acetyltransferase

Chain C: 




- Molecule 1: Streptogramin A acetyltransferase

Chain D: 

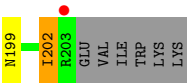


- Molecule 1: Streptogramin A acetyltransferase

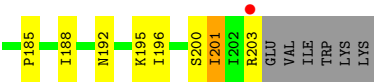
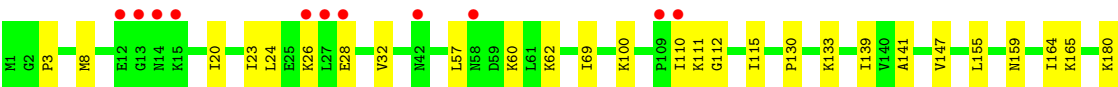
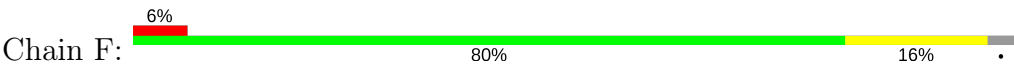
Chain E: 







● Molecule 1: Streptogramin A acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.65Å 183.62Å 183.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.47 – 1.80 25.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.47-1.80) 99.8 (25.46-1.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.213 0.174 , 0.210	Depositor DCC
$R_{free}$ test set	7132 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h 0.014 for k,h,-l 0.015 for -h,-l,-k 0.011 for k,-l,-h 0.011 for -l,h,-k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: FMT, DMS, B2M

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	0.65	0/1648	0.68	0/2234
1	B	0.65	0/1648	0.67	0/2234
1	C	0.65	0/1648	0.70	1/2234 (0.0%)
1	D	0.59	0/1648	0.65	0/2234
1	E	0.60	0/1648	0.64	0/2234
1	F	0.58	0/1648	0.65	0/2234
All	All	0.62	0/9888	0.66	1/13404 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	MET	CG-SD-CE	-6.14	90.37	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	202	ILE	Peptide

## 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	1609	0	1613	21	0
1	B	1609	0	1613	27	0
1	C	1609	0	1613	13	0
1	D	1609	0	1613	19	0
1	E	1609	0	1613	25	0
1	F	1609	0	1613	26	0
2	A	8	0	12	7	0
2	B	8	0	12	0	0
2	C	4	0	6	0	0
2	D	4	0	6	6	0
3	A	26	0	11	3	0
3	B	26	0	11	3	0
3	C	26	0	11	3	0
3	D	26	0	11	5	0
3	E	52	0	22	10	0
4	A	3	0	1	0	0
4	B	6	0	2	3	0
4	C	6	0	2	0	0
4	D	6	0	2	0	0
4	E	3	0	1	0	0
4	F	3	0	1	0	0
5	A	223	0	0	2	0
5	B	236	0	0	6	1
5	C	250	0	0	5	1
5	D	238	0	0	2	0
5	E	199	0	0	2	0
5	F	204	0	0	3	0
All	All	11211	0	9789	141	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 7.

All (141) 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:A:48:LYS:HB2	5:A:602:HOH:O	1.46	1.13
1:B:48:LYS:HB2	5:B:575:HOH:O	1.65	0.95
1:F:110:ILE:HG22	1:F:112:GLY:H	1.29	0.95
2:D:405:DMS:H13	1:F:159:ASN:HD22	1.34	0.91
1:D:154:MET:HE2	1:D:163:GLU:HB3	1.53	0.90
1:E:104:LYS:H	1:E:107:GLN:HE21	1.22	0.87
1:A:104:LYS:H	1:A:107:GLN:HE21	1.24	0.85
1:A:99:GLU:O	1:A:102:MET:HG2	1.78	0.83
1:F:20:ILE:CD1	1:F:69:ILE:HD12	2.07	0.83
1:A:154:MET:HE2	1:A:163:GLU:HB3	1.61	0.81
1:E:154:MET:HE2	1:E:163:GLU:HB3	1.64	0.80
2:D:405:DMS:C1	1:F:159:ASN:HD22	1.96	0.79
1:A:154:MET:CE	1:A:163:GLU:HB3	2.16	0.75
1:D:159:ASN:HD22	2:D:405:DMS:H11	1.52	0.74
1:D:104:LYS:H	1:D:107:GLN:HE21	1.36	0.74
1:E:104:LYS:H	1:E:107:GLN:NE2	1.87	0.73
1:B:20:ILE:HG13	1:B:32:VAL:HG11	1.71	0.72
1:A:179:ILE:HG23	5:A:583:HOH:O	1.92	0.70
1:F:110:ILE:HG22	1:F:112:GLY:N	2.07	0.69
2:A:403:DMS:C1	1:B:159:ASN:HD22	2.06	0.68
3:E:304:B2M:HAJ	5:E:855:HOH:O	1.93	0.68
1:A:159:ASN:HD22	2:A:403:DMS:H12	1.59	0.68
1:B:154:MET:HE2	1:B:163:GLU:HB3	1.76	0.68
1:A:159:ASN:HD22	2:A:403:DMS:C1	2.07	0.67
1:A:111:LYS:HD2	1:A:130:PRO:HB2	1.77	0.67
1:E:80:ALA:HB3	5:E:756:HOH:O	1.93	0.67
1:E:8:MET:CE	1:E:23:ILE:HD13	2.27	0.65
1:E:24:LEU:HD12	1:E:32:VAL:HG21	1.79	0.64
1:D:179:ILE:HD11	1:D:201:ILE:HD12	1.78	0.64
1:F:196:ILE:HA	1:F:201:ILE:HG12	1.78	0.64
2:A:403:DMS:H11	1:B:159:ASN:HD22	1.63	0.64
1:F:57:LEU:HB3	1:F:110:ILE:HD11	1.79	0.63
1:A:104:LYS:H	1:A:107:GLN:NE2	1.97	0.62
1:E:154:MET:CE	1:E:163:GLU:HB3	2.30	0.62
1:E:69:ILE:HD12	1:E:122:ILE:HD12	1.81	0.62
1:B:194:ASP:HB2	4:B:502:FMT:O2	1.99	0.61
1:B:192:ASN:HA	4:B:502:FMT:H	1.81	0.61
1:B:24:LEU:HD12	1:B:32:VAL:HG21	1.82	0.61
1:E:8:MET:HE2	1:E:23:ILE:CD1	2.32	0.60
2:A:403:DMS:C1	1:C:159:ASN:HD22	2.15	0.60
1:D:141:ALA:HB2	3:D:305:B2M:BRAF	2.57	0.60
1:D:31:GLU:HG2	5:D:794:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ASN:HD22	2:D:405:DMS:C1	2.15	0.59
1:D:20:ILE:HD13	1:D:69:ILE:HD12	1.85	0.59
1:D:20:ILE:CD1	1:D:69:ILE:HD12	2.34	0.58
1:C:148:LYS:NZ	5:C:543:HOH:O	2.36	0.58
1:E:8:MET:HE2	1:E:23:ILE:HD13	1.84	0.58
1:A:115:ILE:HB	1:A:133:LYS:HD2	1.87	0.56
3:E:304:B2M:OAC	3:E:304:B2M:NAP	2.37	0.56
1:B:100:LYS:HD3	5:B:591:HOH:O	2.07	0.55
1:E:141:ALA:HB2	3:E:303:B2M:BRAF	2.62	0.55
1:F:24:LEU:HD12	1:F:32:VAL:HG21	1.89	0.54
1:B:69:ILE:HD12	1:B:122:ILE:HD12	1.90	0.54
1:B:128:ILE:HG23	1:B:132:VAL:HG21	1.88	0.54
1:F:20:ILE:HD12	1:F:69:ILE:HD12	1.87	0.54
1:F:20:ILE:HD11	1:F:69:ILE:HD12	1.90	0.53
1:E:22:PRO:HA	1:E:25:GLU:HG3	1.90	0.53
1:B:192:ASN:HA	4:B:502:FMT:C	2.39	0.53
1:F:192:ASN:OD1	1:F:195:LYS:NZ	2.42	0.53
3:A:302:B2M:NAP	3:A:302:B2M:OAC	2.42	0.53
1:C:7:LYS:NZ	5:C:646:HOH:O	2.43	0.52
2:D:405:DMS:H13	1:F:159:ASN:ND2	2.14	0.52
1:A:17:VAL:HG21	1:C:93:LEU:HD21	1.91	0.52
3:D:305:B2M:HNAP	3:D:305:B2M:CAV	2.23	0.51
1:B:102:MET:HG2	5:B:588:HOH:O	2.11	0.51
3:C:301:B2M:OAC	3:C:301:B2M:NAP	2.42	0.51
1:F:180:LYS:HE3	5:F:613:HOH:O	2.09	0.51
1:D:154:MET:CE	1:D:163:GLU:HB3	2.33	0.51
1:A:93:LEU:HG	1:B:11:ILE:HD11	1.94	0.50
1:E:18:GLN:HB3	1:E:23:ILE:HG13	1.94	0.50
1:C:111:LYS:HD2	1:C:130:PRO:HB2	1.94	0.50
3:D:305:B2M:HAJ	5:F:689:HOH:O	2.11	0.50
1:F:62:LYS:HE2	5:F:671:HOH:O	2.11	0.50
1:C:8:MET:HG3	1:C:23:ILE:HG12	1.94	0.49
1:C:141:ALA:HB2	3:C:301:B2M:BRAF	2.67	0.49
1:C:166:GLN:NE2	5:C:634:HOH:O	2.45	0.49
3:E:304:B2M:CAL	1:F:164:ILE:HD13	2.42	0.49
1:F:139:ILE:HB	1:F:155:LEU:HD23	1.94	0.49
1:D:104:LYS:H	1:D:107:GLN:NE2	2.05	0.49
1:E:8:MET:HE3	1:E:23:ILE:HD13	1.94	0.49
3:D:305:B2M:OAC	3:D:305:B2M:NAP	2.42	0.49
3:A:302:B2M:CAV	3:A:302:B2M:HNAP	2.24	0.49
1:B:20:ILE:HG13	1:B:32:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:304:B2M:CAV	3:E:304:B2M:HNAP	2.25	0.49
1:B:115:ILE:HB	1:B:133:LYS:HD2	1.96	0.48
1:F:185:PRO:HD2	1:F:188:ILE:HD12	1.95	0.48
1:F:8:MET:CE	1:F:23:ILE:HD13	2.44	0.47
1:A:139:ILE:HB	1:A:155:LEU:HD23	1.95	0.47
1:D:110:ILE:HD13	5:D:888:HOH:O	2.13	0.47
1:E:104:LYS:N	1:E:107:GLN:HE21	2.02	0.47
1:E:199:ASN:O	1:E:202:ILE:HG12	2.15	0.47
1:B:56:ILE:HA	1:D:104:LYS:HG2	1.97	0.47
1:E:94:PHE:HB3	1:F:3:PRO:HG3	1.97	0.47
1:E:56:ILE:HG13	1:E:105:LEU:HD21	1.96	0.46
3:E:304:B2M:BRAF	1:F:141:ALA:HB2	2.71	0.46
1:C:115:ILE:HB	1:C:133:LYS:HD2	1.97	0.45
3:E:303:B2M:OAC	3:E:303:B2M:NAP	2.48	0.45
2:A:403:DMS:H13	1:C:159:ASN:HD22	1.81	0.45
1:F:115:ILE:HB	1:F:133:LYS:HD2	1.99	0.45
1:D:155:LEU:HD12	1:D:165:LYS:HG3	1.98	0.45
1:F:8:MET:HE3	1:F:23:ILE:HD13	1.99	0.45
1:B:128:ILE:CG2	1:B:132:VAL:HG21	2.46	0.45
1:B:100:LYS:CE	5:B:708:HOH:O	2.65	0.45
1:D:115:ILE:HB	1:D:133:LYS:HD2	1.98	0.45
1:E:18:GLN:HE22	1:E:46:PHE:H	1.66	0.44
2:A:403:DMS:H11	1:C:159:ASN:HD22	1.82	0.44
1:D:90:PRO:HB2	1:D:93:LEU:HG	1.99	0.44
1:E:155:LEU:HD13	1:E:165:LYS:HE3	1.99	0.44
1:B:141:ALA:HB2	3:B:300:B2M:BRAF	2.72	0.44
2:D:405:DMS:C1	1:E:159:ASN:HD22	2.31	0.43
1:E:54:TYR:HA	1:E:55:PRO:HD3	1.89	0.43
1:A:201:ILE:HA	1:A:201:ILE:HD12	1.89	0.43
1:B:180:LYS:NZ	5:B:671:HOH:O	2.52	0.43
1:F:155:LEU:HD12	1:F:165:LYS:HG3	2.00	0.43
1:B:57:LEU:HB3	1:B:110:ILE:HD11	2.01	0.43
1:B:20:ILE:CG1	1:B:32:VAL:HG11	2.46	0.43
3:B:300:B2M:CAV	3:B:300:B2M:HNAP	2.30	0.43
1:D:8:MET:O	1:D:18:GLN:HA	2.19	0.43
3:D:305:B2M:CAJ	1:F:147:VAL:HG11	2.49	0.43
1:E:147:VAL:HG11	3:E:304:B2M:CAV	2.49	0.42
3:E:303:B2M:CAV	3:E:303:B2M:HNAP	2.31	0.42
3:E:304:B2M:HAM	3:E:304:B2M:NAP	2.34	0.42
1:F:200:SER:HA	1:F:203:ARG:HH21	1.84	0.42
1:A:10:PRO:HB3	1:A:19:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:MET:HE2	1:E:23:ILE:HD11	2.02	0.42
1:C:100:LYS:HB3	5:C:657:HOH:O	2.20	0.42
1:C:93:LEU:HD23	1:C:93:LEU:O	2.19	0.42
1:F:111:LYS:HD2	1:F:130:PRO:HB2	2.02	0.42
1:B:56:ILE:CD1	1:D:102:MET:HG3	2.50	0.41
1:A:184:TRP:HH2	1:A:201:ILE:CG1	2.33	0.41
1:A:154:MET:HE3	1:A:163:GLU:HB3	2.01	0.41
1:B:129:MET:HG3	1:B:147:VAL:HG12	2.02	0.41
1:A:184:TRP:HH2	1:A:201:ILE:HG13	1.86	0.41
1:B:84:MET:HE3	5:C:524:HOH:O	2.21	0.41
3:C:301:B2M:HNAP	3:C:301:B2M:CAV	2.31	0.41
1:E:111:LYS:HD2	1:E:130:PRO:HB2	2.03	0.41
1:D:199:ASN:HD22	1:D:199:ASN:HA	1.64	0.40
1:A:199:ASN:O	1:A:202:ILE:HG12	2.21	0.40
3:B:300:B2M:OAC	3:B:300:B2M:NAP	2.51	0.40
1:B:41:LYS:HD3	5:B:585:HOH:O	2.21	0.40
1:A:141:ALA:HB2	3:A:302:B2M:BRFA	2.76	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)
5:B:728:HOH:O	5:C:734:HOH:O[11_555]	1.94	0.26

## 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	201/209 (96%)	197 (98%)	4 (2%)	0	100	100
1	B	201/209 (96%)	199 (99%)	2 (1%)	0	100	100
1	C	201/209 (96%)	199 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	201/209 (96%)	198 (98%)	3 (2%)	0	100	100
1	E	201/209 (96%)	197 (98%)	4 (2%)	0	100	100
1	F	201/209 (96%)	197 (98%)	4 (2%)	0	100	100
All	All	1206/1254 (96%)	1187 (98%)	19 (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	177/183 (97%)	175 (99%)	2 (1%)	78	72
1	B	177/183 (97%)	175 (99%)	2 (1%)	78	72
1	C	177/183 (97%)	176 (99%)	1 (1%)	89	87
1	D	177/183 (97%)	173 (98%)	4 (2%)	56	41
1	E	177/183 (97%)	175 (99%)	2 (1%)	78	72
1	F	177/183 (97%)	172 (97%)	5 (3%)	49	34
All	All	1062/1098 (97%)	1046 (98%)	16 (2%)	70	61

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	203	ARG
1	B	102	MET
1	B	110	ILE
1	C	199	ASN
1	D	165	LYS
1	D	199	ASN
1	D	202	ILE
1	D	203	ARG
1	E	28	GLU

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Mol	Chain	Res	Type
1	E	100	LYS
1	F	26	LYS
1	F	28	GLU
1	F	60	LYS
1	F	100	LYS
1	F	201	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	107	GLN
1	A	159	ASN
1	B	29	ASN
1	B	58	ASN
1	B	159	ASN
1	C	159	ASN
1	C	166	GLN
1	C	170	GLN
1	D	107	GLN
1	D	159	ASN
1	D	162	ASN
1	D	199	ASN
1	E	18	GLN
1	E	29	ASN
1	E	107	GLN
1	E	159	ASN
1	E	162	ASN
1	E	166	GLN
1	E	170	GLN
1	E	174	ASN
1	F	159	ASN
1	F	162	ASN
1	F	166	GLN
1	F	170	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	B2M	A	302	-	28,28,28	2.86	5 (17%)	38,40,40	2.04	10 (26%)
2	DMS	A	401	-	3,3,3	0.30	0	3,3,3	1.41	1 (33%)
2	DMS	A	403	-	3,3,3	0.22	0	3,3,3	1.24	1 (33%)
4	FMT	A	500	-	0,2,2	0.00	-	0,1,1	0.00	-
3	B2M	B	300	-	28,28,28	2.82	4 (14%)	38,40,40	2.19	10 (26%)
2	DMS	B	402	-	3,3,3	0.30	0	3,3,3	1.26	1 (33%)
2	DMS	B	404	-	3,3,3	0.22	0	3,3,3	1.06	0
4	FMT	B	501	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	502	-	0,2,2	0.00	-	0,1,1	0.00	-
3	B2M	C	301	-	28,28,28	2.84	4 (14%)	38,40,40	2.21	13 (34%)
2	DMS	C	400	-	3,3,3	0.35	0	3,3,3	1.61	1 (33%)
4	FMT	C	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	504	-	0,2,2	0.00	-	0,1,1	0.00	-
3	B2M	D	305	-	28,28,28	2.89	4 (14%)	38,40,40	2.09	8 (21%)
2	DMS	D	405	-	3,3,3	0.18	0	3,3,3	1.23	1 (33%)
4	FMT	D	505	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
3	B2M	E	303	-	28,28,28	2.86	5 (17%)	38,40,40	2.03	7 (18%)
3	B2M	E	304	-	28,28,28	2.88	4 (14%)	38,40,40	2.06	12 (31%)
4	FMT	E	507	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FMT	F	508	-	0,2,2	0.00	-	0,1,1	0.00	-

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	B2M	A	302	-	-	0/10/10/10	0/3/3/3
2	DMS	A	401	-	-	0/0/0/0	0/0/0/0
2	DMS	A	403	-	-	0/0/0/0	0/0/0/0
4	FMT	A	500	-	-	0/0/0/0	0/0/0/0
3	B2M	B	300	-	-	0/10/10/10	0/3/3/3
2	DMS	B	402	-	-	0/0/0/0	0/0/0/0
2	DMS	B	404	-	-	0/0/0/0	0/0/0/0
4	FMT	B	501	-	-	0/0/0/0	0/0/0/0
4	FMT	B	502	-	-	0/0/0/0	0/0/0/0
3	B2M	C	301	-	-	0/10/10/10	0/3/3/3
2	DMS	C	400	-	-	0/0/0/0	0/0/0/0
4	FMT	C	503	-	-	0/0/0/0	0/0/0/0
4	FMT	C	504	-	-	0/0/0/0	0/0/0/0
3	B2M	D	305	-	-	0/10/10/10	0/3/3/3
2	DMS	D	405	-	-	0/0/0/0	0/0/0/0
4	FMT	D	505	-	-	0/0/0/0	0/0/0/0
4	FMT	D	506	-	-	0/0/0/0	0/0/0/0
3	B2M	E	303	-	-	0/10/10/10	0/3/3/3
3	B2M	E	304	-	-	0/10/10/10	0/3/3/3
4	FMT	E	507	-	-	0/0/0/0	0/0/0/0
4	FMT	F	508	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	304	B2M	NAP-NAN	-13.39	1.23	1.38
3	D	305	B2M	NAP-NAN	-13.36	1.23	1.38
3	E	303	B2M	NAP-NAN	-13.13	1.23	1.38
3	B	300	B2M	NAP-NAN	-12.76	1.23	1.38
3	C	301	B2M	NAP-NAN	-12.49	1.24	1.38
3	A	302	B2M	NAP-NAN	-12.48	1.24	1.38
3	D	305	B2M	CAW-CAG	-3.08	1.39	1.45
3	A	302	B2M	CAW-CAG	-2.82	1.40	1.45
3	E	304	B2M	CAW-CAG	-2.71	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	303	B2M	CAW-CAG	-2.63	1.40	1.45
3	B	300	B2M	CAW-CAG	-2.56	1.40	1.45
3	C	301	B2M	CAW-CAG	-2.35	1.41	1.45
3	E	303	B2M	CAX-CAQ	2.00	1.54	1.50
3	E	303	B2M	CAM-CAT	2.20	1.39	1.36
3	D	305	B2M	CAM-CAT	2.21	1.39	1.36
3	A	302	B2M	CAM-CAT	2.22	1.39	1.36
3	E	304	B2M	CAM-CAT	2.23	1.39	1.36
3	A	302	B2M	CAX-CAQ	2.51	1.55	1.50
3	B	300	B2M	CAM-CAT	2.64	1.40	1.36
3	C	301	B2M	CAX-CAQ	2.86	1.55	1.50
3	E	304	B2M	CAG-NAN	3.91	1.32	1.28
3	D	305	B2M	CAG-NAN	3.97	1.32	1.28
3	E	303	B2M	CAG-NAN	4.60	1.33	1.28
3	B	300	B2M	CAG-NAN	4.73	1.33	1.28
3	C	301	B2M	CAG-NAN	5.34	1.33	1.28
3	A	302	B2M	CAG-NAN	5.64	1.34	1.28

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	305	B2M	CAL-CAW-CAG	-5.21	111.84	119.60
3	B	300	B2M	CAL-CAW-CAG	-4.75	112.53	119.60
3	E	304	B2M	CAL-CAW-CAG	-4.44	112.99	119.60
3	E	303	B2M	CAL-CAW-CAG	-4.20	113.35	119.60
3	C	301	B2M	CAL-CAW-CAG	-3.95	113.72	119.60
3	A	302	B2M	CAL-CAW-CAG	-3.87	113.84	119.60
3	B	300	B2M	CAK-CAR-NAO	-2.66	119.32	122.61
3	E	304	B2M	CAH-CAT-CAM	-2.61	119.40	121.98
3	B	300	B2M	CAZ-CAY-NAO	-2.60	120.16	122.84
3	C	301	B2M	CAZ-CAY-NAO	-2.51	120.25	122.84
3	E	304	B2M	CAZ-CAY-NAO	-2.34	120.42	122.84
3	A	302	B2M	CAZ-CAY-NAO	-2.29	120.47	122.84
3	E	303	B2M	CAK-CAR-NAO	-2.26	119.81	122.61
3	D	305	B2M	CAK-CAR-NAO	-2.20	119.89	122.61
3	C	301	B2M	CAK-CAR-NAO	-2.11	120.00	122.61
3	E	304	B2M	CAK-CAR-NAO	-2.11	120.00	122.61
3	A	302	B2M	BRAF-CAT-CAM	-2.06	117.10	119.82
3	D	305	B2M	CAZ-CAY-NAO	-2.04	120.73	122.84
3	C	301	B2M	CAL-CAS-CLAD	-2.03	116.61	119.14
2	A	403	DMS	C2-S-C1	2.00	108.83	98.44
2	D	405	DMS	C2-S-C1	2.02	108.92	98.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	DMS	C2-S-C1	2.05	109.05	98.44
3	E	304	B2M	CAA-CAR-NAO	2.06	120.71	117.25
3	B	300	B2M	CAW-CAV-CAU	2.11	119.88	118.36
3	E	304	B2M	CAW-CAV-CAU	2.12	119.89	118.36
3	B	300	B2M	CAA-CAR-NAO	2.21	120.97	117.25
2	A	401	DMS	C2-S-C1	2.26	110.17	98.44
3	A	302	B2M	CAV-CAU-CLAE	2.26	121.99	118.86
2	C	400	DMS	C2-S-C1	2.29	110.30	98.44
3	E	304	B2M	CAZ-CAX-CAQ	2.33	124.14	120.73
3	A	302	B2M	CAX-CAZ-CAY	2.36	119.70	116.91
3	E	304	B2M	CAJ-CAS-CLAD	2.40	122.14	119.14
3	C	301	B2M	CAV-CAU-CLAE	2.42	122.20	118.86
3	E	304	B2M	CAV-CAU-CLAE	2.44	122.23	118.86
3	C	301	B2M	CAX-CAZ-CAY	2.44	119.81	116.91
3	C	301	B2M	CAQ-NAP-NAN	2.54	122.67	118.94
3	A	302	B2M	CAW-CAV-CAU	2.61	120.24	118.36
3	C	301	B2M	CAW-CAV-CAU	3.09	120.58	118.36
3	B	300	B2M	CAV-CAU-CLAE	3.18	123.25	118.86
3	D	305	B2M	CAZ-CAX-CAQ	3.26	125.51	120.73
3	A	302	B2M	CAW-CAG-NAN	3.30	125.64	120.69
3	D	305	B2M	CAW-CAG-NAN	3.35	125.71	120.69
3	B	300	B2M	CAG-NAN-NAP	3.39	121.49	115.91
3	E	303	B2M	CAV-CAU-CLAE	3.42	123.58	118.86
3	C	301	B2M	CAZ-CAX-CAQ	3.51	125.87	120.73
3	E	303	B2M	CAZ-CAX-CAQ	3.52	125.89	120.73
3	E	304	B2M	CAG-NAN-NAP	3.57	121.79	115.91
3	D	305	B2M	CAG-NAN-NAP	3.61	121.86	115.91
3	C	301	B2M	CAJ-CAS-CLAD	3.66	123.72	119.14
3	B	300	B2M	CAZ-CAX-CAQ	3.73	126.19	120.73
3	A	302	B2M	CAG-NAN-NAP	3.82	122.21	115.91
3	D	305	B2M	CAV-CAU-CLAE	3.89	124.23	118.86
3	E	303	B2M	CAW-CAG-NAN	4.07	126.80	120.69
3	B	300	B2M	CAW-CAG-NAN	4.15	126.91	120.69
3	E	303	B2M	CAG-NAN-NAP	4.23	122.88	115.91
3	C	301	B2M	CAW-CAG-NAN	4.23	127.04	120.69
3	C	301	B2M	CAG-NAN-NAP	4.49	123.30	115.91
3	E	304	B2M	CAW-CAG-NAN	4.50	127.43	120.69
3	A	302	B2M	CAZ-CAX-CAQ	5.07	128.16	120.73
3	A	302	B2M	CAV-CAW-CAG	5.89	127.53	121.06
3	C	301	B2M	CAV-CAW-CAG	6.10	127.76	121.06
3	E	304	B2M	CAV-CAW-CAG	6.24	127.91	121.06
3	E	303	B2M	CAV-CAW-CAG	6.37	128.05	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	305	B2M	CAV-CAW-CAG	6.81	128.53	121.06
3	B	300	B2M	CAV-CAW-CAG	7.34	129.12	121.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	B2M	3	0
2	A	403	DMS	7	0
3	B	300	B2M	3	0
4	B	502	FMT	3	0
3	C	301	B2M	3	0
3	D	305	B2M	5	0
2	D	405	DMS	6	0
3	E	303	B2M	3	0
3	E	304	B2M	7	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	203/209 (97%)	-0.22	1 (0%) 90 89	7, 12, 24, 30	0
1	B	203/209 (97%)	-0.12	8 (3%) 40 35	7, 13, 29, 34	0
1	C	203/209 (97%)	-0.24	3 (1%) 74 70	7, 13, 23, 30	0
1	D	203/209 (97%)	-0.11	4 (1%) 65 61	10, 16, 26, 39	0
1	E	203/209 (97%)	0.04	7 (3%) 46 41	9, 16, 33, 42	0
1	F	203/209 (97%)	0.06	12 (5%) 23 19	11, 18, 32, 44	0
All	All	1218/1254 (97%)	-0.10	35 (2%) 52 47	7, 14, 28, 44	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	13	GLY	6.9
1	F	13	GLY	6.4
1	F	203	ARG	5.3
1	E	203	ARG	5.1
1	B	42	ASN	4.3
1	C	42	ASN	4.0
1	F	26	LYS	3.9
1	F	42	ASN	3.6
1	D	109	PRO	3.4
1	A	42	ASN	3.3
1	E	42	ASN	3.2
1	B	13	GLY	3.1
1	E	109	PRO	3.0
1	F	27	LEU	2.9
1	E	110	ILE	2.9
1	F	109	PRO	2.8
1	B	109	PRO	2.7
1	B	105	LEU	2.6
1	F	28	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	41	LYS	2.5
1	B	203	ARG	2.5
1	F	12	GLU	2.5
1	C	109	PRO	2.4
1	F	14	ASN	2.4
1	B	12	GLU	2.4
1	D	42	ASN	2.3
1	E	108	LEU	2.3
1	C	13	GLY	2.3
1	F	110	ILE	2.2
1	F	15	LYS	2.2
1	F	58	ASN	2.1
1	D	13	GLY	2.1
1	B	15	LYS	2.1
1	E	26	LYS	2.1
1	D	110	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DMS	D	405	4/4	0.75	0.30	16.80	62,63,63,64	0
3	B2M	E	303	26/26	0.83	0.50	14.56	11,18,18,18	26
3	B2M	E	304	26/26	0.70	0.58	14.24	16,22,22,23	26
3	B2M	D	305	26/26	0.79	0.52	11.80	15,19,19,20	26
2	DMS	C	400	4/4	0.84	0.26	7.56	44,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FMT	C	504	3/3	0.76	0.16	6.74	24,24,29,32	0
4	FMT	B	501	3/3	0.93	0.17	5.93	25,25,28,28	0
2	DMS	A	403	4/4	0.92	0.17	4.18	28,33,33,34	0
3	B2M	C	301	26/26	0.93	0.19	1.79	16,21,23,23	26
3	B2M	A	302	26/26	0.94	0.17	1.22	14,18,20,21	26
2	DMS	B	404	4/4	0.93	0.17	0.91	33,34,35,35	0
3	B2M	B	300	26/26	0.96	0.14	0.82	13,17,18,20	26
4	FMT	D	505	3/3	0.76	0.16	-	43,43,43,45	0
4	FMT	B	502	3/3	0.90	0.30	-	30,30,32,32	0
4	FMT	D	506	3/3	0.74	0.23	-	31,31,34,35	0
4	FMT	C	503	3/3	0.74	0.18	-	33,33,36,37	0
4	FMT	F	508	3/3	0.90	0.15	-	39,39,40,40	0
4	FMT	E	507	3/3	0.79	0.22	-	34,34,36,38	0
2	DMS	A	401	4/4	0.81	0.20	-	58,58,59,59	0
4	FMT	A	500	3/3	0.59	0.21	-	44,44,46,46	0
2	DMS	B	402	4/4	0.91	0.18	-	57,57,57,57	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.