



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 11:24 pm BST

PDB ID : 3L3T  
Title : Human mesotrypsin complexed with amyloid precursor protein inhibitor variant (APPIR15K)  
Authors : Salameh, M.A.; Soares, A.S.; Radisky, E.S.  
Deposited on : 2009-12-17  
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

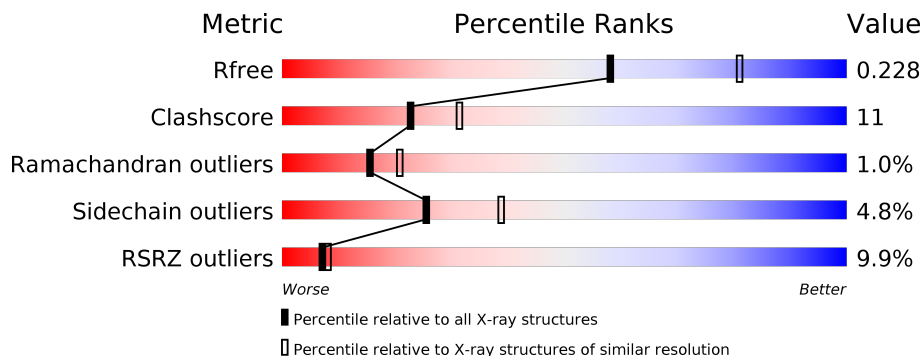
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 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	224	 4% 85% 13%
1	B	224	 10% 83% 15%
1	C	224	 5% 79% 19%
1	D	224	 17% 78% 19%
2	E	57	 12% 72% 21% 7%
2	F	57	 18% 77% 19%

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Mol	Chain	Length	Quality of chain
2	G	57	
2	H	57	

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
3	FMT	A	4	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8967 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 PRSS3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	Total 1706	C 1075	N 294	O 325	S 12	8	1	0
1	B	224	Total 1706	C 1075	N 294	O 325	S 12	13	1	0
1	C	224	Total 1716	C 1082	N 296	O 326	S 12	2	3	0
1	D	224	Total 1714	C 1080	N 297	O 325	S 12	8	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	SER	ENGINEERED MUTATION	UNP Q8N2U3
B	195	ALA	SER	ENGINEERED MUTATION	UNP Q8N2U3
C	195	ALA	SER	ENGINEERED MUTATION	UNP Q8N2U3
D	195	ALA	SER	ENGINEERED MUTATION	UNP Q8N2U3

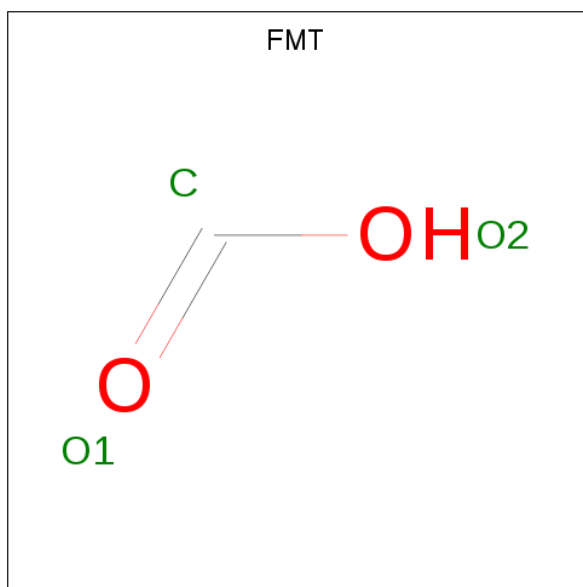
- Molecule 2 is a protein called Protein APP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	57	Total 433	C 268	N 70	O 87	S 8	0	0	0
2	F	57	Total 433	C 268	N 70	O 87	S 8	0	0	0
2	G	57	Total 433	C 268	N 70	O 87	S 8	0	0	0
2	H	57	Total 433	C 268	N 70	O 87	S 8	1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	15	LYS	ARG	ENGINEERED MUTATION	UNP C9JHU0
F	15	LYS	ARG	ENGINEERED MUTATION	UNP C9JHU0
G	15	LYS	ARG	ENGINEERED MUTATION	UNP C9JHU0
H	15	LYS	ARG	ENGINEERED MUTATION	UNP C9JHU0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

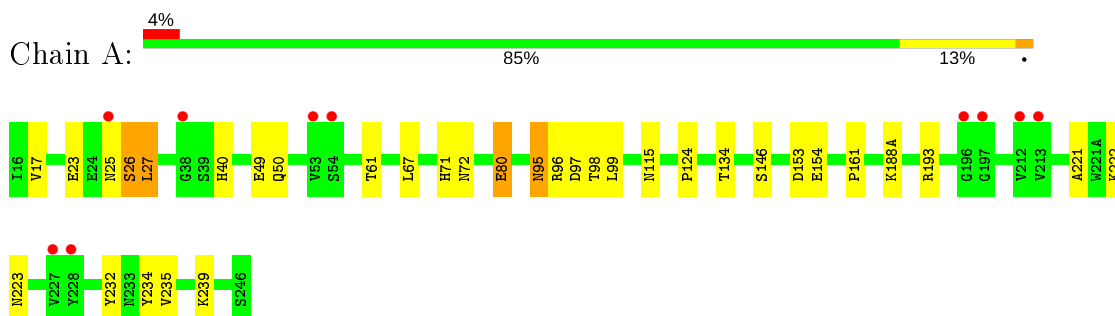
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	104	Total O 106 106	0	2
5	B	83	Total O 84 84	0	1
5	C	69	Total O 71 71	0	2
5	D	41	Total O 41 41	0	0
5	E	18	Total O 18 18	0	0
5	F	10	Total O 10 10	0	0
5	G	11	Total O 11 11	0	0
5	H	9	Total O 9 9	0	0

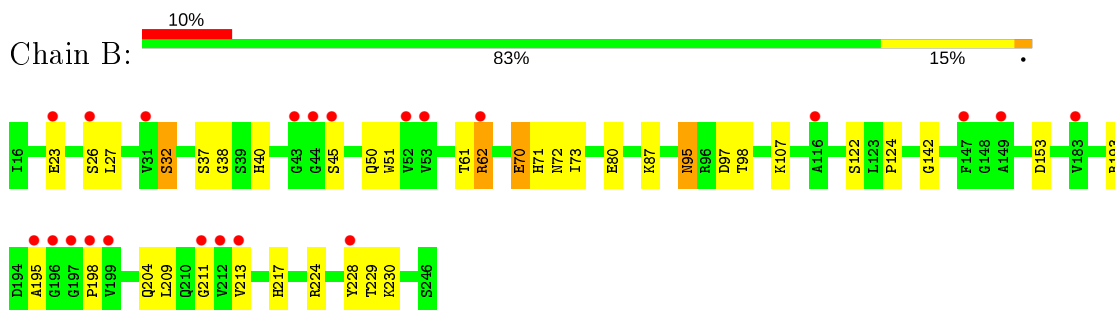
### 3 Residue-property plots [i](#)

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.

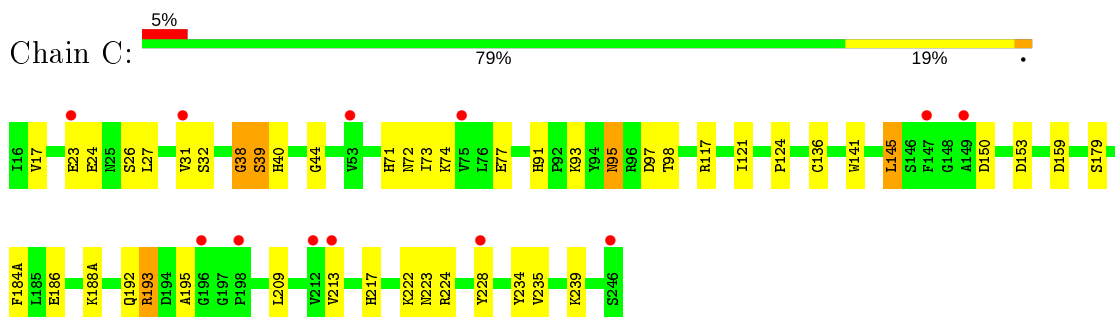
- Molecule 1: PRSS3 protein



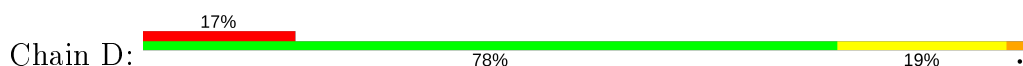
- Molecule 1: PRSS3 protein

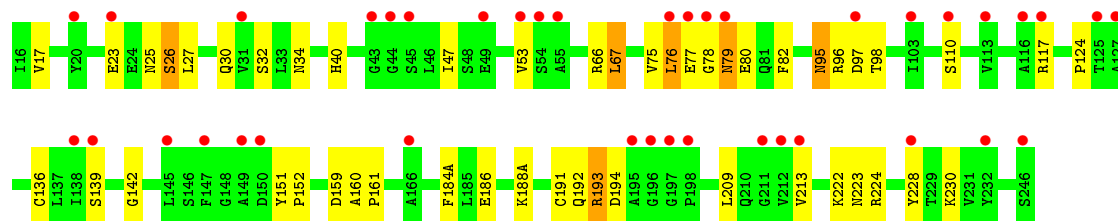


- Molecule 1: PRSS3 protein



- Molecule 1: PRSS3 protein

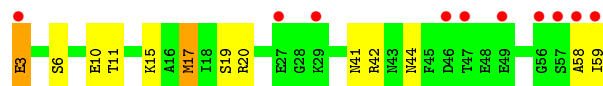
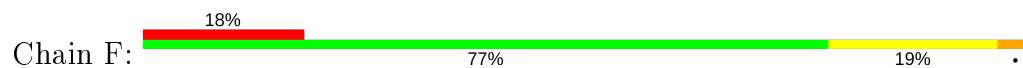




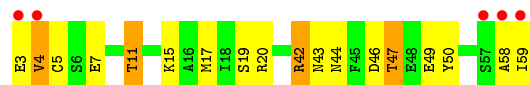
- Molecule 2: Protein APP



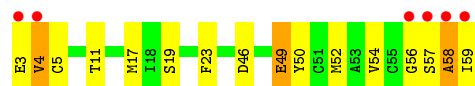
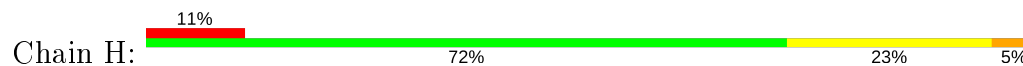
- Molecule 2: Protein APP



- Molecule 2: Protein APP



- Molecule 2: Protein APP





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.79Å 130.07Å 132.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.52 – 2.38 24.52 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.0 (24.52-2.38) 98.0 (24.52-2.38)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.39Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.183 , 0.237 0.172 , 0.228	Depositor DCC
$R_{free}$ test set	3184 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 69.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.025 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: FMT, CA

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	0.42	0/1748	0.57	0/2377
1	B	0.38	0/1748	0.54	0/2377
1	C	0.40	0/1765	0.54	0/2400
1	D	0.32	0/1759	0.53	0/2391
2	E	0.40	0/443	0.55	0/595
2	F	0.37	0/443	0.53	0/595
2	G	0.37	0/443	0.51	0/595
2	H	0.42	0/443	0.58	0/595
All	All	0.38	0/8792	0.55	0/11925

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 [i](#)

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	1706	0	1663	31	0
1	B	1706	0	1663	33	0
1	C	1716	0	1675	40	0
1	D	1714	0	1676	45	0
2	E	433	0	381	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	433	0	381	8	0
2	G	433	0	381	18	0
2	H	433	0	381	13	0
3	A	21	0	7	3	0
3	B	15	0	5	0	0
3	C	3	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	106	0	0	1	0
5	B	84	0	0	3	0
5	C	71	0	0	1	0
5	D	41	0	0	1	0
5	E	18	0	0	3	0
5	F	10	0	0	1	0
5	G	11	0	0	1	0
5	H	9	0	0	0	0
All	All	8967	0	8214	192	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 11.

All (192) 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:D:76:LEU:HB3	1:D:77:GLU:HA	1.14	1.10
1:C:38:GLY:HA3	1:C:39:SER:HB3	1.09	1.07
1:C:38:GLY:HA3	1:C:39:SER:CB	1.95	0.96
1:D:32:SER:HB2	1:D:40:HIS:CD2	2.04	0.93
1:D:76:LEU:CB	1:D:77:GLU:HA	2.02	0.89
2:G:47:THR:HG22	2:G:50:TYR:H	1.37	0.88
2:H:52:MET:HA	2:H:52:MET:HE2	1.56	0.85
1:D:76:LEU:HB3	1:D:77:GLU:CA	2.02	0.85
1:D:95:ASN:HD22	1:D:97:ASP:H	1.20	0.84
1:C:38:GLY:CA	1:C:39:SER:HB3	2.02	0.84
1:D:78:GLY:HA2	1:D:79:ASN:CG	2.01	0.80
1:D:95:ASN:ND2	1:D:97:ASP:H	1.79	0.80
1:C:23:GLU:CD	1:C:23:GLU:H	1.87	0.78
1:D:32:SER:HB2	1:D:40:HIS:HD2	1.48	0.78
1:A:23:GLU:HB2	1:A:26:SER:OG	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:53:ALA:HA	2:E:59:ILE:HD13	1.67	0.76
1:A:95:ASN:ND2	1:A:97:ASP:H	1.84	0.75
1:A:239:LYS:HE2	1:C:235:VAL:HG11	1.71	0.73
1:B:95:ASN:ND2	1:B:97:ASP:H	1.88	0.71
1:A:26:SER:HB3	1:A:27[A]:LEU:HD22	1.72	0.71
2:G:4:VAL:O	2:G:43:ASN:HB2	1.91	0.71
1:B:23:GLU:HB3	1:B:26:SER:OG	1.92	0.70
1:D:78:GLY:HA2	1:D:79:ASN:ND2	2.07	0.70
2:E:20:ARG:HD3	2:E:44:ASN:OD1	1.94	0.68
1:B:193:ARG:HB2	2:F:17:MET:HG3	1.75	0.68
1:C:95:ASN:ND2	1:C:98:THR:H	1.92	0.67
2:G:19:SER:O	2:G:20:ARG:HG2	1.96	0.65
1:B:224:ARG:NE	5:B:265:HOH:O	2.27	0.65
1:B:95:ASN:ND2	1:B:98:THR:H	1.94	0.65
1:D:25:ASN:ND2	1:D:117:ARG:HE	1.94	0.64
1:D:184(A):PHE:HB3	1:D:186:GLU:OE2	1.96	0.64
2:F:20:ARG:HD3	2:F:44:ASN:OD1	1.97	0.64
1:D:124:PRO:HG3	1:D:209:LEU:O	1.97	0.63
1:B:95:ASN:HD21	1:B:97:ASP:HB2	1.64	0.62
2:H:3:GLU:OE1	2:H:5:CYS:HB2	1.99	0.62
1:D:193:ARG:HB2	2:H:17:MET:HB2	1.81	0.62
1:C:192:GLN:O	1:C:193:ARG:HB2	1.99	0.62
1:B:32:SER:HB2	1:B:40:HIS:CE1	2.36	0.60
1:D:66:ARG:HD2	1:D:82:PHE:CD1	2.37	0.60
2:F:42:ARG:HD3	5:F:60:HOH:O	2.02	0.60
1:B:95:ASN:HD22	1:B:97:ASP:H	1.49	0.60
1:A:234:TYR:C	3:A:4:FMT:H	2.22	0.59
2:H:3:GLU:HG2	2:H:4:VAL:N	2.18	0.59
2:H:49:GLU:OE1	2:H:49:GLU:HA	2.02	0.59
1:D:25:ASN:HD21	1:D:117:ARG:HE	1.51	0.59
1:B:95:ASN:HD22	1:B:97:ASP:N	2.01	0.59
1:D:95:ASN:HD22	1:D:97:ASP:N	1.96	0.58
2:G:4:VAL:HG13	2:G:5:CYS:H	1.68	0.58
1:A:193:ARG:HD3	2:E:17:MET:SD	2.43	0.58
1:D:40:HIS:ND1	1:D:193:ARG:HD2	2.19	0.57
1:C:40:HIS:HB2	5:C:304:HOH:O	2.05	0.57
2:E:42:ARG:HD3	5:E:61:HOH:O	2.02	0.57
1:A:95:ASN:HD22	1:A:97:ASP:H	1.51	0.57
1:C:95:ASN:ND2	1:C:97:ASP:H	2.03	0.57
1:C:124:PRO:HG3	1:C:209:LEU:O	2.04	0.56
1:D:78:GLY:HA2	1:D:79:ASN:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:GLU:CD	1:D:186:GLU:H	2.09	0.56
1:B:32:SER:HB2	1:B:40:HIS:ND1	2.21	0.56
1:D:77:GLU:N	5:D:36:HOH:O	2.38	0.56
2:E:3:GLU:HG3	2:E:4:VAL:H	1.70	0.56
2:H:56:GLY:O	2:H:58:ALA:N	2.39	0.56
1:D:23:GLU:HB3	1:D:26:SER:OG	2.06	0.56
1:A:235:VAL:CG1	1:C:239:LYS:HE2	2.36	0.56
2:E:58:ALA:HA	5:E:113:HOH:O	2.05	0.56
1:C:145:LEU:HD22	1:C:150:ASP:HB2	1.87	0.55
1:C:95:ASN:HD22	1:C:97:ASP:H	1.54	0.55
1:B:45:SER:OG	1:B:198:PRO:HB3	2.06	0.55
1:A:95:ASN:HD22	1:A:95:ASN:C	2.09	0.55
1:D:78:GLY:HA3	1:D:80:GLU:OE1	2.06	0.55
1:B:95:ASN:ND2	1:B:97:ASP:N	2.55	0.55
2:F:58:ALA:HB1	2:F:59:ILE:HB	1.87	0.55
2:G:20:ARG:HD3	2:G:44:ASN:OD1	2.07	0.55
2:H:52:MET:HA	2:H:52:MET:CE	2.34	0.55
2:G:4:VAL:HG13	2:G:5:CYS:N	2.22	0.54
1:D:26:SER:HB2	1:D:27[B]:LEU:HD12	1.89	0.54
1:A:95:ASN:ND2	1:A:98:THR:H	2.05	0.54
1:B:87:LYS:HE2	1:B:107:LYS:HD2	1.89	0.54
1:B:70:GLU:HG2	1:B:73:ILE:HG22	1.89	0.54
2:G:3:GLU:O	2:G:5:CYS:N	2.41	0.54
1:D:222:LYS:HG2	1:D:223:ASN:ND2	2.24	0.53
2:G:58:ALA:O	2:G:59:ILE:OXT	2.27	0.52
1:D:78:GLY:HA3	1:D:80:GLU:H	1.74	0.52
2:E:19:SER:C	2:E:20:ARG:HG2	2.28	0.52
1:D:191:CYS:O	1:D:194:ASP:HB2	2.09	0.51
1:D:34:ASN:ND2	1:D:66:ARG:HG3	2.26	0.51
1:D:95:ASN:HD22	1:D:95:ASN:C	2.12	0.51
2:E:49:GLU:H	2:E:49:GLU:CD	2.13	0.51
1:A:115:ASN:HB2	5:A:264:HOH:O	2.09	0.51
1:B:26:SER:HB2	1:B:27[A]:LEU:HD22	1.91	0.51
1:B:71:HIS:HD2	5:B:322:HOH:O	1.92	0.51
1:A:26:SER:HB3	1:A:27[B]:LEU:HD13	1.92	0.51
1:C:195:ALA:HB2	2:G:15:LYS:C	2.31	0.51
2:G:20:ARG:HH21	2:G:46:ASP:CA	2.24	0.51
2:E:3:GLU:HG3	2:E:4:VAL:HG13	1.93	0.50
1:B:72:ASN:HA	1:B:153:ASP:O	2.11	0.50
1:C:23:GLU:O	1:C:26:SER:HB3	2.11	0.50
1:B:142:GLY:HA2	1:B:193:ARG:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:THR:HG23	5:E:63:HOH:O	2.10	0.50
2:G:11:THR:HG23	5:G:117:HOH:O	2.12	0.50
2:G:47:THR:HG23	2:G:49:GLU:OE2	2.11	0.49
1:A:40:HIS:CD2	1:A:193:ARG:HG2	2.47	0.49
1:A:235:VAL:HG11	1:C:239:LYS:HE2	1.94	0.49
1:C:32:SER:HB2	1:C:40:HIS:CD2	2.47	0.49
1:C:23:GLU:HB2	1:C:26:SER:HB2	1.95	0.49
1:C:95:ASN:HD21	1:C:97:ASP:HB2	1.78	0.49
1:C:222:LYS:HG2	1:C:223:ASN:ND2	2.29	0.48
1:A:17:VAL:O	1:A:188(A):LYS:HA	2.13	0.48
1:B:213:VAL:HA	1:B:228:TYR:CD2	2.49	0.48
2:E:53:ALA:HA	2:E:59:ILE:CD1	2.41	0.48
1:B:62:ARG:HA	1:B:62:ARG:HD2	1.53	0.47
1:C:217[A]:HIS:HD2	1:C:224:ARG:CZ	2.27	0.47
1:A:80:GLU:CD	1:A:80:GLU:H	2.18	0.47
1:A:67:LEU:N	1:A:67:LEU:HD12	2.29	0.47
1:C:235:VAL:O	1:C:239:LYS:HG3	2.14	0.47
1:C:95:ASN:C	1:C:95:ASN:HD22	2.18	0.47
2:G:19:SER:C	2:G:20:ARG:HG2	2.35	0.47
1:A:124:PRO:HG2	1:A:232:TYR:HA	1.97	0.47
2:G:20:ARG:HH21	2:G:46:ASP:N	2.12	0.47
1:D:17:VAL:O	1:D:188(A):LYS:HA	2.15	0.46
1:C:213:VAL:HA	1:C:228:TYR:CD2	2.50	0.46
1:C:73:ILE:HG23	1:C:141:TRP:NE1	2.31	0.46
2:F:19:SER:O	2:F:20:ARG:HG3	2.16	0.46
2:H:58:ALA:O	2:H:59:ILE:O	2.33	0.46
1:A:95:ASN:HD22	1:A:97:ASP:N	2.13	0.46
2:G:47:THR:CG2	2:G:49:GLU:HB2	2.45	0.46
1:C:74:LYS:HD2	1:C:153:ASP:OD1	2.16	0.46
1:D:78:GLY:CA	1:D:79:ASN:CG	2.79	0.46
1:B:224:ARG:CZ	5:B:265:HOH:O	2.64	0.46
1:B:211:GLY:HA2	1:B:229:THR:O	2.16	0.46
1:C:31:VAL:HG22	1:C:44:GLY:C	2.36	0.46
3:A:248:FMT:H	1:C:121:ILE:HD12	1.98	0.46
2:E:3:GLU:HG3	2:E:4:VAL:CG1	2.46	0.46
1:A:26:SER:CB	1:A:27[A]:LEU:HD22	2.42	0.45
2:F:10:GLU:HG3	2:F:41:ASN:ND2	2.32	0.45
1:A:146:SER:OG	1:A:221:ALA:HB3	2.16	0.45
1:D:136:CYS:O	1:D:159:ASP:HA	2.17	0.45
1:D:160:ALA:HA	1:D:161:PRO:HD3	1.76	0.45
2:H:49:GLU:OE1	2:H:49:GLU:CA	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HG	1:A:221:ALA:HB3	1.82	0.44
1:D:186:GLU:N	1:D:186:GLU:CD	2.71	0.44
1:B:61:THR:O	1:B:62:ARG:CD	2.66	0.44
1:D:95:ASN:HD21	1:D:97:ASP:HB2	1.82	0.44
1:D:230:LYS:HE3	1:D:230:LYS:HB2	1.78	0.44
1:D:95:ASN:ND2	1:D:98:THR:H	2.16	0.44
2:H:23:PHE:CD1	2:H:52:MET:HE3	2.52	0.44
1:D:151:TYR:HA	1:D:152:PRO:HD3	1.72	0.44
1:A:95:ASN:ND2	1:A:95:ASN:C	2.72	0.43
1:B:51:TRP:CH2	1:B:107:LYS:HB2	2.53	0.43
1:C:72:ASN:HA	1:C:153:ASP:O	2.17	0.43
1:B:195:ALA:HB2	2:F:15:LYS:C	2.38	0.43
1:A:72:ASN:OD1	1:A:153:ASP:HB3	2.19	0.43
1:A:95:ASN:ND2	1:A:97:ASP:N	2.60	0.43
1:C:91:HIS:CE1	1:C:93:LYS:HB2	2.54	0.43
1:C:193:ARG:HG3	2:G:17:MET:SD	2.59	0.43
1:D:75:VAL:HG12	1:D:76:LEU:O	2.19	0.43
1:D:213:VAL:HA	1:D:228:TYR:CD2	2.55	0.42
1:B:124:PRO:HD3	1:B:209:LEU:O	2.19	0.42
1:B:80:GLU:CD	1:B:80:GLU:H	2.21	0.42
2:H:23:PHE:HD1	2:H:52:MET:HE3	1.84	0.42
2:H:46:ASP:N	2:H:46:ASP:OD2	2.51	0.42
1:C:40:HIS:ND1	1:C:193:ARG:HD2	2.34	0.42
2:H:50:TYR:O	2:H:54:VAL:HG23	2.20	0.42
1:A:98:THR:O	1:A:99:LEU:HB2	2.19	0.42
1:C:136:CYS:O	1:C:159:ASP:HA	2.19	0.42
1:B:61:THR:O	1:B:62:ARG:HD3	2.19	0.42
1:D:67:LEU:N	1:D:67:LEU:HD12	2.34	0.42
1:A:23:GLU:O	1:A:26:SER:HB2	2.19	0.42
1:A:134:THR:O	1:A:161:PRO:HA	2.20	0.41
2:G:3:GLU:OE2	2:G:4:VAL:HG12	2.19	0.41
1:A:71:HIS:HE1	1:A:154:GLU:OE2	2.03	0.41
1:C:31:VAL:HG22	1:C:44:GLY:O	2.19	0.41
1:D:192:GLN:O	1:D:193:ARG:HB3	2.20	0.41
2:G:42:ARG:HA	2:G:42:ARG:HD2	1.89	0.41
1:C:17:VAL:O	1:C:188(A):LYS:HA	2.19	0.41
1:B:124:PRO:HA	1:B:204:GLN:OE1	2.20	0.41
1:C:95:ASN:HD22	1:C:97:ASP:N	2.16	0.41
2:F:3:GLU:N	2:F:6:SER:HG	2.18	0.41
1:B:230:LYS:HE3	1:B:230:LYS:HB2	1.79	0.41
1:C:184(A):PHE:CE1	1:C:188(A):LYS:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:SER:C	1:C:27[B]:LEU:HD12	2.40	0.41
1:A:222:LYS:HE2	1:A:223:ASN:HD21	1.86	0.41
2:E:19:SER:O	2:E:20:ARG:HG2	2.21	0.41
1:B:217:HIS:HB3	1:B:224:ARG:HD2	2.02	0.41
1:B:37:SER:HB3	1:B:38:GLY:H	1.73	0.41
1:D:47:ILE:HD13	1:D:53:VAL:HG23	2.02	0.41
1:C:179:SER:HB2	1:C:234:TYR:OH	2.20	0.41
1:D:223:ASN:O	1:D:224:ARG:HD2	2.21	0.40
1:C:24:GLU:HG3	1:C:71:HIS:CG	2.56	0.40
1:D:142:GLY:HA2	1:D:192:GLN:O	2.22	0.40
1:A:235:VAL:N	3:A:4:FMT:H	2.37	0.40
1:B:95:ASN:C	1:B:95:ASN:HD22	2.25	0.40

There are no symmetry-related clashes.

## 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	223/224 (100%)	211 (95%)	9 (4%)	3 (1%)	12 15
1	B	223/224 (100%)	216 (97%)	7 (3%)	0	100 100
1	C	225/224 (100%)	214 (95%)	9 (4%)	2 (1%)	17 23
1	D	224/224 (100%)	210 (94%)	13 (6%)	1 (0%)	34 46
2	E	55/57 (96%)	51 (93%)	2 (4%)	2 (4%)	3 2
2	F	55/57 (96%)	53 (96%)	2 (4%)	0	100 100
2	G	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	8 9
2	H	55/57 (96%)	48 (87%)	5 (9%)	2 (4%)	3 2
All	All	1115/1124 (99%)	1056 (95%)	48 (4%)	11 (1%)	15 21

All (11) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	25	ASN
2	G	4	VAL
1	A	49	GLU
1	C	38	GLY
2	E	56	GLY
2	H	57	SER
1	A	26	SER
1	C	39	SER
1	D	76	LEU
2	E	57	SER
2	H	58	ALA

### 5.3.2 Protein sidechains [i](#)

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	186/185 (100%)	179 (96%)	7 (4%)	33 49
1	B	186/185 (100%)	180 (97%)	6 (3%)	39 56
1	C	188/185 (102%)	182 (97%)	6 (3%)	39 56
1	D	187/185 (101%)	178 (95%)	9 (5%)	25 39
2	E	45/45 (100%)	39 (87%)	6 (13%)	4 4
2	F	45/45 (100%)	42 (93%)	3 (7%)	16 23
2	G	45/45 (100%)	41 (91%)	4 (9%)	9 13
2	H	45/45 (100%)	41 (91%)	4 (9%)	9 13
All	All	927/920 (101%)	882 (95%)	45 (5%)	25 38

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27[A]	LEU
1	A	27[B]	LEU
1	A	50	GLN
1	A	61	THR
1	A	80	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	95	ASN
1	A	96	ARG
1	B	32	SER
1	B	50	GLN
1	B	62	ARG
1	B	70	GLU
1	B	95	ASN
1	B	122	SER
1	C	77	GLU
1	C	95	ASN
1	C	117	ARG
1	C	145	LEU
1	C	186	GLU
1	C	193	ARG
1	D	26	SER
1	D	30	GLN
1	D	67	LEU
1	D	79	ASN
1	D	95	ASN
1	D	96	ARG
1	D	110	SER
1	D	139	SER
1	D	193	ARG
2	E	4	VAL
2	E	7	GLU
2	E	11	THR
2	E	19	SER
2	E	25	VAL
2	E	49	GLU
2	F	3	GLU
2	F	11	THR
2	F	17	MET
2	G	7	GLU
2	G	11	THR
2	G	42	ARG
2	G	47	THR
2	H	4	VAL
2	H	11	THR
2	H	19	SER
2	H	49	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	50	GLN
1	A	71	HIS
1	A	95	ASN
1	A	202	ASN
1	A	223	ASN
1	B	30	GLN
1	B	50	GLN
1	B	71	HIS
1	B	95	ASN
1	C	30	GLN
1	C	95	ASN
1	C	223	ASN
1	D	25	ASN
1	D	95	ASN
1	D	165	GLN
1	D	223	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	FMT	A	248	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	247	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	11	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	3	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	13	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	12	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	2	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	10	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	249	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	6	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	247	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	4	-	0,2,2	0.00	-	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	248	FMT	1	0
3	A	4	FMT	2	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 i

### 6.1 Protein, DNA and RNA chains i

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	224/224 (100%)	0.04	10 (4%) 33 36	20, 33, 53, 75	4 (1%)
1	B	224/224 (100%)	0.32	22 (9%) 7 8	19, 37, 55, 75	4 (1%)
1	C	224/224 (100%)	0.16	12 (5%) 25 28	25, 39, 62, 79	1 (0%)
1	D	224/224 (100%)	0.71	39 (17%) 1 1	27, 54, 83, 113	5 (2%)
2	E	57/57 (100%)	0.43	7 (12%) 4 4	28, 47, 87, 137	0
2	F	57/57 (100%)	0.76	10 (17%) 1 1	25, 58, 95, 147	0
2	G	57/57 (100%)	0.39	5 (8%) 10 11	33, 50, 91, 142	0
2	H	57/57 (100%)	0.10	6 (10%) 6 7	34, 44, 95, 108	0
All	All	1124/1124 (100%)	0.33	111 (9%) 7 8	19, 41, 75, 147	14 (1%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	59	ILE	17.0
2	G	58	ALA	11.1
2	G	59	ILE	8.3
2	E	59	ILE	7.8
2	E	58	ALA	6.9
2	F	57	SER	6.5
2	F	58	ALA	6.3
1	D	246	SER	6.0
2	H	57	SER	5.4
1	C	147	PHE	4.8
1	C	246	SER	4.8
2	H	59	ILE	4.8
1	D	125	THR	4.7
1	D	127	ALA	4.5
1	D	213	VAL	4.4
2	G	3	GLU	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	116	ALA	4.3
1	D	53	VAL	4.3
1	D	23	GLU	4.2
1	C	213	VAL	3.9
1	D	197	GLY	3.9
1	B	31	VAL	3.9
1	D	77	GLU	3.8
1	D	150	ASP	3.7
1	B	213	VAL	3.7
1	D	211	GLY	3.6
1	B	53	VAL	3.6
2	H	3	GLU	3.6
1	D	54	SER	3.5
1	D	212	VAL	3.5
1	B	198	PRO	3.4
1	B	196	GLY	3.4
1	B	212	VAL	3.4
1	B	197	GLY	3.4
1	C	212	VAL	3.2
2	E	3	GLU	3.2
2	H	4	VAL	3.2
1	D	147	PHE	3.2
2	G	4	VAL	3.2
1	D	198	PRO	3.2
1	D	20	TYR	3.1
1	D	196	GLY	3.1
1	B	228	TYR	3.1
1	A	213	VAL	3.1
1	D	49	GLU	3.0
1	B	199	VAL	3.0
1	B	211	GLY	3.0
1	A	25	ASN	3.0
2	E	57	SER	3.0
2	E	50	TYR	3.0
1	A	196	GLY	3.0
1	D	149	ALA	3.0
2	E	49	GLU	3.0
1	D	44	GLY	3.0
1	A	212	VAL	2.9
1	D	79	ASN	2.9
1	D	166	ALA	2.8
2	F	27	GLU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	31	VAL	2.8
1	C	149	ALA	2.7
1	B	44	GLY	2.7
2	F	29	LYS	2.7
1	D	45	SER	2.6
1	A	38	GLY	2.6
1	D	78	GLY	2.6
1	D	138	ILE	2.6
1	D	31	VAL	2.6
1	B	26	SER	2.5
1	C	23	GLU	2.5
1	D	195	ALA	2.5
1	B	23	GLU	2.5
1	A	227	VAL	2.5
1	D	232	TYR	2.5
1	D	43	GLY	2.5
1	C	53	VAL	2.5
1	B	45	SER	2.4
2	H	56	GLY	2.4
2	H	58	ALA	2.4
1	A	197	GLY	2.4
1	A	228	TYR	2.4
1	D	97	ASP	2.4
1	C	198	PRO	2.4
1	D	76	LEU	2.3
1	B	52	VAL	2.3
1	B	116	ALA	2.3
1	B	149	ALA	2.3
1	C	196	GLY	2.3
1	B	195	ALA	2.3
2	F	49	GLU	2.2
1	D	139	SER	2.2
2	F	56	GLY	2.2
1	A	53	VAL	2.2
2	G	57	SER	2.2
2	F	3	GLU	2.1
1	D	145	LEU	2.1
1	B	183	VAL	2.1
1	C	75	VAL	2.1
2	F	46	ASP	2.1
1	B	43	GLY	2.1
1	D	103	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	228	TYR	2.1
1	D	55	ALA	2.1
2	E	53	ALA	2.1
2	F	47	THR	2.1
1	D	113	VAL	2.1
1	B	147	PHE	2.1
1	D	110	SER	2.0
1	B	62	ARG	2.0
1	C	228	TYR	2.0
1	A	54	SER	2.0
1	D	117	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FMT	A	247	3/3	0.72	0.31	66,66,77,79	0
3	FMT	B	11	3/3	0.74	0.19	56,56,64,66	0
4	CA	D	4	1/1	0.76	0.18	120,120,120,120	0
3	FMT	A	2	3/3	0.79	0.24	73,73,77,77	0
3	FMT	A	4	3/3	0.82	0.28	48,48,48,57	0
3	FMT	A	13	3/3	0.82	0.34	66,66,68,72	0
4	CA	C	3	1/1	0.83	0.18	98,98,98,98	0
3	FMT	B	10	3/3	0.83	0.29	76,76,77,79	0
3	FMT	B	6	3/3	0.83	0.16	67,67,69,72	0
3	FMT	A	248	3/3	0.88	0.18	52,52,70,77	0
4	CA	A	250	1/1	0.93	0.18	80,80,80,80	0
3	FMT	C	247	3/3	0.94	0.11	61,61,64,64	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FMT	A	249	3/3	0.94	0.10	56,56,63,69	0
3	FMT	B	12	3/3	0.94	0.16	50,50,51,54	0
4	CA	B	1	1/1	0.95	0.10	68,68,68,68	0
3	FMT	B	3	3/3	0.95	0.22	69,69,70,72	0
3	FMT	A	1	3/3	0.96	0.20	54,54,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.