



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:04 AM BST

PDB ID : 6E1X  
Title : Crystal structure of product-bound complex of spermidine/spermine N-acetyltransferase SpeG  
Authors : Filippova, E.V.; Minasov, G.; Kiryukhina, O.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2018-07-10  
Resolution : 1.35 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

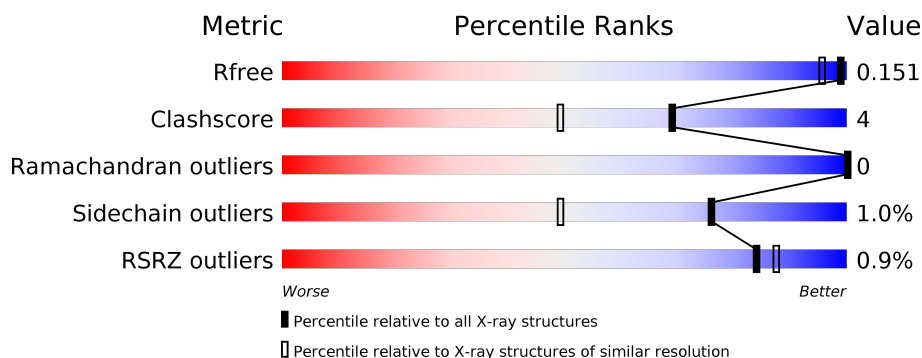
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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))
$R_{free}$	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	176	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>•</div> </div> </div>
1	B	176	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	C	176	<div> <div></div> <div> <div>90%</div> <div>9%</div> <div>•</div> </div> </div>
1	D	176	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>•</div> </div> </div>
1	E	176	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• 5%</div> </div> </div>
1	F	176	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• • 5%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11159 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 Spermidine N(1)-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	14	0
			1557	995	276	283	3			
1	B	169	Total	C	N	O	S	0	15	0
			1557	998	272	284	3			
1	C	176	Total	C	N	O	S	0	13	0
			1588	1011	279	294	4			
1	D	176	Total	C	N	O	S	0	10	0
			1570	998	281	287	4			
1	E	168	Total	C	N	O	S	0	17	0
			1576	1012	280	281	3			
1	F	168	Total	C	N	O	S	0	16	0
			1570	1009	280	278	3			

There are 18 discrepancies between the modelled and reference sequences:

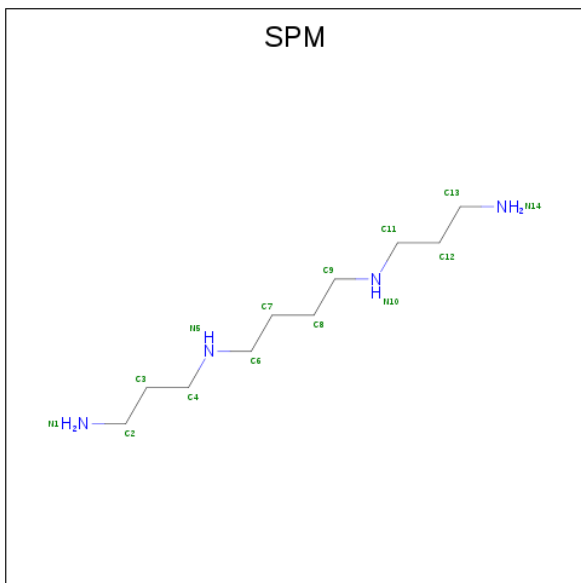
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KL03
A	-1	ASN	-	expression tag	UNP Q9KL03
A	0	ALA	-	expression tag	UNP Q9KL03
B	-2	SER	-	expression tag	UNP Q9KL03
B	-1	ASN	-	expression tag	UNP Q9KL03
B	0	ALA	-	expression tag	UNP Q9KL03
C	-2	SER	-	expression tag	UNP Q9KL03
C	-1	ASN	-	expression tag	UNP Q9KL03
C	0	ALA	-	expression tag	UNP Q9KL03
D	-2	SER	-	expression tag	UNP Q9KL03
D	-1	ASN	-	expression tag	UNP Q9KL03
D	0	ALA	-	expression tag	UNP Q9KL03
E	-2	SER	-	expression tag	UNP Q9KL03
E	-1	ASN	-	expression tag	UNP Q9KL03
E	0	ALA	-	expression tag	UNP Q9KL03
F	-2	SER	-	expression tag	UNP Q9KL03
F	-1	ASN	-	expression tag	UNP Q9KL03

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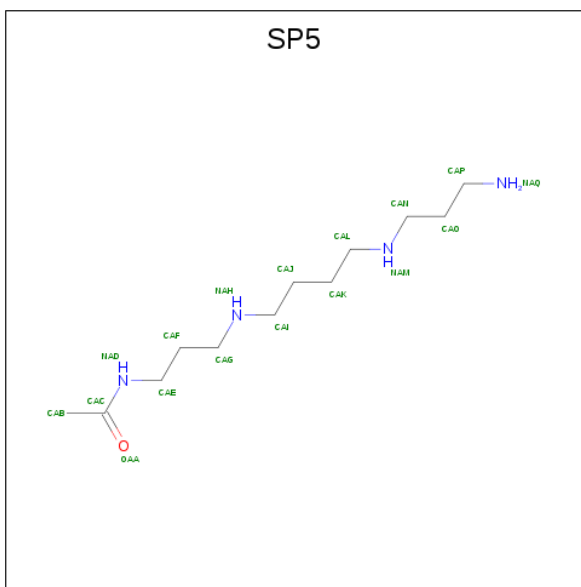
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q9KL03

- Molecule 2 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



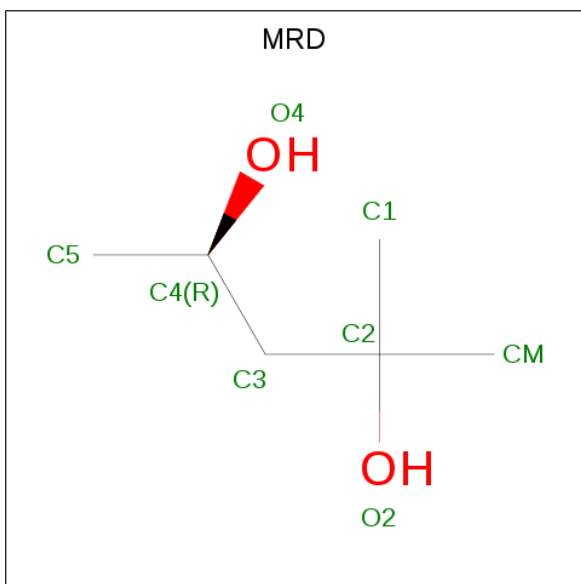
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			14	10	4		
2	B	1	Total	C	N	0	0
			14	10	4		
2	C	1	Total	C	N	0	0
			14	10	4		
2	C	1	Total	C	N	0	0
			10	7	3		
2	D	1	Total	C	N	0	0
			14	10	4		
2	E	1	Total	C	N	0	0
			10	7	3		

- Molecule 3 is N-[3-({4-[(3-aminopropyl)amino]butyl}amino)propyl]acetamide (three-letter code: SP5) (formula:  $C_{12}H_{28}N_4O$ ).



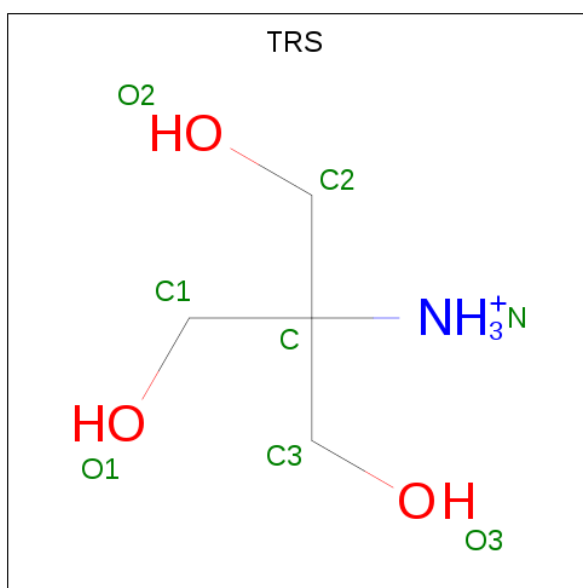
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	12	4	1		
3	B	1	Total	C	N	O	0	1
			25	18	6	1		
3	D	1	Total	C	N	O	0	0
			17	12	4	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



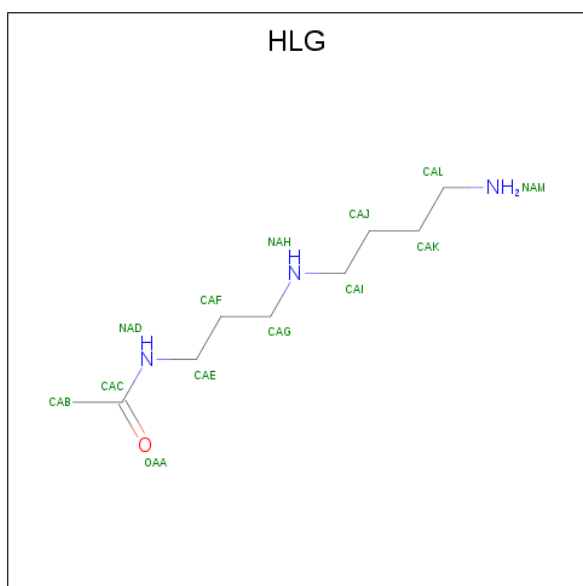
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			8	4	1	3		
5	B	1	Total	C	N	O	0	1
			8	4	1	3		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is N-{3-[(4-aminobutyl)amino]propyl}acetamide (three-letter code: HLG) (formula: C<sub>9</sub>H<sub>21</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			13	9	3	1		

- Molecule 8 is water.

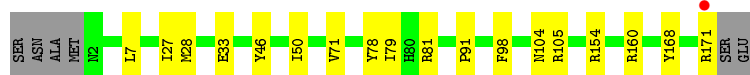
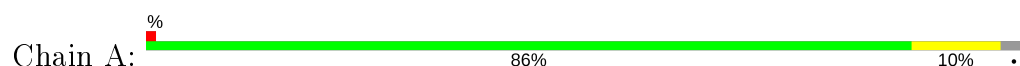
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	243	Total	O	0	15
			253	253		
8	B	240	Total	O	0	13
			246	246		
8	C	267	Total	O	0	13
			276	276		
8	D	259	Total	O	0	10
			268	268		
8	E	232	Total	O	0	8
			239	239		
8	F	228	Total	O	0	6
			231	231		



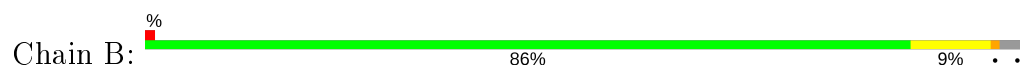
### 3 Residue-property plots [i](#)

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

- Molecule 1: Spermidine N(1)-acetyltransferase



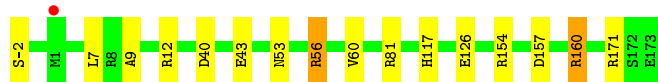
- Molecule 1: Spermidine N(1)-acetyltransferase



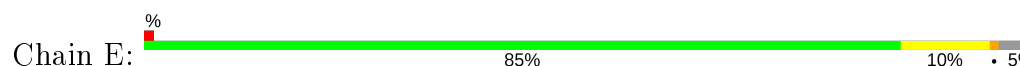
- Molecule 1: Spermidine N(1)-acetyltransferase



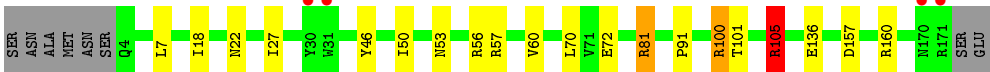
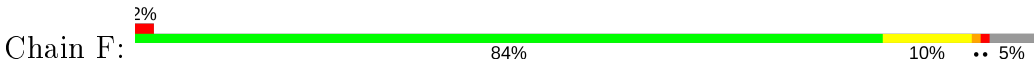
- Molecule 1: Spermidine N(1)-acetyltransferase



- Molecule 1: Spermidine N(1)-acetyltransferase



- Molecule 1: Spermidine N(1)-acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.98Å 186.50Å 73.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.35 29.29 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-1.35) 98.4 (29.29-1.35)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.123 , 0.151 0.123 , 0.151	Depositor DCC
$R_{free}$ test set	13914 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	11159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.45% 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: MPD, SP5, MRD, SPM, HLG, TRS

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	0.72	0/1593	0.97	8/2152 (0.4%)
1	B	0.70	0/1592	1.01	8/2152 (0.4%)
1	C	0.76	0/1622	0.94	8/2188 (0.4%)
1	D	0.78	0/1604	0.95	7/2162 (0.3%)
1	E	0.79	2/1611 (0.1%)	1.00	9/2177 (0.4%)
1	F	0.87	3/1605 (0.2%)	1.01	7/2167 (0.3%)
All	All	0.77	5/9627 (0.1%)	0.98	47/12998 (0.4%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	81[A]	ARG	CZ-NH2	-8.59	1.21	1.33
1	F	81[B]	ARG	CZ-NH2	-8.59	1.21	1.33
1	E	81[A]	ARG	CZ-NH1	-5.24	1.26	1.33
1	E	81[B]	ARG	CZ-NH1	-5.24	1.26	1.33
1	F	105	ARG	CB-CG	-5.00	1.39	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105[A]	ARG	NE-CZ-NH1	12.25	126.42	120.30
1	B	105[B]	ARG	NE-CZ-NH1	12.25	126.42	120.30
1	B	105[A]	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	B	105[B]	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	105[A]	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	105[B]	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	105[A]	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	105[B]	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	E	81[A]	ARG	NE-CZ-NH1	-8.81	115.89	120.30
1	E	81[B]	ARG	NE-CZ-NH1	-8.81	115.89	120.30
1	F	81[A]	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	F	81[B]	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	A	81	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	B	81	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	C	70[A]	LEU	CB-CG-CD1	-7.55	98.16	111.00
1	C	70[B]	LEU	CB-CG-CD1	-7.55	98.16	111.00
1	D	81[A]	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	81[B]	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	81	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	D	56	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	C	40	ASP	CB-CG-OD1	-6.62	112.35	118.30
1	D	160	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	C	56	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	D	40	ASP	CB-CG-OD1	-6.24	112.68	118.30
1	C	160	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	E	105	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	B	81	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	28	MET	CG-SD-CE	-5.70	91.08	100.20
1	F	105	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	E	81[A]	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	E	81[B]	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	A	28	MET	CG-SD-CE	-5.44	91.50	100.20
1	E	16	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	F	105	ARG	CG-CD-NE	-5.38	100.50	111.80
1	A	81	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	98	PHE	CB-CG-CD1	5.35	124.55	120.80
1	E	157	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	F	81[A]	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	F	81[B]	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	D	157	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	160	ARG	CG-CD-NE	5.17	122.65	111.80
1	E	105	ARG	CG-CD-NE	-5.16	100.97	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	157	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	98	PHE	CB-CG-CD1	5.14	124.40	120.80
1	E	8	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	160	ARG	CG-CD-NE	5.05	122.42	111.80
1	C	157	ASP	CB-CG-OD2	-5.05	113.75	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ARG	Sidechain
1	B	160	ARG	Sidechain
1	C	160	ARG	Sidechain
1	D	160	ARG	Sidechain
1	E	160	ARG	Sidechain
1	F	160	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1557	0	1504	10	0
1	B	1557	0	1503	11	0
1	C	1588	0	1535	11	0
1	D	1570	0	1523	9	0
1	E	1576	0	1538	12	0
1	F	1570	0	1538	14	1
2	A	14	0	26	3	0
2	B	14	0	26	3	0
2	C	24	0	43	2	0
2	D	14	0	26	0	0
2	E	10	0	17	0	0
3	A	17	0	28	1	0
3	B	25	0	34	0	0
3	D	17	0	28	0	0
4	A	8	0	14	0	0
4	C	16	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	16	0	28	0	0
5	A	8	0	12	0	0
5	B	8	0	12	3	0
6	B	8	0	14	0	0
6	C	8	0	14	0	0
6	D	8	0	14	0	0
7	C	13	0	0	0	0
8	A	253	0	0	3	0
8	B	246	0	0	6	0
8	C	276	0	0	3	0
8	D	268	0	0	2	1
8	E	239	0	0	3	0
8	F	231	0	0	3	0
All	All	11159	0	9505	72	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 4.

All (72) 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:18[A]:ILE:CD1	1:F:70:LEU:HD21	2.11	0.80
1:B:104[A]:ASN:ND2	8:B:303:HOH:O	2.24	0.69
2:C:201:SPM:N1	8:C:301[A]:HOH:O	2.27	0.67
1:F:81[B]:ARG:NH2	8:F:202:HOH:O	2.28	0.65
1:E:81[B]:ARG:NH2	8:E:303:HOH:O	2.32	0.63
1:E:37[A]:GLU:HG2	1:E:41:GLU:OE2	1.99	0.62
1:E:27[A]:ILE:HD11	1:E:91:PRO:HD3	1.81	0.62
1:A:33[A]:GLU:HG2	2:A:201:SPM:H42	1.81	0.62
1:A:33[A]:GLU:CG	2:A:201:SPM:H42	2.31	0.61
1:E:105:ARG:NH2	8:E:302:HOH:O	2.31	0.59
1:C:59:VAL:HG12	1:C:70[A]:LEU:CD2	2.32	0.59
1:E:37[A]:GLU:OE2	1:E:42:LEU:HD23	2.04	0.58
1:A:7:LEU:HD21	1:A:71[B]:VAL:HG21	1.86	0.57
3:A:202:SP5:NAM	8:A:303:HOH:O	2.24	0.57
1:D:7[A]:LEU:HD23	1:D:60:VAL:HG22	1.87	0.57
1:F:18[A]:ILE:CD1	1:F:70:LEU:CD2	2.82	0.56
1:F:57[B]:ARG:NH2	1:F:72:GLU:OE2	2.39	0.56
1:C:7[A]:LEU:HD23	1:C:60:VAL:HG22	1.88	0.54
1:F:81[B]:ARG:CZ	8:F:202:HOH:O	2.56	0.54
1:B:33[B]:GLU:CG	2:B:201:SPM:H42	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD23	1:B:60:VAL:HG22	1.91	0.53
1:F:7[A]:LEU:HD23	1:F:60:VAL:HG22	1.91	0.53
1:E:57[B]:ARG:NH1	1:E:72:GLU:OE2	2.42	0.52
1:E:81[B]:ARG:CZ	8:E:303:HOH:O	2.58	0.52
1:E:7[A]:LEU:HD23	1:E:60:VAL:HG22	1.91	0.52
1:D:12[B]:ARG:HD3	1:D:43:GLU:OE1	2.11	0.51
1:F:27[B]:ILE:HD11	1:F:91:PRO:HD3	1.93	0.51
1:A:104[A]:ASN:ND2	8:A:306:HOH:O	2.45	0.50
1:C:59:VAL:HG12	1:C:70[A]:LEU:HD23	1.93	0.50
1:E:37[A]:GLU:OE2	1:E:42:LEU:CD2	2.60	0.49
1:F:18[A]:ILE:HD13	1:F:70:LEU:HD21	1.93	0.49
1:C:12[B]:ARG:HD3	1:C:43:GLU:OE1	2.13	0.48
1:C:117[B]:HIS:ND1	8:C:302:HOH:O	2.30	0.48
1:D:53:ASN:HD21	1:D:56:ARG:HH12	1.62	0.47
5:B:204[B]:TRS:O3	5:B:204[B]:TRS:O2	2.10	0.47
1:A:78:TYR:CE2	1:A:79:ILE:HG13	2.49	0.47
1:F:101[B]:THR:HG23	8:F:207:HOH:O	2.14	0.47
1:E:37[A]:GLU:CG	1:E:41:GLU:OE2	2.62	0.47
1:D:9:ALA:HB2	1:E:36:TYR:O	2.15	0.47
1:A:168:TYR:O	1:A:171:ARG:NE	2.40	0.47
1:A:27[B]:ILE:HD11	1:A:91:PRO:HD3	1.97	0.47
5:B:204[B]:TRS:C3	8:B:361[B]:HOH:O	2.62	0.47
1:B:70[A]:LEU:HD12	1:B:70[A]:LEU:C	2.36	0.47
1:C:33[B]:GLU:HG2	2:C:201:SPM:H42	1.98	0.46
1:B:27[A]:ILE:HD11	1:B:91:PRO:HD3	1.98	0.46
1:A:33[A]:GLU:HG2	2:A:201:SPM:H21	1.97	0.46
1:A:46:TYR:CE2	1:A:50[B]:ILE:HD11	2.50	0.46
1:B:78:TYR:CE2	1:B:79:ILE:HG13	2.49	0.46
2:B:201:SPM:N1	8:B:305:HOH:O	2.36	0.45
1:C:89[B]:ILE:HD13	1:C:102:LEU:HD22	1.99	0.45
1:C:12[A]:ARG:HH11	1:C:12[A]:ARG:HG3	1.82	0.45
1:C:17:PHE:HE2	1:C:70[A]:LEU:HD21	1.81	0.45
1:F:18[A]:ILE:HD11	1:F:70:LEU:HD21	1.95	0.45
1:B:105[A]:ARG:HD3	8:B:303:HOH:O	2.16	0.44
1:B:7:LEU:CD2	1:B:60:VAL:HG22	2.47	0.44
1:A:33[B]:GLU:OE1	8:A:301[B]:HOH:O	2.21	0.44
1:D:126:GLU:OE1	1:D:154[B]:ARG:NH2	2.47	0.44
1:D:117[C]:HIS:CE1	8:D:323:HOH:O	2.70	0.43
1:B:33[B]:GLU:HG2	2:B:201:SPM:H42	1.99	0.43
1:C:117[A]:HIS:CD2	8:C:375:HOH:O	2.70	0.43
1:B:46:TYR:CE2	1:B:50[B]:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:204[B]:TRS:H31	8:B:361[B]:HOH:O	2.18	0.42
1:D:117[C]:HIS:HE1	8:D:460:HOH:O	2.00	0.42
1:B:33[A]:GLU:OE1	8:B:301[A]:HOH:O	2.22	0.42
1:E:46:TYR:CE2	1:E:50[B]:ILE:HD11	2.54	0.42
1:F:100[B]:ARG:NH2	1:F:136:GLU:OE1	2.50	0.42
1:F:57[B]:ARG:HD3	1:F:72:GLU:OE1	2.20	0.42
1:C:12[A]:ARG:HG3	1:C:12[A]:ARG:NH1	2.35	0.42
1:F:46:TYR:CE2	1:F:50[B]:ILE:HD11	2.55	0.41
1:D:12[A]:ARG:HG3	1:D:12[A]:ARG:HH11	1.85	0.41
1:D:53:ASN:ND2	1:D:56:ARG:HH12	2.19	0.40
1:F:53:ASN:ND2	1:F:56:ARG:HH12	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ARG:NH1	8:D:317:HOH:O[8_447]	2.19	0.01

## 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	182/176 (103%)	182 (100%)	0	0	100	100
1	B	182/176 (103%)	182 (100%)	0	0	100	100
1	C	187/176 (106%)	187 (100%)	0	0	100	100
1	D	184/176 (104%)	184 (100%)	0	0	100	100
1	E	182/176 (103%)	181 (100%)	1 (0%)	0	100	100
1	F	182/176 (103%)	181 (100%)	1 (0%)	0	100	100
All	All	1099/1056 (104%)	1097 (100%)	2 (0%)	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	168/159 (106%)	167 (99%)	1 (1%)	86	69
1	B	168/159 (106%)	167 (99%)	1 (1%)	86	69
1	C	172/159 (108%)	171 (99%)	1 (1%)	86	69
1	D	169/159 (106%)	167 (99%)	2 (1%)	71	42
1	E	169/159 (106%)	168 (99%)	1 (1%)	86	69
1	F	168/159 (106%)	164 (98%)	4 (2%)	49	15
All	All	1014/954 (106%)	1004 (99%)	10 (1%)	76	49

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

Mol	Chain	Res	Type
1	A	154	ARG
1	B	154	ARG
1	C	-2	SER
1	D	-2	SER
1	D	171	ARG
1	E	22	ASN
1	F	22	ASN
1	F	100[A]	ARG
1	F	100[B]	ARG
1	F	105	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	B	26	ASN
1	B	127	ASN
1	C	20	ASN

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Mol	Chain	Res	Type
1	C	66	ASN
1	D	2	ASN
1	D	20	ASN
1	D	53	ASN
1	F	53	ASN
1	F	170	ASN

### 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 monosaccharides 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	$\# Z  > 2$
7	HLG	C	203	-	12,12,12	0.44	0	12,12,12	0.59	0
2	SPM	E	201	-	9,9,13	0.46	0	8,8,12	1.06	1 (12%)
4	MRD	A	203	-	7,7,7	0.55	0	9,10,10	0.61	0
5	TRS	A	204[A]	-	7,7,7	0.40	0	9,9,9	0.66	0
2	SPM	B	201	-	13,13,13	0.49	0	12,12,12	0.84	0
2	SPM	A	201	-	13,13,13	0.49	0	12,12,12	0.77	0
4	MRD	C	205	-	7,7,7	0.40	0	9,10,10	0.85	0
4	MRD	D	204	-	7,7,7	0.47	0	9,10,10	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MPD	D	205	-	7,7,7	0.26	0	9,10,10	0.42	0
2	SPM	C	202	-	9,9,13	0.35	0	8,8,12	0.90	1 (12%)
3	SP5	D	202	-	16,16,16	0.46	0	16,16,16	0.83	1 (6%)
3	SP5	B	202[B]	-	16,16,16	0.34	0	16,16,16	0.79	0
3	SP5	A	202	-	16,16,16	0.55	0	16,16,16	1.22	2 (12%)
6	MPD	C	206	-	7,7,7	0.28	0	9,10,10	0.32	0
4	MRD	D	203	-	7,7,7	0.22	0	9,10,10	0.48	0
6	MPD	B	203	-	7,7,7	0.57	0	9,10,10	0.49	0
3	SP5	B	202[A]	-	16,16,16	0.46	0	16,16,16	0.92	1 (6%)
5	TRS	B	204[B]	-	7,7,7	0.48	0	9,9,9	1.07	0
4	MRD	C	204	-	7,7,7	0.21	0	9,10,10	0.56	0
2	SPM	D	201	-	13,13,13	0.52	0	12,12,12	1.21	3 (25%)
2	SPM	C	201	-	13,13,13	0.57	0	12,12,12	1.05	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
7	HLG	C	203	-	-	0/10/10/10	-
2	SPM	E	201	-	-	2/7/7/11	-
4	MRD	A	203	-	-	1/5/5/5	-
5	TRS	A	204[A]	-	-	9/9/9/9	-
2	SPM	B	201	-	-	1/11/11/11	-
2	SPM	A	201	-	-	1/11/11/11	-
4	MRD	C	205	-	-	0/5/5/5	-
4	MRD	D	204	-	-	0/5/5/5	-
6	MPD	D	205	-	-	2/5/5/5	-
2	SPM	C	202	-	-	0/7/7/11	-
3	SP5	D	202	-	-	4/14/14/14	-
3	SP5	B	202[B]	-	-	6/14/14/14	-
3	SP5	A	202	-	-	6/14/14/14	-
6	MPD	C	206	-	-	0/5/5/5	-
4	MRD	D	203	-	-	0/5/5/5	-
6	MPD	B	203	-	-	2/5/5/5	-
3	SP5	B	202[A]	-	-	3/14/14/14	-
5	TRS	B	204[B]	-	-	7/9/9/9	-
4	MRD	C	204	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SPM	D	201	-	-	1/11/11/11	-
2	SPM	C	201	-	-	1/11/11/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	SP5	CAN-NAM-CAL	3.06	127.90	113.45
3	A	202	SP5	CAO-CAN-NAM	2.67	119.35	112.14
3	D	202	SP5	CAE-NAD-CAC	2.20	125.95	122.56
2	D	201	SPM	C3-C4-N5	-2.13	106.38	112.14
3	B	202[A]	SP5	CAO-CAN-NAM	2.13	117.89	112.14
2	C	202	SPM	C11-C12-C13	-2.09	106.63	114.28
2	D	201	SPM	C7-C6-N5	2.07	117.72	112.14
2	E	201	SPM	C11-C12-C13	-2.06	106.74	114.28
2	D	201	SPM	C4-C3-C2	-2.04	106.81	114.28

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	204[B]	TRS	C1-C-C2-O2
5	B	204[B]	TRS	C3-C-C2-O2
5	B	204[B]	TRS	N-C-C2-O2
5	B	204[B]	TRS	C1-C-C3-O3
5	B	204[B]	TRS	C2-C-C3-O3
5	B	204[B]	TRS	N-C-C3-O3
6	D	205	MPD	C2-C3-C4-O4
6	B	203	MPD	C2-C3-C4-O4
5	A	204[A]	TRS	C2-C-C1-O1
5	A	204[A]	TRS	C3-C-C1-O1
5	A	204[A]	TRS	N-C-C1-O1
5	A	204[A]	TRS	C1-C-C2-O2
5	A	204[A]	TRS	C3-C-C2-O2
5	A	204[A]	TRS	C2-C-C3-O3
3	B	202[A]	SP5	CAI-CAJ-CAK-CAL
3	B	202[B]	SP5	CAJ-CAK-CAL-NAM
2	C	201	SPM	C2-C3-C4-N5
3	A	202	SP5	CAJ-CAK-CAL-NAM
3	D	202	SP5	CAJ-CAK-CAL-NAM
2	B	201	SPM	C2-C3-C4-N5

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Mol	Chain	Res	Type	Atoms
2	A	201	SPM	C2-C3-C4-N5
2	D	201	SPM	C2-C3-C4-N5
3	D	202	SP5	CAK-CAL-NAM-CAN
3	B	202[B]	SP5	NAH-CAI-CAJ-CAK
3	D	202	SP5	NAM-CAN-CAO-CAP
3	B	202[B]	SP5	NAM-CAN-CAO-CAP
3	A	202	SP5	CAK-CAL-NAM-CAN
2	E	201	SPM	C7-C8-C9-N10
3	A	202	SP5	NAH-CAI-CAJ-CAK
5	A	204[A]	TRS	C1-C-C3-O3
3	B	202[A]	SP5	CAO-CAN-NAM-CAL
3	A	202	SP5	CAI-CAJ-CAK-CAL
3	A	202	SP5	NAM-CAN-CAO-CAP
3	B	202[B]	SP5	CAN-CAO-CAP-NAQ
3	B	202[B]	SP5	CAK-CAL-NAM-CAN
5	A	204[A]	TRS	N-C-C2-O2
4	A	203	MRD	C2-C3-C4-C5
6	D	205	MPD	C2-C3-C4-C5
6	B	203	MPD	C2-C3-C4-C5
2	E	201	SPM	N5-C6-C7-C8
3	B	202[A]	SP5	NAM-CAN-CAO-CAP
5	B	204[B]	TRS	C3-C-C1-O1
3	B	202[B]	SP5	CAO-CAN-NAM-CAL
3	D	202	SP5	CAN-CAO-CAP-NAQ
5	A	204[A]	TRS	N-C-C3-O3
3	A	202	SP5	CAO-CAN-NAM-CAL

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	SPM	3	0
2	A	201	SPM	3	0
3	A	202	SP5	1	0
5	B	204[B]	TRS	3	0
2	C	201	SPM	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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	170/176 (96%)	-0.49	1 (0%) 89 91	10, 14, 31, 54	0
1	B	169/176 (96%)	-0.48	1 (0%) 89 91	10, 14, 30, 54	0
1	C	176/176 (100%)	-0.50	0 100 100	9, 14, 28, 40	0
1	D	176/176 (100%)	-0.53	1 (0%) 89 91	9, 14, 28, 40	0
1	E	168/176 (95%)	-0.30	2 (1%) 79 83	10, 15, 41, 57	0
1	F	168/176 (95%)	-0.32	4 (2%) 59 65	10, 15, 38, 57	0
All	All	1027/1056 (97%)	-0.44	9 (0%) 84 87	9, 14, 33, 57	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ARG	3.5
1	F	171	ARG	2.6
1	E	171	ARG	2.6
1	F	31[A]	TRP	2.5
1	E	31[A]	TRP	2.5
1	F	30	TYR	2.4
1	B	3	SER	2.1
1	F	170	ASN	2.1
1	D	1	MET	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

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
6	MPD	C	206	8/8	0.67	0.14	49,50,51,53	0
5	TRS	B	204[B]	8/8	0.75	0.18	22,26,26,27	8
5	TRS	A	204[A]	8/8	0.79	0.16	21,24,24,25	8
4	MRD	A	203	8/8	0.84	0.15	26,29,41,45	0
6	MPD	D	205	8/8	0.85	0.11	55,56,57,57	0
4	MRD	D	204	8/8	0.86	0.15	22,25,26,26	8
4	MRD	D	203	8/8	0.87	0.12	23,25,26,26	0
4	MRD	C	204	8/8	0.88	0.10	23,25,26,26	0
6	MPD	B	203	8/8	0.89	0.14	25,29,40,41	0
4	MRD	C	205	8/8	0.90	0.15	24,29,29,30	0
2	SPM	C	202	10/14	0.92	0.11	14,21,34,37	0
3	SP5	A	202	17/17	0.93	0.12	13,18,53,55	0
2	SPM	E	201	10/14	0.93	0.11	14,21,35,36	0
3	SP5	B	202[A]	17/17	0.94	0.13	13,16,29,35	8
2	SPM	B	201	14/14	0.94	0.08	12,15,29,30	0
3	SP5	B	202[B]	17/17	0.94	0.13	13,18,31,34	8
2	SPM	A	201	14/14	0.95	0.07	12,15,29,32	0
2	SPM	D	201	14/14	0.95	0.07	13,17,35,40	0
2	SPM	C	201	14/14	0.96	0.06	13,17,36,41	0
3	SP5	D	202	17/17	0.97	0.08	12,16,63,64	0
7	HLG	C	203	13/13	0.97	0.07	13,14,35,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.