



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:30 PM UTC

PDB ID : 3WZ4 / pdb_00003wz4
Title : Structure of the periplasmic domain of DotI (crystal form I)
Authors : Kuroda, T.; Kubori, T.; Uchida, Y.; Nagai, H.; Imada, K.
Deposited on : 2014-09-18
Resolution : 2.20 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

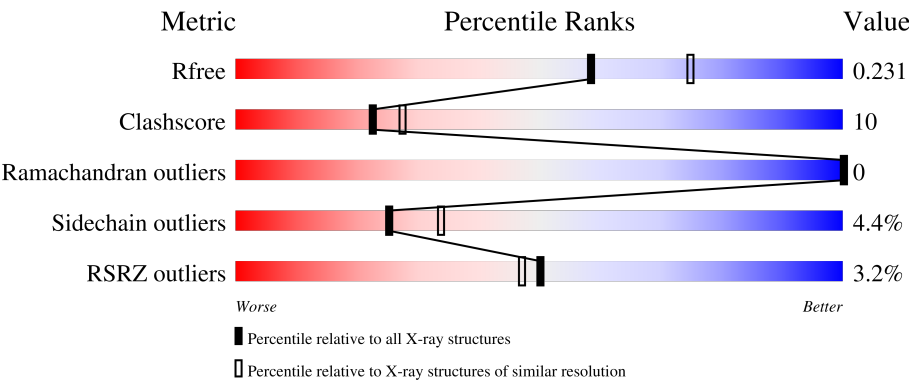
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	144	4% 83% 12% • 5%
1	B	144	3% 80% 13% • 5%
1	C	144	3% 81% 13% • •
1	D	144	% 78% 14% • 6%
1	E	144	3% 82% 12% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	144	 81% 11% 6%
1	G	144	 79% 17% 3%
1	H	144	 81% 15% 4%

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	MPD	A	503	-	-	X	-
3	MPD	B	503	-	-	X	-
3	MPD	C	503	-	-	X	-
3	MPD	E	503	-	-	X	-
3	MPD	G	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10090 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 DotI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	Se	0	2	0
			1075	684	189	199	3			
1	B	137	Total	C	N	O	Se	0	1	0
			1067	679	186	199	3			
1	C	139	Total	C	N	O	Se	0	1	0
			1077	684	188	202	3			
1	D	136	Total	C	N	O	Se	0	1	0
			1057	673	183	198	3			
1	E	139	Total	C	N	O	Se	0	1	0
			1077	684	188	202	3			
1	F	136	Total	C	N	O	Se	0	1	0
			1057	673	183	198	3			
1	G	140	Total	C	N	O	Se	0	1	0
			1083	687	189	204	3			
1	H	139	Total	C	N	O	Se	0	2	0
			1085	689	191	202	3			

There are 32 discrepancies between the modelled and reference sequences:

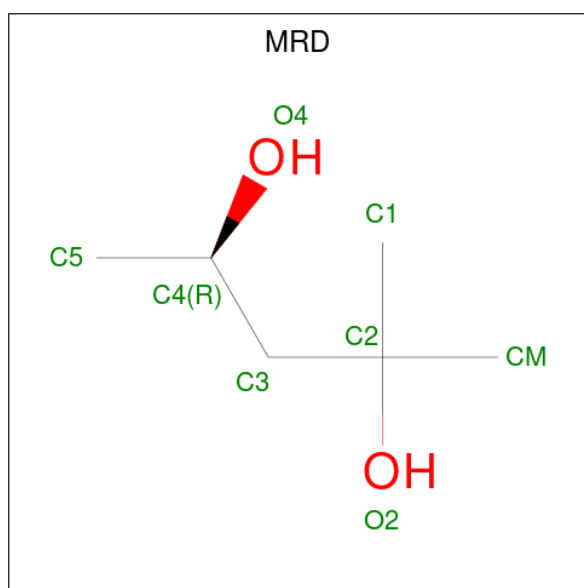
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLY	-	expression tag	UNP O54626
A	70	SER	-	expression tag	UNP O54626
A	71	HIS	-	expression tag	UNP O54626
A	72	MSE	-	expression tag	UNP O54626
B	69	GLY	-	expression tag	UNP O54626
B	70	SER	-	expression tag	UNP O54626
B	71	HIS	-	expression tag	UNP O54626
B	72	MSE	-	expression tag	UNP O54626
C	69	GLY	-	expression tag	UNP O54626
C	70	SER	-	expression tag	UNP O54626
C	71	HIS	-	expression tag	UNP O54626
C	72	MSE	-	expression tag	UNP O54626
D	69	GLY	-	expression tag	UNP O54626

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	SER	-	expression tag	UNP O54626
D	71	HIS	-	expression tag	UNP O54626
D	72	MSE	-	expression tag	UNP O54626
E	69	GLY	-	expression tag	UNP O54626
E	70	SER	-	expression tag	UNP O54626
E	71	HIS	-	expression tag	UNP O54626
E	72	MSE	-	expression tag	UNP O54626
F	69	GLY	-	expression tag	UNP O54626
F	70	SER	-	expression tag	UNP O54626
F	71	HIS	-	expression tag	UNP O54626
F	72	MSE	-	expression tag	UNP O54626
G	69	GLY	-	expression tag	UNP O54626
G	70	SER	-	expression tag	UNP O54626
G	71	HIS	-	expression tag	UNP O54626
G	72	MSE	-	expression tag	UNP O54626
H	69	GLY	-	expression tag	UNP O54626
H	70	SER	-	expression tag	UNP O54626
H	71	HIS	-	expression tag	UNP O54626
H	72	MSE	-	expression tag	UNP O54626

- Molecule 2 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

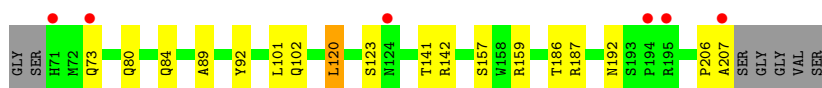
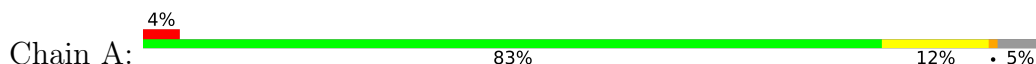
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total	O	0	0
			138	138		
4	B	169	Total	O	0	0
			169	169		
4	C	164	Total	O	0	0
			164	164		
4	D	165	Total	O	0	0
			165	165		
4	E	151	Total	O	0	0
			151	151		
4	F	159	Total	O	0	0
			159	159		
4	G	169	Total	O	0	0
			169	169		
4	H	141	Total	O	0	0
			141	141		

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.

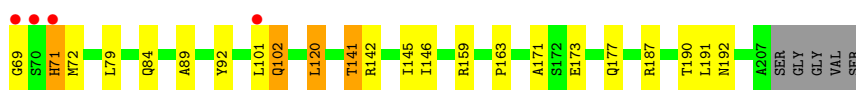
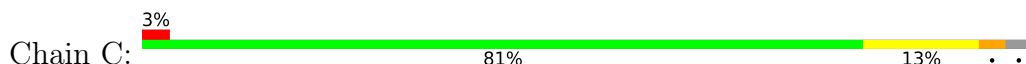
- Molecule 1: DotI



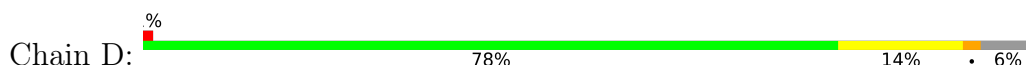
- Molecule 1: DotI



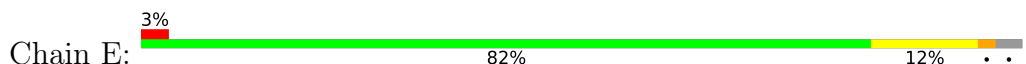
- Molecule 1: DotI



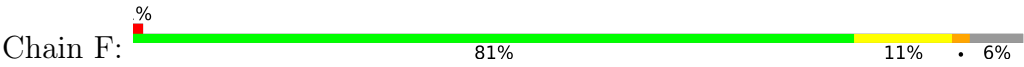
- Molecule 1: DotI



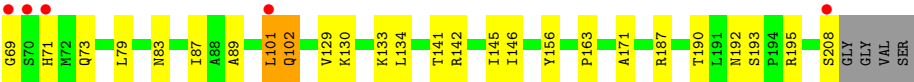
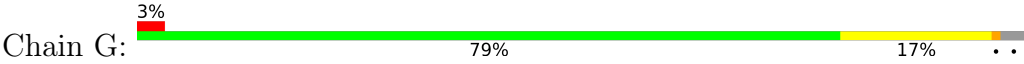
- Molecule 1: DotI



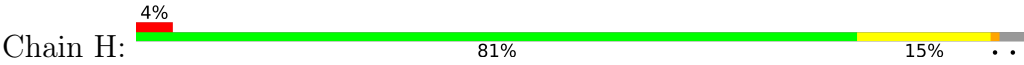
- Molecule 1: DotI



• Molecule 1: DotI



• Molecule 1: DotI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.59Å 207.58Å 58.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.42 – 2.20 37.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.42-2.20) 98.2 (37.42-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.191 , 0.235 0.191 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10090	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MPD, MRD

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	0.28	0/1099	0.67	0/1489
1	B	0.28	0/1088	0.67	0/1475
1	C	0.27	0/1098	0.68	0/1488
1	D	0.27	0/1078	0.67	0/1463
1	E	0.27	0/1098	0.67	0/1488
1	F	0.27	0/1078	0.68	1/1463 (0.1%)
1	G	0.28	0/1104	0.68	0/1496
1	H	0.27	0/1109	0.68	0/1502
All	All	0.27	0/8752	0.68	1/11864 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	169	GLN	N-CA-C	5.10	116.56	108.96

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	1075	0	1075	19	0
1	B	1067	0	1062	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1077	0	1070	24	0
1	D	1057	0	1055	24	0
1	E	1077	0	1070	24	0
1	F	1057	0	1055	19	0
1	G	1083	0	1075	26	0
1	H	1085	0	1083	17	0
2	A	16	0	28	3	0
2	B	16	0	28	3	0
2	C	16	0	28	3	0
2	D	16	0	28	6	0
2	E	16	0	28	5	0
2	F	16	0	28	1	0
2	G	16	0	28	4	0
2	H	16	0	28	3	0
3	A	16	0	28	8	0
3	B	16	0	28	6	0
3	C	16	0	28	7	0
3	D	16	0	28	6	0
3	E	16	0	28	8	0
3	F	16	0	28	3	0
3	G	16	0	28	6	0
3	H	16	0	28	5	0
4	A	138	0	0	5	0
4	B	169	0	0	7	0
4	C	164	0	0	4	0
4	D	165	0	0	11	0
4	E	151	0	0	5	0
4	F	159	0	0	2	0
4	G	169	0	0	6	0
4	H	141	0	0	5	0
All	All	10090	0	8993	187	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 10.

All (187) 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:B:102[B]:GLN:NE2	4:B:745:HOH:O	2.03	0.90
1:H:159[A]:ARG:NH2	4:H:670:HOH:O	2.09	0.85
2:G:502:MRD:O4	4:G:769:HOH:O	1.97	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159[B]:ARG:NH2	3:A:504:MPD:O2	2.13	0.81
1:C:102[A]:GLN:NE2	4:C:627:HOH:O	2.14	0.80
1:C:69:GLY:O	1:C:187:ARG:NH2	2.15	0.80
1:E:87:ILE:HG22	4:E:739:HOH:O	1.84	0.77
2:H:502:MRD:O4	4:H:741:HOH:O	2.01	0.77
1:E:142:ARG:HH11	1:E:142:ARG:HG2	1.50	0.76
1:D:177:GLN:NE2	4:D:616:HOH:O	2.19	0.75
1:D:101:LEU:HA	3:D:503:MPD:H11	1.68	0.75
1:C:173:GLU:OE2	2:C:501:MRD:H5C1	1.88	0.73
2:B:502:MRD:O4	4:B:619:HOH:O	2.06	0.72
2:A:502:MRD:O4	4:A:725:HOH:O	2.08	0.71
1:G:73:GLN:NE2	4:G:763:HOH:O	2.24	0.70
2:D:501:MRD:O2	2:D:501:MRD:O4	2.05	0.70
1:G:129:VAL:HA	1:G:134:LEU:HD12	1.72	0.70
1:G:69:GLY:O	1:G:187:ARG:NH2	2.25	0.69
1:H:159[B]:ARG:NH1	3:H:504:MPD:O2	2.25	0.69
1:E:102[B]:GLN:HG2	1:F:145:ILE:HA	1.75	0.69
1:B:101:LEU:HA	3:B:503:MPD:H11	1.75	0.68
1:F:142:ARG:HG2	1:F:142:ARG:HH11	1.57	0.68
1:B:89:ALA:O	2:B:502:MRD:H5C1	1.93	0.68
3:C:503:MPD:O4	3:C:503:MPD:O2	2.07	0.67
1:D:133:LYS:HD2	1:E:171:ALA:HA	1.77	0.67
1:D:159:ARG:HD2	4:D:756:HOH:O	1.95	0.67
1:D:189:SER:O	4:D:765:HOH:O	2.12	0.67
1:A:101:LEU:HB2	3:A:503:MPD:H52	1.78	0.66
1:G:89:ALA:O	2:G:502:MRD:H5C1	1.96	0.66
1:H:195:ARG:NH2	4:H:703:HOH:O	2.28	0.66
1:D:89:ALA:O	2:D:502:MRD:H5C1	1.95	0.66
1:H:92:TYR:CD1	3:H:503:MPD:HM1	2.31	0.65
2:B:501:MRD:O4	2:B:501:MRD:O2	2.13	0.65
1:D:148:GLN:OE1	4:D:756:HOH:O	2.14	0.64
1:D:101:LEU:HA	3:D:503:MPD:C1	2.26	0.64
1:D:134:LEU:HD11	2:D:501:MRD:H5C3	1.79	0.64
1:E:142:ARG:HG2	1:E:142:ARG:NH1	2.10	0.64
2:E:502:MRD:H5C1	3:E:503:MPD:O2	1.98	0.64
1:C:69:GLY:N	1:C:190:THR:HG1	1.96	0.63
1:B:126:LEU:O	1:B:130:LYS:HG3	1.99	0.63
1:F:142:ARG:HG2	1:F:142:ARG:NH1	2.14	0.62
1:E:159:ARG:NE	4:E:682:HOH:O	2.31	0.62
1:F:102[B]:GLN:HG2	1:G:145:ILE:HA	1.81	0.62
1:H:148:GLN:OE1	1:H:159[B]:ARG:NH2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HA	3:C:503:MPD:H11	1.81	0.61
1:B:194:PRO:HB3	4:B:712:HOH:O	2.01	0.61
1:D:126:LEU:O	1:D:130:LYS:HG3	2.00	0.61
1:B:101:LEU:HA	3:B:503:MPD:C1	2.30	0.61
1:A:101:LEU:HA	3:A:503:MPD:H31	1.81	0.60
1:C:102[B]:GLN:HG2	1:D:145:ILE:HA	1.82	0.60
2:A:501:MRD:O2	2:A:501:MRD:O4	2.20	0.60
1:E:101:LEU:HA	3:E:503:MPD:H11	1.83	0.59
1:G:102[B]:GLN:HG2	1:H:145:ILE:HA	1.82	0.59
1:D:159:ARG:NE	4:D:642:HOH:O	2.30	0.59
1:H:89:ALA:O	2:H:502:MRD:H5C1	2.02	0.59
1:D:138:ALA:O	4:D:747:HOH:O	2.17	0.58
1:G:69:GLY:N	1:G:190:THR:HG1	2.02	0.58
1:A:101:LEU:CA	3:A:503:MPD:H31	2.33	0.58
3:E:503:MPD:O2	3:E:503:MPD:O4	2.19	0.58
1:F:187:ARG:NH1	4:F:654:HOH:O	2.37	0.57
3:F:503:MPD:O4	3:F:503:MPD:O2	2.23	0.57
1:A:142:ARG:NH1	4:A:727:HOH:O	2.37	0.57
1:C:84:GLN:HB2	4:C:723:HOH:O	2.04	0.56
1:C:89:ALA:O	2:C:502:MRD:H5C1	2.05	0.56
1:A:192:ASN:ND2	4:A:659:HOH:O	2.31	0.56
2:E:501:MRD:O4	2:E:501:MRD:O2	2.17	0.56
1:G:192:ASN:HB2	4:G:661:HOH:O	2.06	0.56
1:A:92:TYR:CD1	3:A:503:MPD:HM1	2.41	0.56
3:G:503:MPD:O4	3:G:503:MPD:O2	2.19	0.55
3:A:503:MPD:O4	3:A:503:MPD:O2	2.24	0.55
1:E:190:THR:HA	1:E:193:SER:O	2.06	0.55
1:B:102[A]:GLN:HG2	1:C:145:ILE:HA	1.88	0.55
1:B:71:HIS:HB3	1:B:187:ARG:NH2	2.23	0.54
4:B:712:HOH:O	1:C:72:MSE:HE2	2.06	0.54
1:F:101:LEU:HA	3:F:503:MPD:H11	1.89	0.54
1:F:157:SER:OG	1:F:186:THR:HG22	2.08	0.54
1:C:101:LEU:HA	3:C:503:MPD:C1	2.38	0.54
1:F:126:LEU:O	1:F:130:LYS:HG3	2.08	0.53
1:H:190:THR:HA	1:H:193:SER:O	2.07	0.53
1:G:190:THR:HA	1:G:193:SER:O	2.08	0.53
1:H:156:TYR:H	1:H:187:ARG:HH21	1.55	0.53
1:A:102[A]:GLN:HG2	1:B:145:ILE:HA	1.91	0.52
1:B:132:LYS:HD3	1:B:173:GLU:OE1	2.10	0.52
1:H:101:LEU:HA	3:H:503:MPD:H11	1.91	0.52
1:H:101:LEU:HA	3:H:503:MPD:C1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD12	2:D:502:MRD:H3C2	1.91	0.52
1:G:101:LEU:HA	3:G:503:MPD:H31	1.91	0.52
1:C:159:ARG:NH2	4:C:727:HOH:O	2.37	0.52
1:G:195:ARG:HG2	4:G:723:HOH:O	2.10	0.52
1:B:124:ASN:HB2	4:B:669:HOH:O	2.10	0.51
2:F:501:MRD:O4	2:F:501:MRD:O2	2.27	0.51
1:G:130:LYS:HE2	4:H:679:HOH:O	2.10	0.51
1:C:79:LEU:HD21	1:C:146:ILE:HG13	1.93	0.51
1:H:129:VAL:HA	1:H:134:LEU:HD12	1.92	0.51
1:E:69:GLY:HA3	1:E:190:THR:OG1	2.11	0.50
1:G:156:TYR:HB3	1:G:187:ARG:HD3	1.94	0.50
2:C:501:MRD:O4	2:C:501:MRD:O2	2.13	0.50
1:D:155:ARG:NE	4:D:658:HOH:O	2.42	0.49
1:E:190:THR:O	4:E:720:HOH:O	2.20	0.49
1:A:101:LEU:HA	3:A:503:MPD:C1	2.42	0.49
1:E:120:LEU:HD11	3:E:503:MPD:H4	1.94	0.49
1:E:142:ARG:HH11	1:E:142:ARG:CG	2.22	0.49
1:C:101:LEU:CA	3:C:503:MPD:H31	2.43	0.49
1:B:101:LEU:HB2	3:B:503:MPD:H52	1.95	0.49
1:E:101:LEU:CA	3:E:503:MPD:H31	2.41	0.49
1:C:120:LEU:HD11	3:C:503:MPD:H4	1.95	0.49
1:C:141:THR:HG22	1:C:163:PRO:HG2	1.93	0.49
1:G:192:ASN:ND2	4:G:691:HOH:O	2.22	0.48
1:G:101:LEU:CA	3:G:503:MPD:H31	2.44	0.48
2:E:501:MRD:H2	2:E:501:MRD:HA	1.57	0.48
1:B:171:ALA:HA	1:G:133:LYS:HD2	1.96	0.48
2:H:501:MRD:O4	2:H:501:MRD:O2	2.29	0.48
3:D:504:MPD:O2	4:D:756:HOH:O	2.20	0.47
2:G:501:MRD:O4	2:G:501:MRD:O2	2.32	0.47
1:D:180:VAL:HG23	1:D:207:ALA:HA	1.97	0.47
1:A:89:ALA:O	2:A:502:MRD:H5C1	2.14	0.47
1:A:206:PRO:O	1:A:207:ALA:C	2.58	0.47
1:F:142:ARG:HH11	1:F:142:ARG:CG	2.26	0.47
1:G:101:LEU:HA	3:G:503:MPD:H11	1.96	0.47
1:E:114:ASP:OD1	4:E:627:HOH:O	2.20	0.46
1:A:157:SER:OG	1:A:186:THR:HG22	2.14	0.46
1:D:152:LEU:HD22	3:D:504:MPD:HM1	1.96	0.46
1:B:159:ARG:NH2	4:B:657:HOH:O	2.39	0.46
3:B:503:MPD:O4	3:B:503:MPD:O2	2.32	0.46
1:E:142:ARG:NH1	4:E:687:HOH:O	2.41	0.46
1:A:192:ASN:HB2	4:A:637:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:LEU:HA	3:E:503:MPD:H31	1.98	0.45
1:B:101:LEU:CA	3:B:503:MPD:H31	2.45	0.45
1:C:69:GLY:C	1:C:71:HIS:H	2.24	0.45
1:A:101:LEU:HA	3:A:503:MPD:H11	1.98	0.45
2:D:502:MRD:H5C3	3:D:503:MPD:O2	2.16	0.45
1:C:92:TYR:CD1	3:C:503:MPD:HM1	2.52	0.45
1:G:134:LEU:HD11	2:G:501:MRD:H5C2	1.99	0.45
1:F:102[B]:GLN:CD	1:G:146:ILE:H	2.25	0.45
1:A:73:GLN:HG2	1:A:187:ARG:HH11	1.81	0.45
1:F:192:ASN:OD1	1:G:187:ARG:HD2	2.17	0.45
1:A:120:LEU:HD22	1:A:120:LEU:O	2.17	0.44
1:G:83:ASN:O	1:G:87:ILE:HG12	2.18	0.44
1:D:134:LEU:CD1	2:D:501:MRD:H5C3	2.46	0.44
1:E:157:SER:OG	1:E:186:THR:HG22	2.17	0.44
1:A:80:GLN:O	1:A:84:GLN:HG3	2.18	0.44
1:E:71:HIS:HB2	1:E:190:THR:HG21	2.00	0.44
1:G:79:LEU:HD21	1:G:146:ILE:HG13	1.99	0.44
1:H:97:TYR:CZ	1:H:130:LYS:HD3	2.53	0.43
1:B:92:TYR:CD1	3:B:503:MPD:HM1	2.53	0.43
1:E:101:LEU:HA	3:E:503:MPD:C1	2.47	0.43
3:D:503:MPD:O2	3:D:503:MPD:O4	2.35	0.43
1:B:142:ARG:NE	4:B:754:HOH:O	2.41	0.43
1:C:101:LEU:HA	3:C:503:MPD:H31	2.00	0.43
1:F:99:ASP:OD2	4:F:619:HOH:O	2.21	0.43
1:B:133:LYS:HD2	1:G:171:ALA:HA	2.00	0.43
1:E:141:THR:O	1:E:142:ARG:HG3	2.18	0.43
1:G:141:THR:HG22	1:G:163:PRO:C	2.44	0.43
1:D:102[A]:GLN:NE2	4:D:635:HOH:O	2.52	0.42
1:E:79:LEU:HD21	1:E:146:ILE:HG13	2.01	0.42
1:H:159[A]:ARG:HG3	4:H:670:HOH:O	2.18	0.42
1:A:142:ARG:HG2	4:A:727:HOH:O	2.19	0.42
1:E:69:GLY:HA3	1:E:190:THR:H	1.84	0.42
1:H:193:SER:HA	1:H:194:PRO:HD2	1.81	0.42
1:C:192:ASN:HB2	4:C:672:HOH:O	2.19	0.42
1:B:193:SER:HA	1:B:194:PRO:HD2	1.84	0.42
1:C:171:ALA:HA	1:F:133:LYS:HD2	2.01	0.42
1:H:81:TRP:NE1	1:H:195:ARG:HG2	2.35	0.42
1:A:102[B]:GLN:HG3	1:B:79:LEU:HD13	2.02	0.42
1:H:132:LYS:HB2	1:H:134:LEU:HG	2.02	0.42
1:B:79:LEU:HD21	1:B:146:ILE:HG13	2.01	0.41
1:C:142:ARG:HB2	1:C:163:PRO:CG	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ARG:NH2	4:D:639:HOH:O	2.51	0.41
2:E:502:MRD:H1C3	2:E:502:MRD:H4	1.87	0.41
1:F:120:LEU:HD23	1:F:120:LEU:HA	1.83	0.41
1:G:101:LEU:HA	3:G:503:MPD:C1	2.51	0.41
1:F:101:LEU:HA	3:F:503:MPD:C1	2.51	0.41
1:D:142:ARG:NH1	4:D:746:HOH:O	2.54	0.41
3:G:503:MPD:HO2	3:G:503:MPD:HO4	1.61	0.41
1:E:102[A]:GLN:HG3	1:F:79:LEU:HD13	2.03	0.41
2:E:502:MRD:C5	3:E:503:MPD:O2	2.65	0.41
1:D:142:ARG:HB2	1:D:163:PRO:HG2	2.03	0.40
1:F:73:GLN:HG2	1:F:187:ARG:NH2	2.35	0.40
1:E:69:GLY:O	1:E:70:SER:HB2	2.21	0.40
1:G:141:THR:HG21	4:G:759:HOH:O	2.20	0.40
3:H:504:MPD:O2	3:H:504:MPD:O4	2.33	0.40
1:B:192:ASN:OD1	1:C:187:ARG:HD2	2.21	0.40
1:D:166:VAL:O	1:D:176:GLN:HA	2.21	0.40
1:B:102[A]:GLN:CD	1:C:146:ILE:H	2.30	0.40
1:F:142:ARG:HB2	1:F:163:PRO:CG	2.52	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	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
1	B	136/144 (94%)	134 (98%)	2 (2%)	0	100	100
1	C	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
1	D	135/144 (94%)	134 (99%)	1 (1%)	0	100	100
1	E	138/144 (96%)	137 (99%)	1 (1%)	0	100	100
1	F	135/144 (94%)	132 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
1	H	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
All	All	1097/1152 (95%)	1079 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	115/114 (101%)	112 (97%)	3 (3%)	40	55
1	B	114/114 (100%)	110 (96%)	4 (4%)	32	43
1	C	115/114 (101%)	108 (94%)	7 (6%)	17	20
1	D	113/114 (99%)	108 (96%)	5 (4%)	25	34
1	E	115/114 (101%)	108 (94%)	7 (6%)	17	20
1	F	113/114 (99%)	107 (95%)	6 (5%)	20	26
1	G	116/114 (102%)	110 (95%)	6 (5%)	21	26
1	H	116/114 (102%)	108 (93%)	8 (7%)	14	16
All	All	917/912 (100%)	871 (95%)	46 (5%)	25	28

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LEU
1	A	123	SER
1	A	141	THR
1	B	71	HIS
1	B	120	LEU
1	B	130	LYS
1	B	187	ARG
1	C	71	HIS
1	C	102[A]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	102[B]	GLN
1	C	120	LEU
1	C	141	THR
1	C	177	GLN
1	C	191	LEU
1	D	73	GLN
1	D	102[A]	GLN
1	D	102[B]	GLN
1	D	130	LYS
1	D	142	ARG
1	E	102[A]	GLN
1	E	102[B]	GLN
1	E	120	LEU
1	E	121	GLU
1	E	142	ARG
1	E	173	GLU
1	E	187	ARG
1	F	102[A]	GLN
1	F	102[B]	GLN
1	F	120	LEU
1	F	142	ARG
1	F	173	GLU
1	F	190	THR
1	G	71	HIS
1	G	101	LEU
1	G	102[A]	GLN
1	G	102[B]	GLN
1	G	142	ARG
1	G	208	SER
1	H	71	HIS
1	H	102[A]	GLN
1	H	102[B]	GLN
1	H	120	LEU
1	H	132	LYS
1	H	141	THR
1	H	142	ARG
1	H	187	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	84	GLN
1	B	176	GLN
1	B	179	ASN
1	C	71	HIS
1	C	80	GLN
1	C	125	ASN
1	C	179	ASN
1	D	84	GLN
1	D	148	GLN
1	D	161	GLN
1	D	176	GLN
1	D	177	GLN
1	D	179	ASN
1	E	125	ASN
1	E	176	GLN
1	F	80	GLN
1	F	176	GLN
1	F	179	ASN
1	G	73	GLN
1	G	161	GLN
1	H	125	ASN
1	H	161	GLN
1	H	179	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 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	$\# Z > 2$
2	MRD	D	501	-	7,7,7	0.30	0	9,10,10	0.24	0
2	MRD	H	502	-	7,7,7	0.29	0	9,10,10	0.36	0
2	MRD	F	502	-	7,7,7	0.34	0	9,10,10	0.36	0
3	MPD	H	504	-	7,7,7	0.29	0	9,10,10	0.23	0
2	MRD	G	501	-	7,7,7	0.33	0	9,10,10	0.25	0
3	MPD	H	503	-	7,7,7	0.30	0	9,10,10	0.23	0
3	MPD	D	504	-	7,7,7	0.29	0	9,10,10	0.23	0
3	MPD	G	504	-	7,7,7	0.28	0	9,10,10	0.29	0
2	MRD	D	502	-	7,7,7	0.31	0	9,10,10	0.38	0
2	MRD	C	501	-	7,7,7	0.31	0	9,10,10	0.26	0
3	MPD	B	504	-	7,7,7	0.27	0	9,10,10	0.22	0
3	MPD	C	503	-	7,7,7	0.27	0	9,10,10	0.21	0
3	MPD	F	504	-	7,7,7	0.27	0	9,10,10	0.28	0
3	MPD	D	503	-	7,7,7	0.26	0	9,10,10	0.24	0
2	MRD	A	501	-	7,7,7	0.31	0	9,10,10	0.25	0
3	MPD	G	503	-	7,7,7	0.29	0	9,10,10	0.22	0
3	MPD	E	504	-	7,7,7	0.29	0	9,10,10	0.24	0
3	MPD	B	503	-	7,7,7	0.30	0	9,10,10	0.27	0
3	MPD	A	504	-	7,7,7	0.27	0	9,10,10	0.22	0
3	MPD	E	503	-	7,7,7	0.27	0	9,10,10	0.18	0
2	MRD	B	501	-	7,7,7	0.29	0	9,10,10	0.32	0
2	MRD	C	502	-	7,7,7	0.31	0	9,10,10	0.35	0
2	MRD	E	501	-	7,7,7	0.30	0	9,10,10	0.22	0
3	MPD	A	503	-	7,7,7	0.29	0	9,10,10	0.24	0
3	MPD	F	503	-	7,7,7	0.30	0	9,10,10	0.19	0
2	MRD	A	502	-	7,7,7	0.29	0	9,10,10	0.38	0
2	MRD	F	501	-	7,7,7	0.33	0	9,10,10	0.25	0
2	MRD	H	501	-	7,7,7	0.30	0	9,10,10	0.25	0
2	MRD	G	502	-	7,7,7	0.33	0	9,10,10	0.37	0
3	MPD	C	504	-	7,7,7	0.30	0	9,10,10	0.20	0
2	MRD	B	502	-	7,7,7	0.32	0	9,10,10	0.39	0
2	MRD	E	502	-	7,7,7	0.32	0	9,10,10	0.32	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
2	MRD	D	501	-	-	1/5/5/5	-
2	MRD	H	502	-	-	3/5/5/5	-
2	MRD	F	502	-	-	3/5/5/5	-
3	MPD	H	504	-	-	0/5/5/5	-
2	MRD	G	501	-	-	0/5/5/5	-
3	MPD	H	503	-	-	2/5/5/5	-
3	MPD	D	504	-	-	0/5/5/5	-
3	MPD	G	504	-	-	0/5/5/5	-
2	MRD	D	502	-	-	3/5/5/5	-
2	MRD	C	501	-	-	0/5/5/5	-
3	MPD	B	504	-	-	0/5/5/5	-
3	MPD	C	503	-	-	3/5/5/5	-
3	MPD	F	504	-	-	0/5/5/5	-
3	MPD	D	503	-	-	3/5/5/5	-
2	MRD	A	501	-	-	1/5/5/5	-
3	MPD	G	503	-	-	3/5/5/5	-
3	MPD	E	504	-	-	0/5/5/5	-
3	MPD	B	503	-	-	3/5/5/5	-
3	MPD	A	504	-	-	0/5/5/5	-
3	MPD	E	503	-	-	3/5/5/5	-
2	MRD	B	501	-	-	2/5/5/5	-
2	MRD	C	502	-	-	2/5/5/5	-
2	MRD	E	501	-	-	0/5/5/5	-
3	MPD	A	503	-	-	2/5/5/5	-
3	MPD	F	503	-	-	2/5/5/5	-
2	MRD	A	502	-	-	1/5/5/5	-
2	MRD	F	501	-	-	0/5/5/5	-
2	MRD	H	501	-	-	0/5/5/5	-
2	MRD	G	502	-	-	3/5/5/5	-
3	MPD	C	504	-	-	0/5/5/5	-
2	MRD	B	502	-	-	2/5/5/5	-
2	MRD	E	502	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	MRD	C1-C2-C3-C4
2	C	502	MRD	C1-C2-C3-C4
2	D	502	MRD	CM-C2-C3-C4
2	F	502	MRD	C1-C2-C3-C4
2	F	502	MRD	CM-C2-C3-C4
2	H	502	MRD	C1-C2-C3-C4
3	A	503	MPD	C1-C2-C3-C4
3	C	503	MPD	C1-C2-C3-C4
3	F	503	MPD	CM-C2-C3-C4
3	G	503	MPD	CM-C2-C3-C4
3	H	503	MPD	C1-C2-C3-C4
2	A	501	MRD	O2-C2-C3-C4
2	B	502	MRD	O2-C2-C3-C4
2	D	502	MRD	O2-C2-C3-C4
2	F	502	MRD	O2-C2-C3-C4
2	G	502	MRD	O2-C2-C3-C4
2	H	502	MRD	O2-C2-C3-C4
3	B	503	MPD	O2-C2-C3-C4
3	D	503	MPD	O2-C2-C3-C4
3	E	503	MPD	O2-C2-C3-C4
3	G	503	MPD	O2-C2-C3-C4
2	B	502	MRD	C2-C3-C4-O4
2	D	501	MRD	C2-C3-C4-O4
3	C	503	MPD	C2-C3-C4-O4
2	A	502	MRD	C1-C2-C3-C4
2	B	501	MRD	CM-C2-C3-C4
2	C	502	MRD	CM-C2-C3-C4
2	D	502	MRD	C1-C2-C3-C4
2	G	502	MRD	C1-C2-C3-C4
2	G	502	MRD	CM-C2-C3-C4
2	H	502	MRD	CM-C2-C3-C4
3	A	503	MPD	CM-C2-C3-C4
3	B	503	MPD	C1-C2-C3-C4
3	B	503	MPD	CM-C2-C3-C4
3	C	503	MPD	CM-C2-C3-C4
3	D	503	MPD	C1-C2-C3-C4
3	D	503	MPD	CM-C2-C3-C4
3	E	503	MPD	C1-C2-C3-C4
3	E	503	MPD	CM-C2-C3-C4
3	F	503	MPD	C1-C2-C3-C4
3	G	503	MPD	C1-C2-C3-C4
3	H	503	MPD	CM-C2-C3-C4

There are no ring outliers.

26 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	MRD	3	0
2	H	502	MRD	2	0
3	H	504	MPD	2	0
2	G	501	MRD	2	0
3	H	503	MPD	3	0
3	D	504	MPD	2	0
2	D	502	MRD	3	0
2	C	501	MRD	2	0
3	C	503	MPD	7	0
3	D	503	MPD	4	0
2	A	501	MRD	1	0
3	G	503	MPD	6	0
3	B	503	MPD	6	0
3	A	504	MPD	1	0
3	E	503	MPD	8	0
2	B	501	MRD	1	0
2	C	502	MRD	1	0
2	E	501	MRD	2	0
3	A	503	MPD	7	0
3	F	503	MPD	3	0
2	A	502	MRD	2	0
2	F	501	MRD	1	0
2	H	501	MRD	1	0
2	G	502	MRD	2	0
2	B	502	MRD	2	0
2	E	502	MRD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q < 0.9
1	A	134/144 (93%)	-0.15	6 (4%)	38	35	10, 18, 37, 59	2 (1%)
1	B	134/144 (93%)	-0.14	5 (3%)	45	42	9, 17, 37, 58	1 (0%)
1	C	136/144 (94%)	-0.10	4 (2%)	53	50	10, 17, 38, 64	1 (0%)
1	D	133/144 (92%)	-0.23	1 (0%)	82	80	8, 16, 35, 40	1 (0%)
1	E	136/144 (94%)	-0.16	5 (3%)	45	42	9, 16, 38, 59	1 (0%)
1	F	133/144 (92%)	-0.18	2 (1%)	72	69	10, 17, 35, 42	1 (0%)
1	G	137/144 (95%)	-0.13	5 (3%)	46	43	9, 16, 39, 63	1 (0%)
1	H	136/144 (94%)	-0.08	6 (4%)	39	36	10, 18, 38, 59	2 (1%)
All	All	1079/1152 (93%)	-0.14	34 (3%)	50	47	8, 17, 37, 64	10 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	70	SER	6.0
1	E	70	SER	4.7
1	E	71	HIS	4.2
1	G	71	HIS	4.2
1	C	70	SER	4.2
1	C	69	GLY	4.0
1	G	69	GLY	3.9
1	C	71	HIS	3.8
1	H	69	GLY	3.7
1	H	71	HIS	3.5
1	A	71	HIS	3.5
1	B	73	GLN	3.2
1	F	101	LEU	3.2
1	H	70	SER	3.1
1	B	207	ALA	3.1
1	F	207	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	207	ALA	3.0
1	B	71	HIS	3.0
1	E	69	GLY	2.8
1	B	101	LEU	2.8
1	A	73	GLN	2.7
1	E	101	LEU	2.7
1	A	195	ARG	2.6
1	H	207	ALA	2.6
1	B	195	ARG	2.6
1	H	101	LEU	2.5
1	G	208	SER	2.5
1	G	101	LEU	2.5
1	A	194	PRO	2.4
1	E	207	ALA	2.2
1	C	101	LEU	2.2
1	H	195	ARG	2.1
1	D	207	ALA	2.0
1	A	124	ASN	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	MRD	A	501	8/8	0.67	0.22	33,40,48,52	0
2	MRD	F	501	8/8	0.73	0.17	36,38,46,51	0
2	MRD	H	501	8/8	0.76	0.20	32,37,40,47	0
2	MRD	B	501	8/8	0.78	0.20	32,38,41,51	0
2	MRD	D	501	8/8	0.78	0.18	32,36,43,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MRD	D	502	8/8	0.79	0.16	16,21,25,34	0
2	MRD	C	501	8/8	0.80	0.20	32,39,42,46	0
3	MPD	A	503	8/8	0.81	0.27	23,28,32,35	0
2	MRD	G	501	8/8	0.82	0.15	29,31,37,46	0
2	MRD	E	501	8/8	0.82	0.16	30,35,43,49	0
2	MRD	F	502	8/8	0.82	0.15	21,26,31,32	0
2	MRD	G	502	8/8	0.83	0.13	17,25,28,37	0
3	MPD	C	503	8/8	0.83	0.23	19,22,30,32	0
3	MPD	G	503	8/8	0.84	0.20	19,21,28,32	0
3	MPD	E	503	8/8	0.85	0.24	18,21,30,31	0
2	MRD	E	502	8/8	0.85	0.13	20,23,26,31	0
3	MPD	B	503	8/8	0.86	0.23	17,25,28,29	0
2	MRD	A	502	8/8	0.86	0.12	19,24,28,29	0
3	MPD	D	503	8/8	0.87	0.20	19,22,31,32	0
2	MRD	H	502	8/8	0.87	0.13	24,27,29,36	0
2	MRD	C	502	8/8	0.87	0.12	21,22,24,32	0
3	MPD	H	504	8/8	0.87	0.12	10,18,20,28	0
2	MRD	B	502	8/8	0.88	0.11	24,25,27,36	0
3	MPD	H	503	8/8	0.88	0.18	17,23,27,33	0
3	MPD	A	504	8/8	0.88	0.12	17,22,23,31	0
3	MPD	B	504	8/8	0.89	0.11	15,18,22,30	0
3	MPD	E	504	8/8	0.90	0.09	14,21,22,33	0
3	MPD	D	504	8/8	0.90	0.10	18,21,22,31	0
3	MPD	F	503	8/8	0.91	0.19	17,21,29,29	0
3	MPD	G	504	8/8	0.91	0.10	14,19,22,32	0
3	MPD	C	504	8/8	0.93	0.09	16,20,21,26	0
3	MPD	F	504	8/8	0.93	0.10	18,20,21,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.