Full wwPDB X-ray Structure Validation Report (i)

Jan 29, 2024 – 12:22 am GMT

PDB ID	:	7ZB0
Title	:	macrocyclase OphP with 15mer
Authors	:	Song, H.; Naismith, J.H.
Deposited on	:	2022-03-23
Resolution	:	2.47 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 (i) 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 (1)) were used in the production of this report:

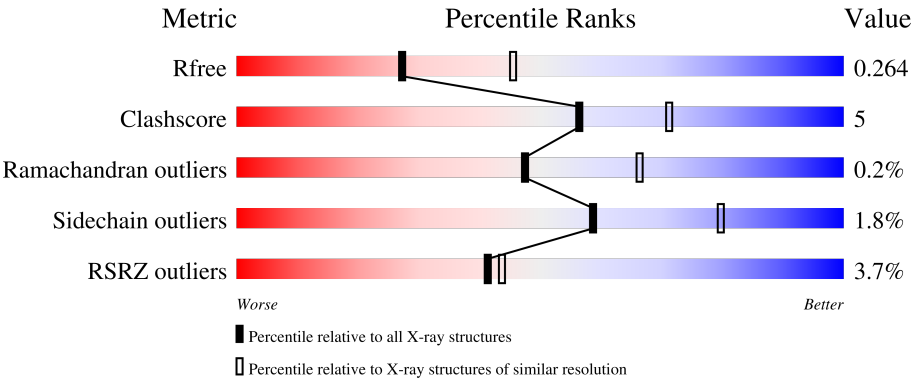
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	745	2% 86% 10%
1	B	745	3% 87% 9%
1	C	745	6% 84% 11% 5%
1	D	745	3% 86% 10%
2	E	15	7% 13% 20% 67%

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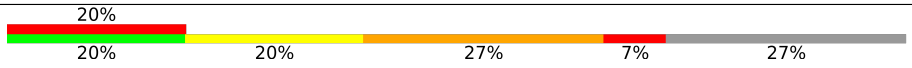
Mol	Chain	Length	Quality of chain
2	F	15	
2	G	15	
2	H	15	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MVA	E	807	-	-	X	-
2	SAR	G	809	-	-	X	-
2	MVA	H	807	-	-	X	-
2	MVA	H	808	-	-	X	-
2	SAR	H	809	-	-	X	-
6	NA	D	806	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23277 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.

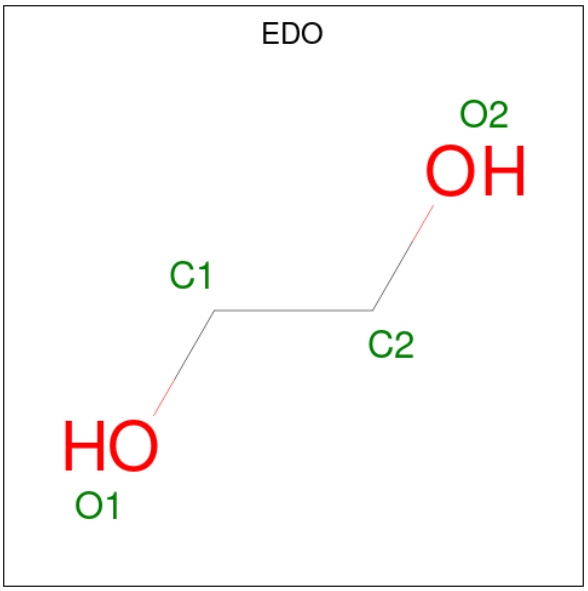
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	0	0
			5769	3686	970	1087	26			
1	B	718	Total	C	N	O	S	0	0	0
			5750	3673	968	1083	26			
1	C	706	Total	C	N	O	S	0	0	0
			5667	3627	950	1064	26			
1	D	719	Total	C	N	O	S	0	0	0
			5762	3680	970	1086	26			

- Molecule 2 is a protein called 15mer.

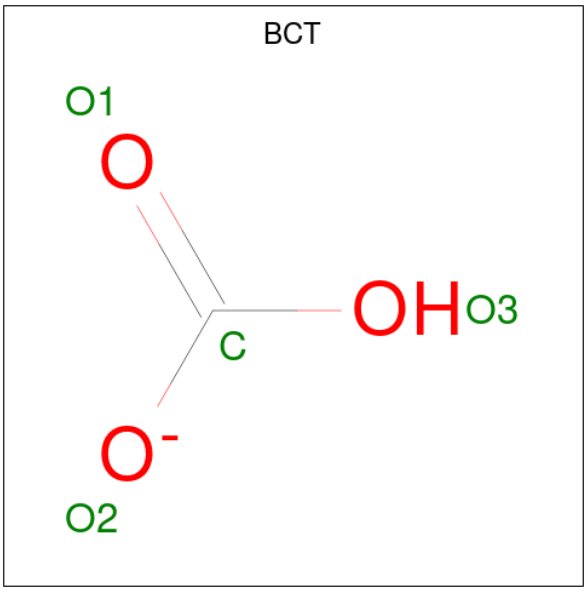
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			37	27	5	5			
2	F	7	Total	C	N	O	0	0	0
			64	49	8	7			
2	G	5	Total	C	N	O	0	0	0
			37	27	5	5			
2	H	11	Total	C	N	O	0	0	0
			90	67	12	11			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



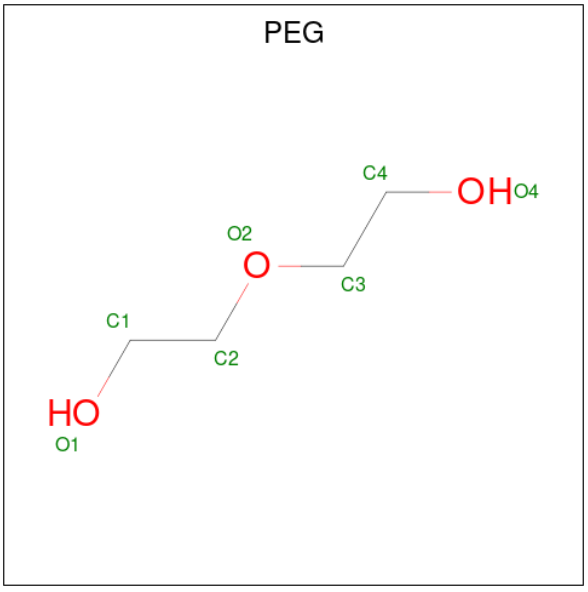
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	3	Total Na 3 3	0	0
6	D	3	Total Na 3 3	0	0

- Molecule 7 is water.

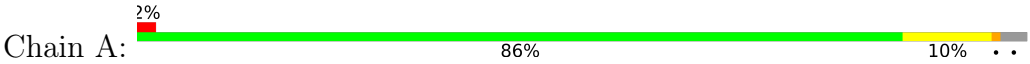
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O 7 7	0	0
7	B	18	Total O 18 18	0	0
7	C	11	Total O 11 11	0	0
7	D	17	Total O 17 17	0	0

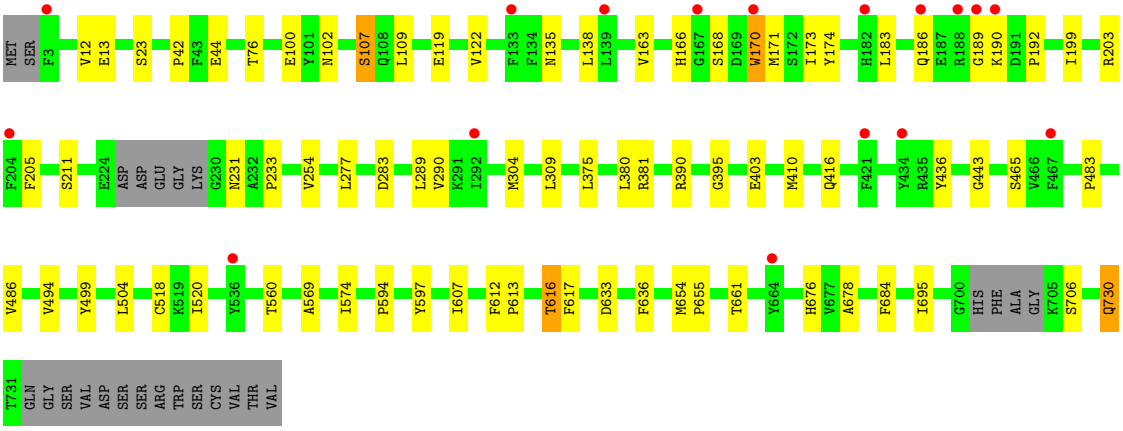
3 Residue-property plots (i)

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: Prolyl endopeptidase

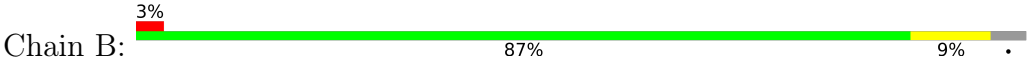
Chain A:

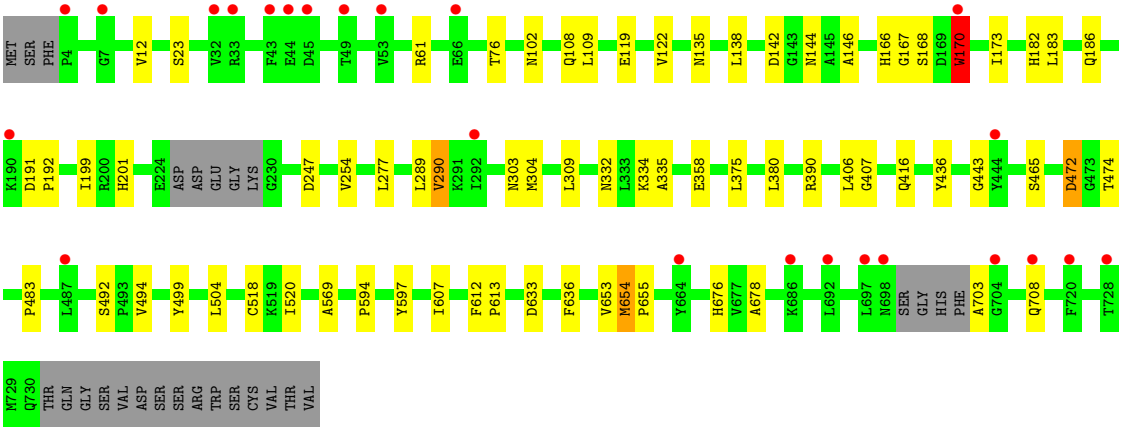




• Molecule 1: Prolyl endopeptidase

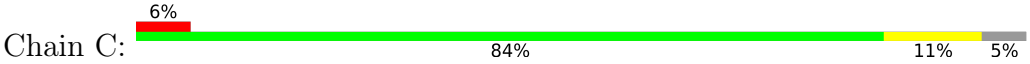
Chain B:

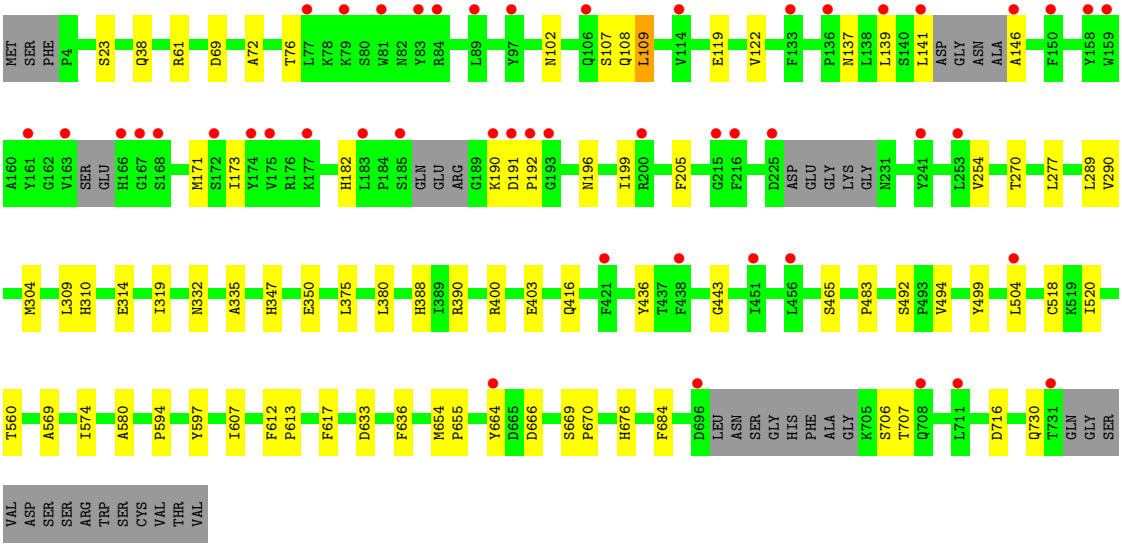




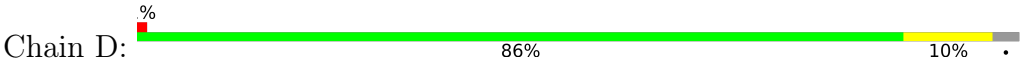
• Molecule 1: Prolyl endopeptidase

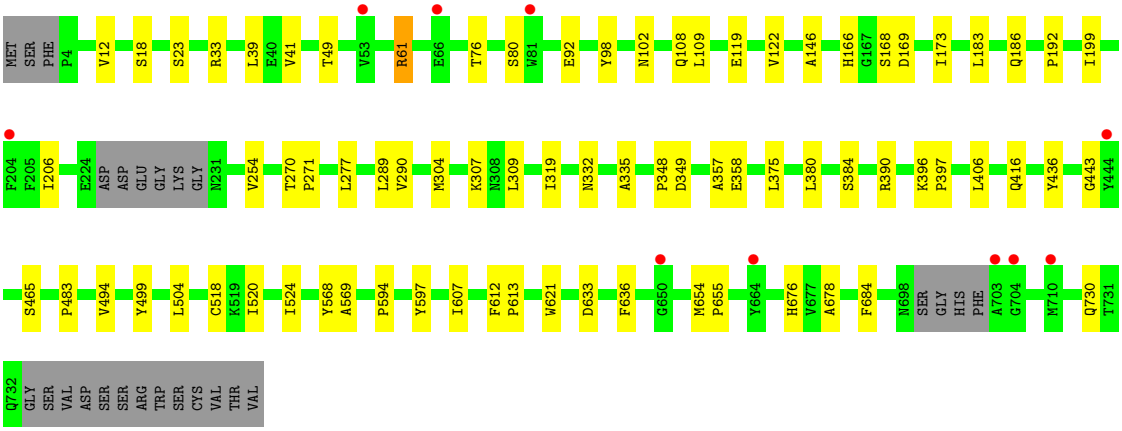
Chain C:



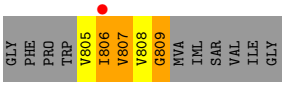


• Molecule 1: Prolyl endopeptidase

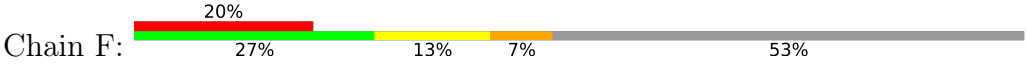


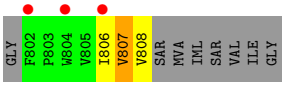


• Molecule 2: 15mer



• Molecule 2: 15mer



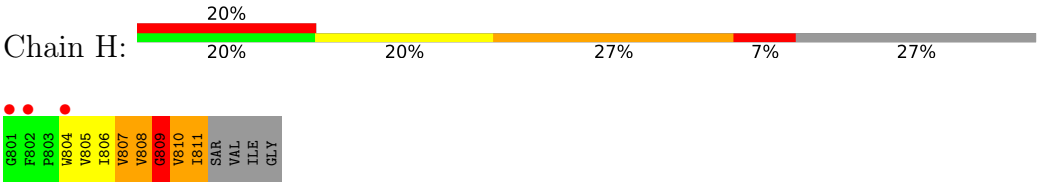


• Molecule 2: 15mer

Chain G:

• Molecule 2: 15mer

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.22Å 106.18Å 114.79Å 113.04° 101.67° 93.24°	Depositor
Resolution (Å)	64.35 – 2.47 64.35 – 2.47	Depositor EDS
% Data completeness (in resolution range)	98.6 (64.35-2.47) 98.6 (64.35-2.47)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.229 , 0.266 0.228 , 0.264	Depositor DCC
R_{free} test set	5223 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23277	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, MVA, BCT, IML, PEG, SAR, NA

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	0.69	0/5937	0.83	0/8053
1	B	0.66	0/5917	0.81	1/8025 (0.0%)
1	C	0.66	0/5831	0.81	0/7906
1	D	0.68	0/5929	0.82	1/8042 (0.0%)
2	E	0.50	0/7	1.68	0/8
2	F	0.50	0/42	0.55	0/56
2	G	0.11	0/7	0.76	0/8
2	H	0.52	0/46	0.84	0/61
All	All	0.67	0/23716	0.82	2/32159 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	G	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	170	TRP	CA-CB-CG	5.79	124.70	113.70
1	D	61	ARG	CG-CD-NE	-5.12	101.05	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	730	GLN	Peptide
2	G	808	MVA	Peptide
2	H	809	SAR	Peptide

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	5769	0	5512	47	0
1	B	5750	0	5497	43	0
1	C	5667	0	5420	51	0
1	D	5762	0	5509	53	0
2	E	37	0	50	14	0
2	F	64	0	69	4	0
2	G	37	0	50	11	0
2	H	90	0	101	21	0
3	B	4	0	6	0	0
3	C	8	0	12	0	0
3	D	12	0	18	0	0
4	B	4	0	0	0	0
5	C	7	0	10	0	0
5	D	7	0	10	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
7	A	7	0	0	1	0
7	B	18	0	0	1	0
7	C	11	0	0	0	0
7	D	17	0	0	0	0
All	All	23277	0	22264	228	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 5.

All (228) 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:621:TRP:HE1	2:H:808:MVA:HN2	1.14	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:807:MVA:HG12	2:F:807:MVA:HN2	1.50	0.93
2:H:807:MVA:HN3	2:H:808:MVA:HN1	1.48	0.93
1:D:206:ILE:HD11	2:H:804:TRP:CD2	2.12	0.83
1:D:621:TRP:NE1	2:H:808:MVA:HN2	1.95	0.80
2:H:807:MVA:CN	2:H:808:MVA:HN1	2.11	0.80
1:D:41:VAL:O	1:D:49:THR:HG21	1.84	0.76
1:D:621:TRP:HE1	2:H:808:MVA:CN	1.98	0.73
1:D:277:LEU:HD11	1:D:290:VAL:HG22	1.73	0.71
1:A:100:GLU:OE2	1:A:109:LEU:HD13	1.91	0.70
1:A:594:PRO:HB3	1:A:654:MET:HE2	1.75	0.69
1:B:277:LEU:HD11	1:B:290:VAL:HG22	1.73	0.69
1:A:277:LEU:HD11	1:A:290:VAL:HG22	1.74	0.69
1:C:277:LEU:HD11	1:C:290:VAL:HG22	1.75	0.69
1:A:290:VAL:HG13	1:A:309:LEU:HB3	1.76	0.68
1:C:594:PRO:HB3	1:C:654:MET:HE1	1.75	0.68
2:E:806:ILE:CG1	2:E:807:MVA:HN1	2.24	0.67
1:D:166:HIS:NE2	1:D:168:SER:HB3	2.08	0.67
2:E:806:ILE:O	2:E:807:MVA:HG12	1.94	0.66
1:C:388:HIS:CE1	1:C:400:ARG:HD3	2.29	0.66
1:D:290:VAL:HG13	1:D:309:LEU:HB3	1.77	0.66
1:B:183:LEU:O	1:B:186:GLN:HG3	1.96	0.65
1:B:144:ASN:ND2	1:B:166:HIS:HA	2.12	0.63
1:D:183:LEU:O	1:D:186:GLN:HG3	1.97	0.63
1:A:654:MET:HG3	1:A:684:PHE:CE2	2.33	0.62
1:B:290:VAL:HG13	1:B:309:LEU:HB3	1.81	0.62
2:H:807:MVA:N	2:H:808:MVA:HN1	2.15	0.61
1:A:183:LEU:O	1:A:186:GLN:HG3	2.01	0.61
1:A:483:PRO:HD3	1:A:518:CYS:HB3	1.82	0.61
1:A:42:PRO:HG3	1:A:231:ASN:HB2	1.82	0.61
1:C:290:VAL:HG13	1:C:309:LEU:HB3	1.80	0.61
1:C:654:MET:HG3	1:C:684:PHE:CE2	2.36	0.61
1:C:664:TYR:O	1:C:664:TYR:CD1	2.54	0.61
2:H:809:SAR:HN2	2:H:809:SAR:O	2.01	0.61
1:B:406:LEU:C	1:B:406:LEU:HD23	2.21	0.60
2:E:806:ILE:HG23	2:E:807:MVA:HN1	1.81	0.60
2:G:805:MVA:HG12	2:G:805:MVA:HN3	1.84	0.60
1:A:617:PHE:HB3	2:E:807:MVA:HG21	1.84	0.60
2:F:807:MVA:HG12	2:F:807:MVA:CN	2.29	0.59
1:D:206:ILE:HD11	2:H:804:TRP:CG	2.36	0.59
1:C:310:HIS:HE1	1:C:314:GLU:OE1	1.85	0.59
1:B:142:ASP:OD1	1:B:144:ASN:OD1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:THR:HG21	1:D:520:ILE:HD11	1.85	0.58
1:D:654:MET:HG3	1:D:684:PHE:CE2	2.38	0.58
2:E:805:MVA:HG12	2:E:805:MVA:HN3	1.84	0.58
2:G:808:MVA:HN2	2:G:808:MVA:HG23	1.85	0.58
1:C:171:MET:HE3	1:C:205:PHE:HD1	1.69	0.57
2:H:808:MVA:HN3	2:H:808:MVA:HG23	1.85	0.57
1:D:33:ARG:HG2	1:D:33:ARG:HH11	1.69	0.57
1:A:163:VAL:CG2	1:A:174:TYR:CE1	2.88	0.57
1:A:173:ILE:HB	1:A:199:ILE:HB	1.88	0.56
1:D:483:PRO:HD3	1:D:518:CYS:HB3	1.87	0.56
2:E:806:ILE:CB	2:E:807:MVA:HN1	2.36	0.56
1:C:483:PRO:HD3	1:C:518:CYS:HB3	1.89	0.55
1:B:472:ASP:OD2	1:B:474:THR:OG1	2.19	0.55
1:A:283:ASP:O	2:E:806:ILE:HD13	2.06	0.55
1:C:76:THR:HG21	1:C:520:ILE:HD11	1.88	0.55
2:G:806:ILE:HG13	2:G:808:MVA:HG12	1.87	0.55
1:A:163:VAL:CG2	1:A:174:TYR:HE1	2.20	0.54
1:D:166:HIS:CE1	1:D:168:SER:HB3	2.42	0.54
1:B:254:VAL:HG13	1:B:304:MET:CE	2.37	0.54
1:C:61:ARG:NH2	1:C:716:ASP:OD1	2.40	0.54
1:D:39:LEU:HA	1:D:49:THR:HG22	1.89	0.54
1:B:483:PRO:HD3	1:B:518:CYS:HB3	1.88	0.54
1:C:182:HIS:HE2	1:C:191:ASP:HB2	1.72	0.54
1:C:347:HIS:HB3	1:C:350:GLU:HG3	1.90	0.54
1:D:173:ILE:HB	1:D:199:ILE:HB	1.90	0.54
2:E:806:ILE:CG1	2:E:807:MVA:CN	2.86	0.54
1:C:173:ILE:HB	1:C:199:ILE:HB	1.88	0.54
1:C:580:ALA:CB	2:G:809:SAR:HA2	2.38	0.54
1:B:173:ILE:HB	1:B:199:ILE:HB	1.91	0.53
1:B:182:HIS:HE2	1:B:191:ASP:HB2	1.72	0.53
1:C:119:GLU:O	1:C:122:VAL:HG22	2.08	0.53
1:A:138:LEU:HD13	1:A:186:GLN:OE1	2.09	0.53
1:B:375:LEU:HB3	1:B:390:ARG:HB2	1.90	0.53
1:D:76:THR:HG21	1:D:520:ILE:CD1	2.39	0.53
1:D:375:LEU:HB3	1:D:390:ARG:HB2	1.91	0.53
1:A:375:LEU:HB3	1:A:390:ARG:HB2	1.91	0.53
1:B:119:GLU:O	1:B:122:VAL:HG22	2.09	0.53
1:A:254:VAL:HG13	1:A:304:MET:CE	2.39	0.52
1:D:166:HIS:CD2	1:D:168:SER:HB3	2.44	0.52
1:D:633:ASP:HA	1:D:636:PHE:CE2	2.45	0.52
1:B:633:ASP:HA	1:B:636:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:806:ILE:CG2	2:E:807:MVA:HN1	2.40	0.52
1:A:119:GLU:O	1:A:122:VAL:HG22	2.10	0.51
1:C:375:LEU:HB3	1:C:390:ARG:HB2	1.92	0.51
1:C:76:THR:HG21	1:C:520:ILE:CD1	2.40	0.51
2:H:809:SAR:O	2:H:810:MVA:HG12	2.11	0.51
1:A:494:VAL:CG2	1:A:569:ALA:HB2	2.41	0.51
1:A:633:ASP:HA	1:A:636:PHE:CE2	2.46	0.51
1:D:307:LYS:HG2	1:D:348:PRO:CB	2.41	0.51
1:C:254:VAL:HG13	1:C:304:MET:CE	2.42	0.50
2:H:808:MVA:O	2:H:808:MVA:HG13	2.11	0.50
1:B:167:GLY:O	1:B:703:ALA:HB2	2.11	0.50
1:D:102:ASN:HB2	1:D:109:LEU:HD23	1.94	0.50
1:D:349:ASP:OD1	1:D:349:ASP:N	2.42	0.50
1:C:633:ASP:HA	1:C:636:PHE:CE2	2.47	0.50
1:B:102:ASN:HB2	1:B:109:LEU:HD23	1.93	0.50
1:D:607:ILE:HG21	1:D:676:HIS:CG	2.47	0.50
1:A:12:VAL:HG21	1:A:678:ALA:HB1	1.93	0.50
1:B:654:MET:HG3	1:B:655:PRO:HD2	1.93	0.50
1:D:119:GLU:O	1:D:122:VAL:HG22	2.11	0.50
1:D:12:VAL:HG21	1:D:678:ALA:HB1	1.94	0.49
1:C:597:TYR:O	1:C:655:PRO:HB3	2.13	0.49
1:D:384:SER:OG	1:D:406:LEU:HD12	2.12	0.49
1:D:524:ILE:CD1	1:D:568:TYR:HB3	2.43	0.49
2:G:808:MVA:HN2	2:G:808:MVA:CG2	2.42	0.49
2:H:807:MVA:HN2	2:H:807:MVA:HG22	1.93	0.49
2:H:809:SAR:O	2:H:809:SAR:CN	2.60	0.49
1:A:607:ILE:HG21	1:A:676:HIS:CG	2.47	0.49
1:B:12:VAL:HG21	1:B:678:ALA:HB1	1.94	0.49
1:C:607:ILE:HG21	1:C:676:HIS:CG	2.48	0.49
1:D:494:VAL:CG2	1:D:569:ALA:HB2	2.43	0.49
1:B:494:VAL:CG2	1:B:569:ALA:HB2	2.42	0.49
1:C:254:VAL:HG13	1:C:304:MET:HE2	1.94	0.49
1:C:664:TYR:O	1:C:664:TYR:CG	2.66	0.48
1:A:189:GLY:O	1:A:190:LYS:HG3	2.14	0.48
1:A:594:PRO:HB3	1:A:654:MET:CE	2.43	0.48
1:A:107:SER:HB3	1:A:706:SER:HB2	1.96	0.48
1:B:472:ASP:O	1:B:472:ASP:OD1	2.31	0.48
1:B:607:ILE:HG21	1:B:676:HIS:CG	2.49	0.48
1:C:69:ASP:HA	1:C:72:ALA:HB3	1.96	0.48
1:A:171:MET:HE3	1:A:205:PHE:HD1	1.78	0.48
1:A:170:TRP:HB3	1:A:203:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:SER:O	1:D:33:ARG:HD3	2.14	0.47
1:B:597:TYR:O	1:B:655:PRO:HB3	2.14	0.47
1:C:107:SER:HB2	1:C:137:ASN:OD1	2.14	0.47
1:C:580:ALA:HB1	2:G:809:SAR:HA2	1.96	0.47
1:A:163:VAL:HG22	1:A:174:TYR:CE1	2.49	0.47
1:A:597:TYR:O	1:A:655:PRO:HB3	2.15	0.47
1:D:597:TYR:O	1:D:655:PRO:HB3	2.14	0.47
1:D:254:VAL:HG13	1:D:304:MET:CE	2.45	0.47
1:C:580:ALA:CB	2:G:809:SAR:C	2.94	0.46
1:D:289:LEU:HD23	1:D:290:VAL:N	2.30	0.46
2:H:810:MVA:HA	2:H:811:IML:HN1	1.80	0.46
2:E:806:ILE:HG13	2:E:807:MVA:CN	2.45	0.46
1:B:76:THR:HG21	1:B:520:ILE:HD11	1.97	0.46
1:D:307:LYS:HG2	1:D:348:PRO:HB3	1.97	0.46
2:H:808:MVA:HN3	2:H:808:MVA:CG2	2.41	0.46
1:C:520:ILE:O	1:C:730:GLN:HG3	2.16	0.45
1:A:135:ASN:HB3	1:A:138:LEU:HD12	1.98	0.45
1:B:76:THR:HG21	1:B:520:ILE:CD1	2.47	0.45
1:C:499:TYR:CD2	1:C:504:LEU:HD23	2.52	0.45
1:C:580:ALA:HB3	2:G:809:SAR:C	2.46	0.45
1:C:494:VAL:CG2	1:C:569:ALA:HB2	2.47	0.45
2:E:806:ILE:HG12	2:E:807:MVA:HN1	1.95	0.45
1:A:254:VAL:HG13	1:A:304:MET:HE2	1.98	0.45
1:B:289:LEU:HD23	1:B:290:VAL:N	2.32	0.45
1:B:254:VAL:HG13	1:B:304:MET:HE2	1.99	0.45
1:B:612:PHE:N	1:B:613:PRO:CD	2.80	0.44
1:D:206:ILE:CD1	2:H:804:TRP:CG	2.99	0.44
1:B:406:LEU:C	1:B:406:LEU:CD2	2.86	0.44
1:A:76:THR:HG21	1:A:520:ILE:HD11	2.00	0.44
1:B:406:LEU:HD23	1:B:407:GLY:N	2.32	0.44
1:D:436:TYR:CZ	1:D:443:GLY:HA3	2.52	0.44
1:B:499:TYR:CD2	1:B:504:LEU:HD23	2.52	0.44
1:C:664:TYR:CD1	1:C:664:TYR:C	2.90	0.44
1:A:499:TYR:CD2	1:A:504:LEU:HD23	2.53	0.44
1:B:594:PRO:HB3	1:B:654:MET:CE	2.47	0.44
1:D:520:ILE:O	1:D:730:GLN:HG3	2.18	0.44
1:C:436:TYR:CZ	1:C:443:GLY:HA3	2.53	0.43
2:E:808:MVA:HA	2:E:809:SAR:HN1	1.65	0.43
1:A:289:LEU:HD23	1:A:289:LEU:C	2.38	0.43
1:B:436:TYR:CZ	1:B:443:GLY:HA3	2.53	0.43
2:H:804:TRP:HA	2:H:805:MVA:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD23	1:A:290:VAL:N	2.34	0.43
1:B:135:ASN:HB3	1:B:138:LEU:HD12	1.99	0.43
1:C:612:PHE:N	1:C:613:PRO:CD	2.81	0.43
1:A:233:PRO:HA	1:A:616:THR:O	2.18	0.43
1:A:381:ARG:NH2	7:A:802:HOH:O	2.51	0.43
1:B:332:ASN:HA	1:B:335:ALA:O	2.17	0.43
1:C:107:SER:HB3	1:C:706:SER:HB2	2.00	0.43
1:D:396:LYS:HG3	1:D:397:PRO:HD2	2.01	0.43
1:A:612:PHE:N	1:A:613:PRO:CD	2.82	0.43
1:C:102:ASN:HD22	1:C:109:LEU:HD12	1.83	0.43
1:D:612:PHE:CG	1:D:613:PRO:HD3	2.54	0.43
2:E:808:MVA:O	2:E:808:MVA:HG12	2.19	0.43
1:B:108:GLN:HE22	1:B:146:ALA:HA	1.84	0.42
1:D:594:PRO:HB3	1:D:654:MET:CE	2.48	0.42
1:B:182:HIS:HE2	1:B:191:ASP:CB	2.31	0.42
1:C:594:PRO:HB3	1:C:654:MET:CE	2.44	0.42
1:B:334:LYS:HG2	1:D:357:ALA:HB1	2.02	0.42
2:H:806:ILE:HA	2:H:807:MVA:HN1	1.72	0.42
1:C:107:SER:O	1:C:707:THR:HG23	2.19	0.42
1:C:612:PHE:CG	1:C:613:PRO:HD3	2.55	0.42
1:D:206:ILE:CD1	2:H:804:TRP:CD2	2.92	0.42
1:D:332:ASN:HA	1:D:335:ALA:O	2.19	0.42
1:C:171:MET:HE3	1:C:205:PHE:CD1	2.52	0.42
1:C:332:ASN:HA	1:C:335:ALA:O	2.18	0.42
1:D:335:ALA:HB1	1:D:358:GLU:HB2	2.02	0.42
1:B:289:LEU:HD23	1:B:289:LEU:C	2.40	0.42
1:A:436:TYR:CZ	1:A:443:GLY:HA3	2.55	0.42
1:B:186:GLN:NE2	1:B:192:PRO:HG2	2.35	0.42
1:B:612:PHE:CG	1:B:613:PRO:HD3	2.55	0.42
2:H:807:MVA:HG13	2:H:809:SAR:HN1	2.02	0.42
1:A:102:ASN:HB2	1:A:109:LEU:HD23	2.01	0.42
1:C:289:LEU:HD23	1:C:290:VAL:N	2.34	0.42
1:D:499:TYR:CD2	1:D:504:LEU:HD23	2.54	0.42
1:D:612:PHE:N	1:D:613:PRO:CD	2.82	0.42
2:F:807:MVA:HA	2:F:808:MVA:HN1	1.77	0.41
1:A:612:PHE:CG	1:A:613:PRO:HD3	2.55	0.41
1:D:92:GLU:HG3	1:D:98:TYR:CD1	2.55	0.41
1:B:170:TRP:HZ2	1:B:201:HIS:CD2	2.38	0.41
1:C:139:LEU:CD2	1:C:191:ASP:HB3	2.50	0.41
1:D:108:GLN:HE22	1:D:146:ALA:HA	1.86	0.41
2:E:807:MVA:HA	2:E:808:MVA:HN1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:807:MVA:HA	2:G:808:MVA:HN1	1.74	0.41
1:A:168:SER:HB3	1:A:170:TRP:CE2	2.55	0.41
1:B:334:LYS:NZ	7:B:901:HOH:O	2.52	0.41
1:A:483:PRO:HB2	1:A:486:VAL:HG13	2.03	0.41
1:C:108:GLN:HE22	1:C:146:ALA:HA	1.86	0.41
1:C:499:TYR:HH	2:G:809:SAR:C	2.34	0.41
1:C:669:SER:HA	1:C:670:PRO:HD3	1.96	0.41
1:D:166:HIS:NE2	1:D:168:SER:CB	2.81	0.41
1:D:289:LEU:HD23	1:D:289:LEU:C	2.41	0.41
1:A:520:ILE:O	1:A:730:GLN:HG3	2.22	0.40
1:D:270:THR:HA	1:D:319:ILE:HG21	2.02	0.40
2:F:806:ILE:HA	2:F:807:MVA:HN1	1.76	0.40
1:A:390:ARG:NH1	1:A:395:GLY:O	2.53	0.40
1:A:494:VAL:HG23	1:A:569:ALA:CB	2.52	0.40
1:A:560:THR:HG23	1:A:574:ILE:HG21	2.03	0.40
1:A:661:THR:HG23	1:A:695:ILE:HD13	2.03	0.40
1:C:560:THR:HG23	1:C:574:ILE:HG21	2.02	0.40
1:C:182:HIS:HE2	1:C:191:ASP:CB	2.32	0.40
1:B:335:ALA:HB1	1:B:358:GLU:HB2	2.03	0.40
1:C:270:THR:HA	1:C:319:ILE:HG21	2.03	0.40
1:C:617:PHE:CD1	2:G:807:MVA:HG21	2.57	0.40
1:D:594:PRO:HB3	1:D:654:MET:HE1	2.03	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	714/745 (96%)	673 (94%)	38 (5%)	3 (0%)	34	52
1	B	712/745 (96%)	674 (95%)	37 (5%)	1 (0%)	51	71
1	C	694/745 (93%)	652 (94%)	41 (6%)	1 (0%)	51	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	713/745 (96%)	673 (94%)	38 (5%)	2 (0%)	41 59
2	E	1/15 (7%)	0	1 (100%)	0	100 100
2	F	3/15 (20%)	3 (100%)	0	0	100 100
2	G	1/15 (7%)	1 (100%)	0	0	100 100
2	H	4/15 (27%)	4 (100%)	0	0	100 100
All	All	2842/3040 (94%)	2680 (94%)	155 (6%)	7 (0%)	47 66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	192	PRO
1	C	192	PRO
1	D	192	PRO
1	D	169	ASP
1	B	653	VAL
1	A	616	THR

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	623/644 (97%)	612 (98%)	11 (2%)	59 80
1	B	620/644 (96%)	606 (98%)	14 (2%)	50 74
1	C	613/644 (95%)	601 (98%)	12 (2%)	55 77
1	D	622/644 (97%)	615 (99%)	7 (1%)	73 88
2	E	1/6 (17%)	0	1 (100%)	0 0
2	F	4/6 (67%)	4 (100%)	0	100 100
2	G	1/6 (17%)	1 (100%)	0	100 100
2	H	4/6 (67%)	4 (100%)	0	100 100
All	All	2488/2600 (96%)	2443 (98%)	45 (2%)	59 80

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

Mol	Chain	Res	Type
1	A	13	GLU
1	A	23	SER
1	A	44	GLU
1	A	107	SER
1	A	170	TRP
1	A	211	SER
1	A	380	LEU
1	A	403	GLU
1	A	410	MET
1	A	416	GLN
1	A	465	SER
1	B	23	SER
1	B	61	ARG
1	B	168	SER
1	B	170	TRP
1	B	247	ASP
1	B	290	VAL
1	B	303	ASN
1	B	380	LEU
1	B	416	GLN
1	B	465	SER
1	B	472	ASP
1	B	492	SER
1	B	654	MET
1	B	708	GLN
1	C	23	SER
1	C	38	GLN
1	C	109	LEU
1	C	141	LEU
1	C	190	LYS
1	C	196	ASN
1	C	380	LEU
1	C	403	GLU
1	C	416	GLN
1	C	465	SER
1	C	492	SER
1	C	666	ASP
1	D	23	SER
1	D	61	ARG
1	D	80	SER
1	D	271	PRO
1	D	380	LEU

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Mol	Chain	Res	Type
1	D	416	GLN
1	D	465	SER
2	E	806	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	GLN
1	B	201	HIS
1	B	308	ASN
1	C	38	GLN
1	C	310	HIS
1	C	408	GLN
1	D	408	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAR	E	809	2	4,4,5	1.27	1 (25%)	1,3,5	1.13	0
2	MVA	E	807	2	6,7,8	0.95	0	7,8,10	2.22	2 (28%)
2	MVA	E	808	2	6,7,8	0.67	0	7,8,10	1.18	0
2	MVA	F	805	2	6,7,8	0.58	0	7,8,10	0.83	0
2	MVA	H	807	2	6,7,8	1.21	1 (16%)	7,8,10	0.89	0
2	MVA	G	808	2	6,7,8	0.71	0	7,8,10	0.91	0
2	MVA	H	805	2	6,7,8	0.50	0	7,8,10	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MVA	H	808	2	6,7,8	0.89	0	7,8,10	2.29	3 (42%)
2	MVA	F	808	2	6,7,8	0.78	0	7,8,10	1.05	0
2	SAR	G	809	2	4,4,5	1.19	0	1,3,5	1.58	0
2	MVA	G	805	2	6,7,8	0.47	0	7,8,10	0.92	0
2	MVA	F	807	2	6,7,8	0.67	0	7,8,10	1.56	2 (28%)
2	SAR	H	809	2	4,4,5	1.35	1 (25%)	1,3,5	1.38	0
2	MVA	E	805	2	6,7,8	0.58	0	7,8,10	0.98	0
2	IML	H	811	2	7,8,9	0.81	0	7,9,11	1.10	1 (14%)
2	MVA	G	807	2	6,7,8	0.63	0	7,8,10	2.17	3 (42%)
2	MVA	H	810	2	6,7,8	0.67	0	7,8,10	1.18	1 (14%)

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	SAR	E	809	2	-	1/1/2/3	-
2	MVA	E	807	2	-	6/6/8/10	-
2	MVA	E	808	2	-	5/6/8/10	-
2	MVA	F	805	2	-	2/6/8/10	-
2	MVA	H	807	2	-	2/6/8/10	-
2	MVA	G	808	2	-	2/6/8/10	-
2	MVA	H	805	2	-	3/6/8/10	-
2	MVA	H	808	2	-	2/6/8/10	-
2	MVA	F	808	2	-	4/6/8/10	-
2	SAR	G	809	2	-	1/1/2/3	-
2	MVA	G	805	2	-	5/6/8/10	-
2	MVA	F	807	2	-	5/6/8/10	-
2	SAR	H	809	2	-	1/1/2/3	-
2	MVA	E	805	2	-	5/6/8/10	-
2	IML	H	811	2	-	1/8/10/12	-
2	MVA	G	807	2	-	1/6/8/10	-
2	MVA	H	810	2	-	1/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	807	MVA	CA-N	2.56	1.51	1.47
2	H	809	SAR	CA-N	2.34	1.49	1.46
2	E	809	SAR	CA-N	2.05	1.48	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	807	MVA	CB-CA-C	-4.56	107.32	113.04
2	H	808	MVA	C-CA-N	3.86	123.79	110.88
2	G	807	MVA	CB-CA-N	3.83	116.16	111.17
2	H	808	MVA	CB-CA-N	-3.80	106.22	111.17
2	G	807	MVA	CB-CA-C	-2.92	109.38	113.04
2	G	807	MVA	O-C-CA	-2.69	117.32	124.83
2	H	811	IML	CB-CA-C	-2.68	109.16	112.82
2	E	807	MVA	CG1-CB-CA	2.61	115.21	111.21
2	F	807	MVA	O-C-CA	-2.49	117.89	124.83
2	H	810	MVA	O-C-CA	-2.42	118.09	124.83
2	H	808	MVA	CB-CA-C	-2.27	110.20	113.04
2	F	807	MVA	CB-CA-C	-2.20	110.28	113.04

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	805	MVA	N-CA-CB-CG1
2	E	805	MVA	N-CA-CB-CG2
2	E	805	MVA	C-CA-CB-CG1
2	E	805	MVA	C-CA-CB-CG2
2	F	805	MVA	N-CA-CB-CG2
2	G	805	MVA	N-CA-CB-CG1
2	G	805	MVA	N-CA-CB-CG2
2	G	805	MVA	C-CA-CB-CG1
2	G	805	MVA	C-CA-CB-CG2
2	H	805	MVA	N-CA-CB-CG2
2	E	807	MVA	CB-CA-N-CN
2	E	807	MVA	N-CA-CB-CG1
2	E	807	MVA	N-CA-CB-CG2
2	E	807	MVA	C-CA-CB-CG1
2	E	807	MVA	C-CA-CB-CG2
2	F	807	MVA	CB-CA-N-CN
2	F	807	MVA	N-CA-CB-CG1
2	F	807	MVA	C-CA-CB-CG1

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Mol	Chain	Res	Type	Atoms
2	G	807	MVA	CB-CA-N-CN
2	H	807	MVA	CB-CA-N-CN
2	H	807	MVA	C-CA-CB-CG1
2	E	808	MVA	N-CA-CB-CG1
2	E	808	MVA	N-CA-CB-CG2
2	E	808	MVA	C-CA-CB-CG2
2	F	808	MVA	CB-CA-N-CN
2	F	808	MVA	N-CA-CB-CG1
2	F	808	MVA	N-CA-CB-CG2
2	G	808	MVA	CB-CA-N-CN
2	H	808	MVA	CB-CA-N-CN
2	E	809	SAR	C-CA-N-CN
2	G	809	SAR	C-CA-N-CN
2	H	809	SAR	C-CA-N-CN
2	H	810	MVA	CB-CA-N-CN
2	H	811	IML	CB-CA-N-CN
2	F	807	MVA	C-CA-CB-CG2
2	H	808	MVA	C-CA-CB-CG2
2	F	807	MVA	N-CA-CB-CG2
2	E	805	MVA	CB-CA-N-CN
2	F	805	MVA	CB-CA-N-CN
2	G	805	MVA	CB-CA-N-CN
2	H	805	MVA	CB-CA-N-CN
2	E	808	MVA	CB-CA-N-CN
2	E	807	MVA	O-C-CA-CB
2	E	808	MVA	O-C-CA-CB
2	F	808	MVA	O-C-CA-CB
2	G	808	MVA	O-C-CA-CB
2	H	805	MVA	N-CA-CB-CG1

There are no ring outliers.

16 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	809	SAR	1	0
2	E	807	MVA	10	0
2	E	808	MVA	3	0
2	H	807	MVA	6	0
2	G	808	MVA	4	0
2	H	805	MVA	1	0
2	H	808	MVA	9	0
2	F	808	MVA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	809	SAR	5	0
2	G	805	MVA	1	0
2	F	807	MVA	4	0
2	H	809	SAR	4	0
2	E	805	MVA	1	0
2	H	811	IML	1	0
2	G	807	MVA	2	0
2	H	810	MVA	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	EDO	D	801	-	3,3,3	0.09	0	2,2,2	0.15	0
3	EDO	B	801	-	3,3,3	0.05	0	2,2,2	0.09	0
3	EDO	D	802	-	3,3,3	0.05	0	2,2,2	0.24	0
3	EDO	C	801	-	3,3,3	0.11	0	2,2,2	0.28	0
4	BCT	B	802	-	2,3,3	1.06	0	2,3,3	1.15	0
5	PEG	D	807	-	6,6,6	0.17	0	5,5,5	0.11	0
5	PEG	C	802	-	6,6,6	0.24	0	5,5,5	0.11	0
3	EDO	C	806	-	3,3,3	0.09	0	2,2,2	0.24	0
3	EDO	D	803	-	3,3,3	0.13	0	2,2,2	0.31	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
3	EDO	D	801	-	-	1/1/1/1	-
3	EDO	B	801	-	-	1/1/1/1	-
3	EDO	D	802	-	-	1/1/1/1	-
3	EDO	C	801	-	-	1/1/1/1	-
5	PEG	D	807	-	-	2/4/4/4	-
5	PEG	C	802	-	-	1/4/4/4	-
3	EDO	C	806	-	-	0/1/1/1	-
3	EDO	D	803	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	807	PEG	O2-C3-C4-O4
5	D	807	PEG	C4-C3-O2-C2
3	D	801	EDO	O1-C1-C2-O2
3	D	802	EDO	O1-C1-C2-O2
3	B	801	EDO	O1-C1-C2-O2
3	C	801	EDO	O1-C1-C2-O2
5	C	802	PEG	C1-C2-O2-C3
3	D	803	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	720/745 (96%)	0.13	17 (2%) 59 61	54, 74, 98, 131	0
1	B	718/745 (96%)	0.28	24 (3%) 46 49	59, 79, 112, 135	0
1	C	706/745 (94%)	0.42	48 (6%) 17 17	52, 80, 117, 145	0
1	D	719/745 (96%)	0.06	10 (1%) 75 77	48, 68, 95, 112	0
2	E	1/15 (6%)	4.17	1 (100%) 0 0	112, 112, 112, 112	0
2	F	4/15 (26%)	3.77	3 (75%) 0 0	124, 125, 126, 131	0
2	G	1/15 (6%)	0.57	0 100 100	107, 107, 107, 107	0
2	H	5/15 (33%)	1.76	3 (60%) 0 0	93, 93, 95, 98	0
All	All	2874/3040 (94%)	0.23	106 (3%) 41 44	48, 75, 111, 145	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	664	TYR	7.6
2	F	804	TRP	5.9
1	C	225	ASP	5.0
1	C	161	TYR	5.0
1	C	191	ASP	4.9
1	D	81	TRP	4.8
2	F	802	PHE	4.7
1	A	170	TRP	4.7
1	B	4	PRO	4.4
1	C	185	SER	4.3
2	E	806	ILE	4.2
1	B	664	TYR	4.1
1	C	175	VAL	4.1
1	C	167	GLY	4.0
1	A	3	PHE	3.9
1	A	664	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	703	ALA	3.7
1	C	421	PHE	3.6
1	C	114	VAL	3.6
1	C	190	LYS	3.6
1	C	77	LEU	3.6
1	B	704	GLY	3.5
1	C	253	LEU	3.5
2	H	804	TRP	3.5
1	D	704	GLY	3.4
1	C	168	SER	3.4
1	C	146	ALA	3.4
1	B	53	VAL	3.3
1	B	170	TRP	3.3
1	C	81	TRP	3.3
1	C	216	PHE	3.2
1	B	444	TYR	3.2
1	C	158	TYR	3.1
1	A	186	GLN	3.1
1	B	720	PHE	3.1
1	D	650	GLY	3.1
1	D	444	TYR	3.1
1	C	97	TYR	3.0
1	C	133	PHE	3.0
1	B	487	LEU	2.9
1	C	438	PHE	2.9
1	C	192	PRO	2.9
1	C	504	LEU	2.9
1	C	89	LEU	2.9
1	C	136	PRO	2.8
1	B	33	ARG	2.8
2	F	806	ILE	2.7
1	C	163	VAL	2.7
1	C	451	ILE	2.7
1	B	692	LEU	2.7
2	H	801	GLY	2.7
1	D	664	TYR	2.7
1	A	421	PHE	2.6
1	D	204	PHE	2.6
1	C	215	GLY	2.6
1	C	200	ARG	2.6
1	C	696	ASP	2.6
1	B	698	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	697	LEU	2.5
1	B	43	PHE	2.5
1	A	536	TYR	2.5
1	D	53	VAL	2.5
1	C	106	GLN	2.5
1	A	139	LEU	2.4
1	A	188	ARG	2.4
1	C	183	LEU	2.4
1	A	292	ILE	2.4
1	A	434	TYR	2.4
1	A	167	GLY	2.4
1	C	141	LEU	2.4
1	C	159	TRP	2.4
1	C	84	ARG	2.3
2	H	802	PHE	2.3
1	B	728	THR	2.3
1	C	79	LYS	2.3
1	C	139	LEU	2.3
1	A	204	PHE	2.3
1	C	174	TYR	2.3
1	B	190	LYS	2.2
1	A	189	GLY	2.2
1	C	193	GLY	2.2
1	C	731	THR	2.2
1	C	177	LYS	2.2
1	B	7	GLY	2.2
1	C	166	HIS	2.2
1	C	172	SER	2.2
1	A	182	HIS	2.2
1	C	150	PHE	2.2
1	C	83	TYR	2.2
1	C	711	LEU	2.2
1	B	45	ASP	2.1
1	A	467	PHE	2.1
1	B	44	GLU	2.1
1	B	66	GLU	2.1
1	B	686	LYS	2.1
1	C	708	GLN	2.1
1	D	710	MET	2.1
1	B	292	ILE	2.1
1	A	133	PHE	2.1
1	B	49	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	241	TYR	2.1
1	B	32	VAL	2.1
1	B	708	GLN	2.0
1	C	456	LEU	2.0
1	D	66	GLU	2.0
1	A	190	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	MVA	G	805	8/9	0.53	0.33	101,104,108,108	0
2	SAR	E	809	5/6	0.68	0.33	98,102,105,105	0
2	MVA	F	808	8/9	0.74	0.28	106,113,116,117	0
2	MVA	E	805	8/9	0.77	0.27	105,109,110,110	0
2	MVA	E	808	8/9	0.81	0.24	104,106,109,109	0
2	MVA	F	807	8/9	0.83	0.37	121,122,124,125	0
2	MVA	E	807	8/9	0.86	0.31	109,111,113,113	0
2	MVA	F	805	8/9	0.87	0.25	122,124,126,127	0
2	MVA	H	810	8/9	0.89	0.19	100,101,102,103	0
2	MVA	G	807	8/9	0.90	0.28	106,107,108,109	0
2	MVA	G	808	8/9	0.90	0.28	108,109,110,112	0
2	IML	H	811	9/10	0.90	0.20	92,94,98,98	0
2	SAR	H	809	5/6	0.91	0.13	99,99,100,102	0
2	SAR	G	809	5/6	0.92	0.28	92,97,103,104	0
2	MVA	H	808	8/9	0.92	0.22	97,99,99,100	0
2	MVA	H	807	8/9	0.93	0.14	93,96,97,98	0
2	MVA	H	805	8/9	0.97	0.28	93,95,98,99	0

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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
3	EDO	C	806	4/4	0.55	0.26	82,84,85,85	0
3	EDO	D	801	4/4	0.66	0.20	77,79,81,83	0
3	EDO	D	803	4/4	0.66	0.27	77,77,77,78	0
3	EDO	D	802	4/4	0.67	0.20	82,85,87,91	0
4	BCT	B	802	4/4	0.76	0.32	83,83,85,87	0
3	EDO	B	801	4/4	0.80	0.18	81,81,83,83	0
6	NA	D	806	1/1	0.80	0.46	58,58,58,58	0
3	EDO	C	801	4/4	0.83	0.27	74,74,75,75	0
6	NA	D	804	1/1	0.86	0.18	62,62,62,62	0
5	PEG	D	807	7/7	0.86	0.25	101,102,104,105	0
5	PEG	C	802	7/7	0.87	0.16	88,88,89,90	0
6	NA	D	805	1/1	0.92	0.55	64,64,64,64	0
6	NA	C	804	1/1	0.94	0.20	61,61,61,61	0
6	NA	C	803	1/1	0.94	0.29	60,60,60,60	0
6	NA	C	805	1/1	0.96	0.44	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.