



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 PM GMT

PDB ID : 4GCL
Title : structure of no-dna factor
Authors : Schumacher, M.A.
Deposited on : 2012-07-30
Resolution : 2.65 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

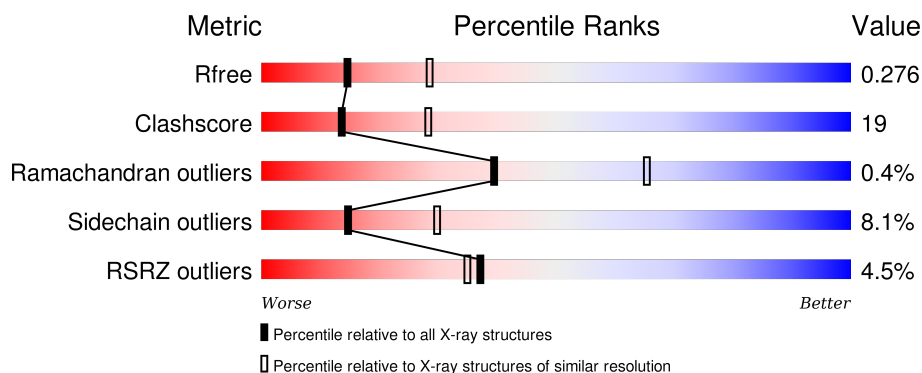
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	212	<div> <div>2%</div> <div>55%</div> <div>31%</div> <div>•</div> <div>10%</div> </div>
1	B	212	<div> <div>9%</div> <div>48%</div> <div>40%</div> <div>• •</div> <div>8%</div> </div>
1	C	212	<div> <div>64%</div> <div>21%</div> <div>5%</div> <div>10%</div> </div>
1	D	212	<div> <div>3%</div> <div>55%</div> <div>31%</div> <div>•</div> <div>11%</div> </div>
1	E	212	<div> <div>•</div> <div>49%</div> <div>37%</div> <div>•</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	212	
1	G	212	
1	H	212	
2	R	14	
2	T	14	
2	W	14	
2	Z	14	

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	MES	A	201	-	-	-	X
3	MES	F	201	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13922 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 Nucleoid occlusion factor SlmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1535	966	278	285	6			
1	B	196	Total	C	N	O	S	0	0	0
			1587	997	290	294	6			
1	C	190	Total	C	N	O	S	0	0	0
			1541	969	281	285	6			
1	D	189	Total	C	N	O	S	0	0	0
			1530	963	277	284	6			
1	E	190	Total	C	N	O	S	0	0	0
			1541	969	281	285	6			
1	F	189	Total	C	N	O	S	0	0	0
			1530	963	277	284	6			
1	G	190	Total	C	N	O	S	0	0	0
			1541	969	281	285	6			
1	H	190	Total	C	N	O	S	0	0	0
			1541	969	281	285	6			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			
2	Z	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			
2	R	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			
2	T	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	33	Total	O	0	0
			33	33		
4	C	67	Total	O	0	0
			67	67		
4	D	49	Total	O	0	0
			49	49		
4	E	41	Total	O	0	0
			41	41		
4	F	38	Total	O	0	0
			38	38		
4	G	43	Total	O	0	0
			43	43		
4	H	62	Total	O	0	0
			62	62		

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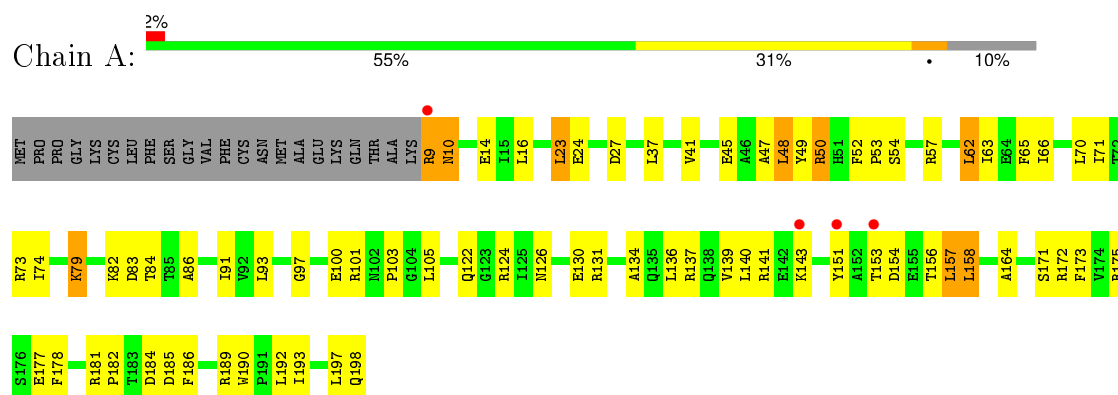
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	7	Total 7	O 7	0	0
4	Z	10	Total 10	O 10	0	0
4	R	10	Total 10	O 10	0	0
4	T	10	Total 10	O 10	0	0

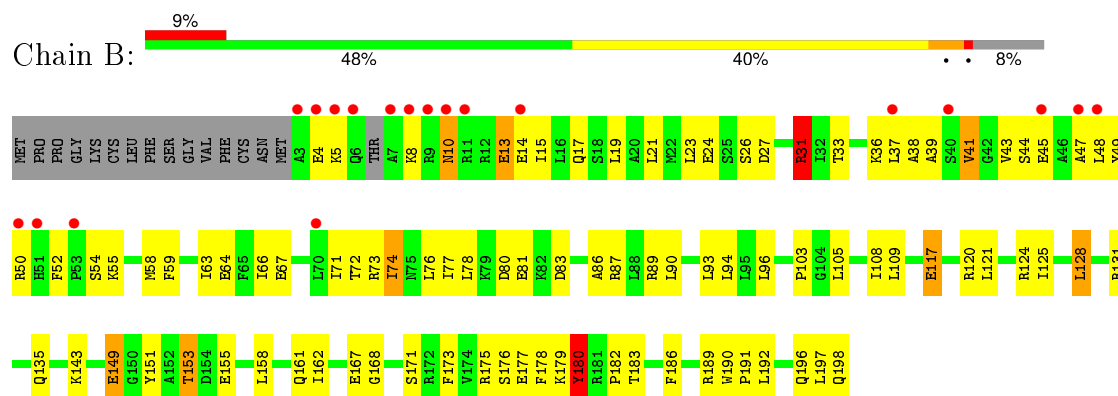
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

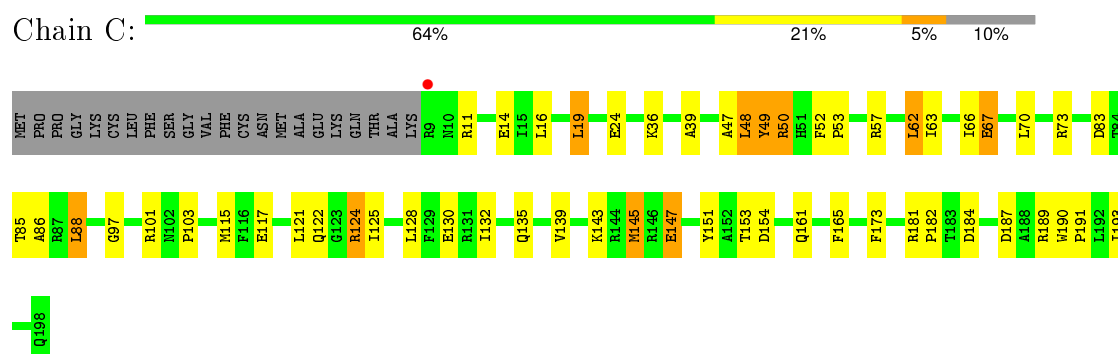
• Molecule 1: Nucleoid occlusion factor SlmA



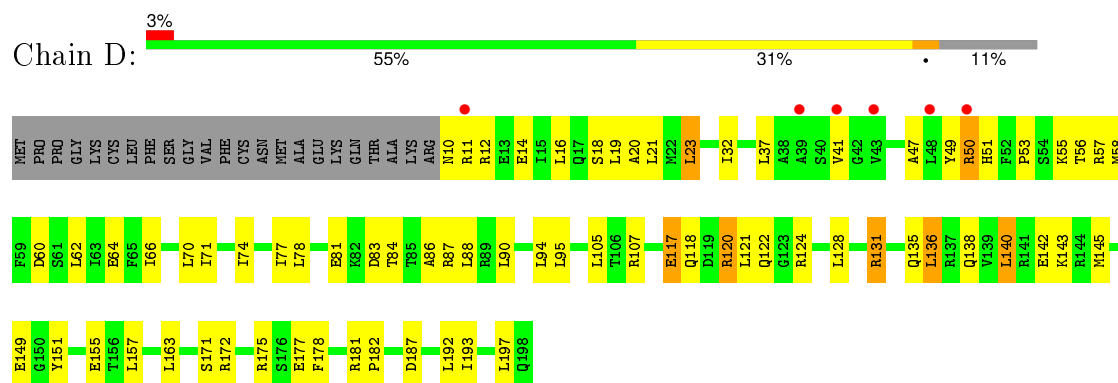
• Molecule 1: Nucleoid occlusion factor SlmA



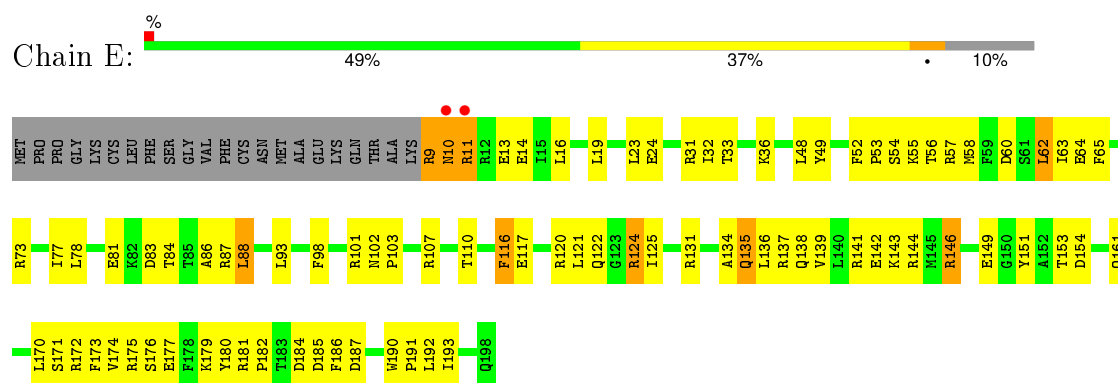
• Molecule 1: Nucleoid occlusion factor SlmA



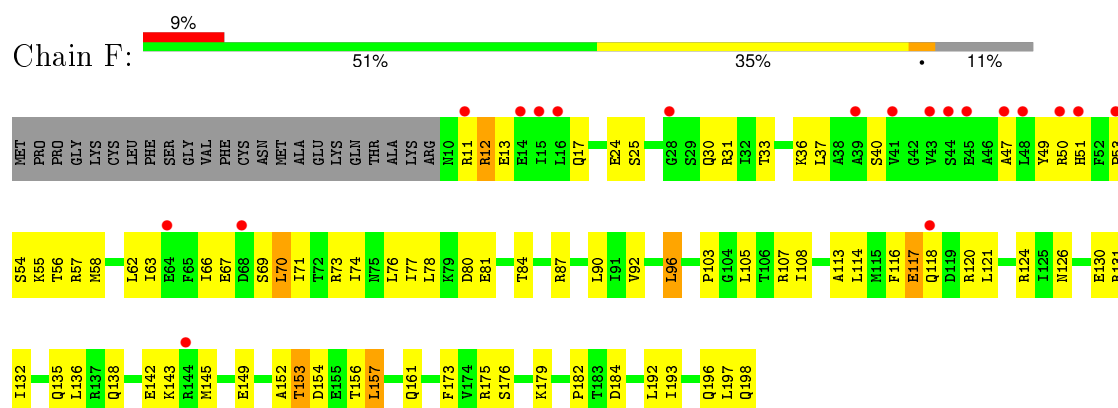
- Molecule 1: Nucleoid occlusion factor SlmA



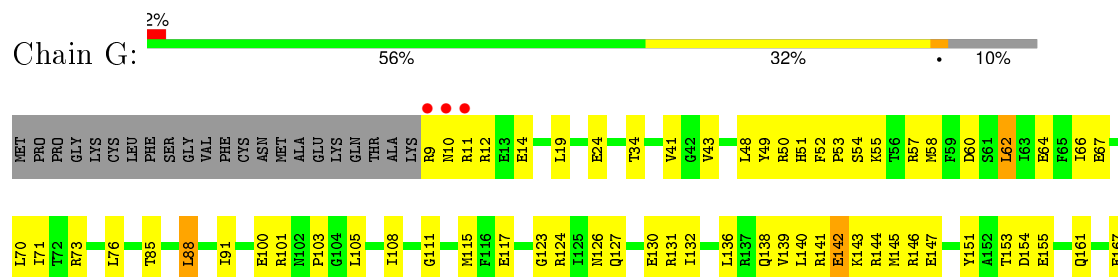
- Molecule 1: Nucleoid occlusion factor SlmA

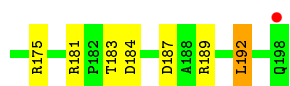


- Molecule 1: Nucleoid occlusion factor SlmA

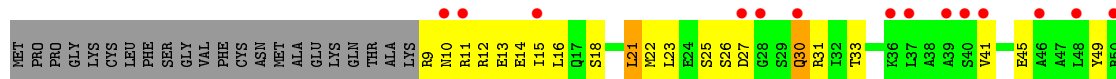


- Molecule 1: Nucleoid occlusion factor SlmA





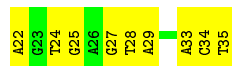
- Molecule 1: Nucleoid occlusion factor SlmA



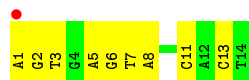
- Molecule 2: DNA (5'-D(*AP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP*T)-3')



- Molecule 2: DNA (5'-D(*AP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP*T)-3')



- Molecule 2: DNA (5'-D(*AP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP*T)-3')



- Molecule 2: DNA (5'-D(*AP*GP*TP*GP*AP*GP*TP*AP*CP*TP*CP*AP*CP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.29Å 160.52Å 201.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.39 – 2.65 64.39 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.4 (64.39-2.65) 91.5 (64.39-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.65Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.230 , 0.276 0.230 , 0.276	Depositor DCC
R_{free} test set	6993 reflections (11.40%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	1.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	16 of 61488 reflections (0.026%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13922	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.80 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4681e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MES

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	0.55	0/1555	0.61	0/2088
1	B	0.66	3/1607 (0.2%)	0.66	2/2155 (0.1%)
1	C	0.63	0/1561	0.69	0/2095
1	D	0.69	2/1550 (0.1%)	0.81	3/2081 (0.1%)
1	E	0.58	0/1561	0.64	0/2095
1	F	0.59	0/1550	0.63	0/2081
1	G	0.58	0/1561	0.65	0/2095
1	H	0.60	0/1561	0.65	0/2095
2	R	0.68	0/318	0.76	0/489
2	T	0.64	0/318	0.72	0/489
2	W	0.67	0/318	0.78	0/489
2	Z	0.65	0/318	0.72	0/489
All	All	0.62	5/13778 (0.0%)	0.68	5/18741 (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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	TYR	CE2-CZ	8.97	1.50	1.38
1	D	12	ARG	CZ-NH2	8.76	1.44	1.33
1	B	180	TYR	CE1-CZ	7.92	1.48	1.38
1	B	13	GLU	CD-OE1	-6.44	1.18	1.25
1	D	12	ARG	NE-CZ	6.37	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	D	12	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	B	13	GLU	CG-CD-OE1	-5.72	106.85	118.30
1	B	41	VAL	CB-CA-C	-5.54	100.87	111.40
1	D	12	ARG	NH1-CZ-NH2	-5.54	113.31	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	180	TYR	Sidechain

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	1535	0	1566	59	0
1	B	1587	0	1627	84	0
1	C	1541	0	1577	48	0
1	D	1530	0	1564	61	0
1	E	1541	0	1577	79	0
1	F	1530	0	1564	57	0
1	G	1541	0	1577	57	0
1	H	1541	0	1577	56	0
2	R	284	0	160	10	0
2	T	284	0	160	13	0
2	W	284	0	160	15	0
2	Z	284	0	160	9	0
3	A	12	0	13	1	0
3	C	12	0	13	0	0
3	E	12	0	13	4	0
3	F	12	0	13	0	0
4	A	22	0	0	0	0
4	B	33	0	0	0	0
4	C	67	0	0	9	0
4	D	49	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	41	0	0	3	0
4	F	38	0	0	3	0
4	G	43	0	0	1	0
4	H	62	0	0	7	0
4	R	10	0	0	0	0
4	T	10	0	0	2	0
4	W	7	0	0	0	0
4	Z	10	0	0	0	0
All	All	13922	0	13321	498	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 19.

All (498) 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:64:GLU:HG3	1:D:124:ARG:HH22	1.26	1.01
1:H:64:GLU:HG3	1:H:124:ARG:HH22	1.24	0.99
1:B:176:SER:HB3	1:B:180:TYR:CD2	2.04	0.92
1:E:192:LEU:HD11	1:F:153:THR:HG21	1.53	0.91
1:A:73:ARG:NH1	1:A:101:ARG:HH22	1.70	0.88
1:A:9:ARG:HE	1:A:10:ASN:HB2	1.37	0.88
1:F:69:SER:HB3	1:F:73:ARG:HH12	1.38	0.88
1:B:176:SER:HB3	1:B:180:TYR:HD2	1.36	0.86
1:E:9:ARG:HH21	1:E:11:ARG:HB2	1.39	0.86
1:D:57:ARG:HH21	1:D:120:ARG:HH12	1.24	0.82
1:A:73:ARG:HH12	1:A:101:ARG:HH22	1.26	0.81
1:A:140:LEU:HD13	1:A:158:LEU:HB3	1.63	0.81
1:C:145:MET:HE2	4:C:365:HOH:O	1.81	0.81
1:C:143:LYS:HG2	1:C:147:GLU:HG3	1.61	0.80
2:Z:28:DT:H2"	2:Z:29:DA:C8	2.18	0.79
1:G:64:GLU:HG3	1:G:124:ARG:HH22	1.48	0.79
1:E:73:ARG:HH12	1:E:101:ARG:HH22	1.28	0.79
1:B:176:SER:CB	1:B:180:TYR:CD2	2.67	0.78
1:B:176:SER:CB	1:B:180:TYR:HD2	1.97	0.78
1:E:81:GLU:O	1:E:87:ARG:HD2	1.85	0.77
1:A:71:ILE:HD11	1:A:131:ARG:HG2	1.65	0.76
1:B:13:GLU:O	1:B:17:GLN:HG2	1.85	0.76
1:B:71:ILE:HD11	1:B:131:ARG:HD3	1.68	0.76
1:E:161:GLN:HG2	1:F:192:LEU:HD23	1.65	0.76
1:D:56:THR:HG21	1:D:118:GLN:OE1	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:28:DT:H2"	2:T:29:DA:C8	2.22	0.75
1:F:108:ILE:HG23	1:F:114:LEU:HD21	1.68	0.75
4:E:314:HOH:O	1:F:175:ARG:HG2	1.85	0.75
1:C:153:THR:HG22	1:C:154:ASP:H	1.53	0.73
1:E:172:ARG:HD3	1:E:175:ARG:NH2	2.03	0.73
1:C:145:MET:CE	4:C:365:HOH:O	2.34	0.72
1:D:70:LEU:O	1:D:74:ILE:HG12	1.88	0.72
1:F:126:ASN:O	1:F:130:GLU:HG2	1.90	0.72
1:C:88:LEU:HD13	1:C:139:VAL:HG11	1.70	0.72
1:F:80:ASP:HB3	4:F:313:HOH:O	1.90	0.71
1:A:192:LEU:HD11	1:B:153:THR:HG21	1.72	0.71
1:C:16:LEU:HD22	1:C:62:LEU:HD13	1.71	0.71
1:H:16:LEU:HD22	1:H:62:LEU:HD13	1.72	0.70
1:E:31:ARG:HB3	1:E:116:PHE:CD2	2.25	0.70
1:C:117:GLU:HB3	4:C:306:HOH:O	1.91	0.70
1:C:24:GLU:HG3	1:C:103:PRO:HB2	1.74	0.69
1:G:142:GLU:HG2	1:G:146:ARG:HE	1.57	0.69
1:A:172:ARG:HG2	1:B:167:GLU:OE2	1.93	0.69
1:E:9:ARG:HD2	1:E:10:ASN:H	1.56	0.69
1:F:152:ALA:HB3	1:F:198:GLN:O	1.93	0.69
1:E:16:LEU:HD22	1:E:62:LEU:HD13	1.73	0.68
1:F:13:GLU:O	1:F:17:GLN:HG2	1.94	0.68
1:H:64:GLU:HG3	1:H:124:ARG:NH2	2.04	0.68
1:D:136:LEU:O	1:D:140:LEU:HG	1.94	0.68
1:H:25:SER:HB2	4:H:207:HOH:O	1.92	0.67
1:B:47:ALA:HA	1:B:50:ARG:NH1	2.09	0.67
1:F:62:LEU:O	1:F:66:ILE:HG12	1.94	0.67
1:A:154:ASP:HB3	1:A:157:LEU:HB2	1.75	0.67
1:B:73:ARG:O	1:B:77:ILE:HG13	1.95	0.67
1:B:171:SER:O	1:B:175:ARG:HG3	1.95	0.66
1:G:161:GLN:HG2	1:H:192:LEU:HD23	1.76	0.66
1:G:9:ARG:HD2	1:G:11:ARG:H	1.61	0.66
1:C:189:ARG:HG3	1:D:157:LEU:HD11	1.78	0.66
1:B:41:VAL:HG12	1:B:41:VAL:O	1.96	0.66
1:B:176:SER:HB2	1:B:179:LYS:HB3	1.77	0.66
1:H:64:GLU:HB3	4:H:224:HOH:O	1.97	0.65
1:G:88:LEU:HD13	1:G:139:VAL:HG11	1.78	0.65
1:H:13:GLU:HB3	4:H:231:HOH:O	1.96	0.65
1:A:140:LEU:HD22	1:A:158:LEU:HD13	1.78	0.64
1:F:50:ARG:HD2	4:F:308:HOH:O	1.97	0.64
1:F:132:ILE:O	1:F:136:LEU:HD13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:LEU:O	1:D:41:VAL:HG23	1.98	0.64
1:G:73:ARG:HH12	1:G:101:ARG:HH12	1.46	0.64
1:B:33:THR:HG22	2:W:11:DC:H3'	1.80	0.64
1:A:192:LEU:HD23	1:B:161:GLN:HG2	1.80	0.63
1:C:53:PRO:HG2	1:C:57:ARG:HG3	1.81	0.63
1:E:63:ILE:HD13	1:E:125:ILE:HG12	1.80	0.63
1:F:55:LYS:HD2	1:F:117:GLU:OE2	1.97	0.62
1:B:67:GLU:HG3	1:B:128:LEU:HG	1.81	0.62
1:D:64:GLU:HG3	1:D:124:ARG:NH2	2.07	0.62
1:B:190:TRP:HB3	1:B:191:PRO:HD3	1.82	0.62
1:E:13:GLU:OE1	3:E:201:MES:H72	2.00	0.62
1:E:88:LEU:HD13	1:E:139:VAL:HG11	1.81	0.62
1:D:57:ARG:NH2	1:D:120:ARG:HH12	1.97	0.61
1:E:11:ARG:HE	1:E:11:ARG:HA	1.65	0.61
1:A:158:LEU:HD21	1:A:197:LEU:HD23	1.82	0.61
1:A:24:GLU:HG3	1:A:103:PRO:HB2	1.82	0.61
1:D:49:TYR:OH	2:Z:33:DA:H2''	2.01	0.61
1:A:140:LEU:CD1	1:A:158:LEU:HB3	2.29	0.61
1:F:74:ILE:HG21	1:F:135:GLN:HG2	1.81	0.61
1:E:83:ASP:HB3	1:E:86:ALA:HB3	1.83	0.61
1:E:33:THR:OG1	1:E:36:LYS:HG3	2.01	0.60
1:E:73:ARG:NH1	1:E:101:ARG:HH22	1.99	0.60
2:W:5:DA:H1'	2:W:6:DG:H5'	1.80	0.60
1:G:138:GLN:O	1:G:141:ARG:HG2	2.01	0.60
1:G:73:ARG:NH1	1:G:101:ARG:HH12	2.00	0.60
1:G:49:TYR:HA	1:G:52:PHE:O	2.01	0.60
1:C:173:PHE:CD1	1:C:182:PRO:HD3	2.36	0.60
1:G:55:LYS:HA	1:G:58:MET:CE	2.33	0.59
1:E:176:SER:O	1:E:179:LYS:HE3	2.02	0.59
2:T:22:DA:H5'	4:T:109:HOH:O	2.03	0.59
2:W:1:DA:H61	2:Z:35:DT:H3	1.50	0.59
1:G:9:ARG:HD2	1:G:11:ARG:N	2.18	0.59
1:A:83:ASP:HB3	1:A:86:ALA:HB3	1.84	0.59
1:E:143:LYS:HD2	1:E:149:GLU:O	2.01	0.59
1:E:73:ARG:O	1:E:77:ILE:HG13	2.02	0.59
1:D:71:ILE:HD11	1:D:131:ARG:HG2	1.83	0.59
1:B:37:LEU:HD23	1:B:48:LEU:HD21	1.85	0.59
1:G:34:THR:HG21	1:G:49:TYR:OH	2.03	0.59
1:H:64:GLU:CG	1:H:124:ARG:HH22	2.06	0.58
1:B:86:ALA:O	1:B:90:LEU:HG	2.03	0.58
1:B:176:SER:HB3	1:B:180:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:GLN:HA	4:H:209:HOH:O	2.03	0.58
1:E:24:GLU:HG3	1:E:103:PRO:HB2	1.84	0.58
1:D:78:LEU:HD11	1:D:135:GLN:OE1	2.03	0.58
1:B:143:LYS:HE3	1:B:149:GLU:OE2	2.03	0.58
1:E:78:LEU:HD11	1:E:135:GLN:NE2	2.19	0.58
1:C:73:ARG:HH12	1:C:101:ARG:HH12	1.52	0.58
1:E:93:LEU:HD13	1:E:186:PHE:CD2	2.38	0.58
1:F:81:GLU:O	1:F:87:ARG:HD2	2.03	0.58
1:H:117:GLU:HB3	1:H:121:LEU:HD12	1.85	0.58
1:E:142:GLU:O	1:E:146:ARG:HD3	2.04	0.58
2:Z:24:DT:H2"	2:Z:25:DG:N7	2.19	0.57
1:B:71:ILE:CD1	1:B:131:ARG:HD3	2.34	0.57
1:D:23:LEU:HD13	1:D:32:ILE:HD11	1.86	0.57
1:F:84:THR:HG21	1:F:143:LYS:HB2	1.86	0.57
1:C:143:LYS:HD2	1:C:151:TYR:CZ	2.39	0.57
1:H:45:GLU:CD	2:R:13:DC:H41	2.08	0.57
1:H:57:ARG:HD3	4:H:217:HOH:O	2.05	0.57
1:B:73:ARG:HD2	1:B:94:LEU:HD11	1.87	0.57
1:C:53:PRO:CG	1:C:57:ARG:HG3	2.35	0.57
1:H:127:GLN:HE21	1:H:131:ARG:HH22	1.53	0.56
1:B:74:ILE:HA	1:B:77:ILE:HD12	1.87	0.56
1:F:63:ILE:HG21	1:F:124:ARG:HG2	1.88	0.56
1:E:185:ASP:HB3	1:F:157:LEU:HD11	1.86	0.56
1:B:72:THR:O	1:B:76:LEU:HG	2.05	0.56
1:G:51:HIS:CE1	2:R:1:DA:H3'	2.40	0.56
1:D:11:ARG:HB3	1:D:51:HIS:NE2	2.21	0.56
1:H:70:LEU:O	1:H:74:ILE:HG12	2.06	0.56
1:H:33:THR:HG22	2:R:11:DC:H3'	1.87	0.56
1:G:9:ARG:HG2	1:G:10:ASN:H	1.70	0.56
1:F:56:THR:HG23	1:F:121:LEU:HD11	1.88	0.56
1:H:141:ARG:O	1:H:144:ARG:HG3	2.05	0.56
1:G:73:ARG:HH12	1:G:101:ARG:NH1	2.03	0.56
1:D:19:LEU:HD12	1:D:19:LEU:O	2.05	0.56
1:B:10:ASN:O	1:B:14:GLU:HB2	2.05	0.56
1:E:170:LEU:O	1:E:174:VAL:HG23	2.06	0.56
1:C:49:TYR:OH	2:W:8:DA:H2"	2.04	0.56
1:H:69:SER:O	1:H:73:ARG:HG2	2.05	0.56
1:A:131:ARG:O	1:A:134:ALA:HB3	2.06	0.56
1:D:74:ILE:HD13	1:D:94:LEU:HD23	1.88	0.56
1:H:81:GLU:O	1:H:87:ARG:HD2	2.06	0.55
1:F:73:ARG:O	1:F:77:ILE:HG13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:SER:O	1:B:58:MET:HE2	2.07	0.55
1:E:110:THR:HG21	1:E:174:VAL:HG21	1.87	0.55
1:F:33:THR:OG1	1:F:36:LYS:HD3	2.07	0.55
1:F:107:ARG:HB3	1:F:113:ALA:HB2	1.88	0.55
2:W:14:DT:H3	2:Z:22:DA:H2	1.51	0.55
1:G:143:LYS:HD2	1:G:151:TYR:CZ	2.41	0.55
1:D:47:ALA:O	1:D:50:ARG:HG2	2.06	0.55
1:E:143:LYS:HG3	1:E:151:TYR:CZ	2.41	0.55
1:D:55:LYS:HG3	1:D:58:MET:HE3	1.88	0.55
1:F:138:GLN:HE21	1:F:142:GLU:HG3	1.72	0.55
1:H:143:LYS:HE3	1:H:147:GLU:HG3	1.88	0.54
1:B:73:ARG:HD2	1:B:94:LEU:CD1	2.38	0.54
2:T:34:DC:H1'	2:T:35:DT:H5'	1.88	0.54
1:C:161:GLN:HE22	1:D:193:ILE:HD11	1.73	0.54
1:B:81:GLU:O	1:B:87:ARG:HD2	2.07	0.54
1:A:9:ARG:NE	1:A:10:ASN:H	2.05	0.53
1:C:19:LEU:HD13	1:C:62:LEU:CD2	2.38	0.53
1:G:51:HIS:HE1	2:R:1:DA:H3'	1.74	0.53
1:E:117:GLU:HB3	1:E:121:LEU:HD12	1.90	0.53
1:F:69:SER:HB3	1:F:73:ARG:NH1	2.17	0.53
1:B:47:ALA:O	1:B:50:ARG:HG2	2.08	0.53
1:D:74:ILE:CD1	1:D:94:LEU:HD23	2.38	0.53
1:B:89:ARG:HG3	1:B:190:TRP:CE2	2.44	0.53
1:G:55:LYS:HA	1:G:58:MET:HE3	1.91	0.53
1:A:192:LEU:O	1:B:196:GLN:HG2	2.09	0.53
1:H:15:ILE:HG12	1:H:41:VAL:HG21	1.91	0.53
2:W:1:DA:N6	2:Z:35:DT:H3	2.06	0.52
1:B:66:ILE:HG21	1:B:109:LEU:HD21	1.90	0.52
1:C:143:LYS:HG2	1:C:147:GLU:CG	2.35	0.52
1:E:84:THR:HG21	1:E:143:LYS:HG2	1.91	0.52
1:A:66:ILE:HD11	1:A:105:LEU:HB3	1.91	0.52
1:A:16:LEU:HD22	1:A:62:LEU:HD13	1.91	0.52
1:G:9:ARG:HG2	1:G:10:ASN:N	2.25	0.52
1:B:143:LYS:HD2	1:B:151:TYR:CE2	2.44	0.52
1:A:173:PHE:CD1	1:A:182:PRO:HD3	2.44	0.52
1:B:5:LYS:HA	1:B:8:LYS:HE3	1.92	0.52
1:B:196:GLN:O	1:B:198:GLN:N	2.39	0.52
1:E:53:PRO:HG2	1:E:57:ARG:HG3	1.92	0.52
1:B:93:LEU:HB2	1:B:186:PHE:CE2	2.44	0.52
1:G:91:ILE:HG21	1:G:136:LEU:HD21	1.92	0.52
1:C:115:MET:CE	4:C:360:HOH:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:LEU:HD23	1:H:87:ARG:HG2	1.92	0.52
1:H:74:ILE:CD1	1:H:91:ILE:HG23	2.40	0.52
1:H:26:SER:HA	4:H:201:HOH:O	2.09	0.51
1:D:57:ARG:HH21	1:D:120:ARG:NH1	2.02	0.51
1:D:55:LYS:HG3	1:D:58:MET:CE	2.39	0.51
1:G:62:LEU:O	1:G:66:ILE:HG13	2.10	0.51
1:A:154:ASP:OD1	1:A:156:THR:HG23	2.11	0.51
1:B:41:VAL:CG1	1:B:41:VAL:O	2.57	0.51
1:D:117:GLU:HB3	1:D:121:LEU:HD12	1.92	0.51
1:F:37:LEU:O	1:F:40:SER:HB3	2.10	0.51
1:B:93:LEU:HD13	1:B:186:PHE:CD2	2.46	0.51
1:C:48:LEU:C	1:C:50:ARG:H	2.13	0.51
1:E:23:LEU:CD1	1:E:32:ILE:HG13	2.40	0.51
1:G:70:LEU:HD23	1:G:132:ILE:HD11	1.92	0.51
2:R:7:DT:H5'	4:T:101:HOH:O	2.10	0.50
1:F:92:VAL:HG12	1:F:96:LEU:HD22	1.92	0.50
1:F:55:LYS:HG3	1:F:58:MET:HE3	1.93	0.50
1:F:49:TYR:CE1	2:T:34:DC:H2'	2.46	0.50
1:E:181:ARG:HB2	1:E:184:ASP:OD1	2.12	0.50
1:F:67:GLU:O	1:F:71:ILE:HG12	2.11	0.50
1:E:9:ARG:HD2	1:E:10:ASN:ND2	2.26	0.50
1:G:24:GLU:HG3	1:G:103:PRO:HB2	1.94	0.50
1:H:72:THR:O	1:H:76:LEU:HG	2.12	0.50
1:E:135:GLN:HE21	1:E:135:GLN:HA	1.76	0.50
1:C:97:GLY:O	1:C:101:ARG:HG2	2.12	0.50
1:D:77:ILE:HD12	1:D:90:LEU:HB3	1.93	0.50
1:A:50:ARG:NH2	2:W:1:DA:N7	2.60	0.50
1:H:67:GLU:O	1:H:71:ILE:HG12	2.12	0.50
1:E:19:LEU:CD1	1:E:32:ILE:HG21	2.42	0.50
1:A:10:ASN:O	1:A:14:GLU:HB2	2.12	0.49
1:F:54:SER:HB2	2:T:34:DC:OP1	2.12	0.49
2:T:24:DT:H2''	2:T:25:DG:N7	2.27	0.49
1:E:192:LEU:O	1:F:196:GLN:HG2	2.12	0.49
1:A:151:TYR:C	1:A:153:THR:H	2.16	0.49
1:C:165:PHE:CE2	1:C:193:ILE:HD11	2.47	0.49
1:E:33:THR:HA	2:R:8:DA:OP1	2.13	0.49
2:T:23:DG:C2'	2:T:24:DT:H71	2.42	0.49
4:C:304:HOH:O	1:D:172:ARG:HB2	2.12	0.49
1:B:49:TYR:OH	2:W:13:DC:H6	1.95	0.49
1:E:23:LEU:O	1:E:107:ARG:HD2	2.11	0.49
1:B:173:PHE:CD1	1:B:182:PRO:HD3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:PRO:HG2	1:G:54:SER:H	1.77	0.49
1:F:196:GLN:C	1:F:198:GLN:H	2.16	0.49
1:G:9:ARG:HB3	1:G:12:ARG:H	1.76	0.49
1:A:100:GLU:OE1	1:A:181:ARG:HB3	2.13	0.49
1:F:53:PRO:HD2	1:F:57:ARG:HG3	1.94	0.49
1:E:190:TRP:HB3	1:E:191:PRO:HD3	1.95	0.49
1:F:196:GLN:O	1:F:198:GLN:N	2.35	0.49
1:B:196:GLN:O	1:B:198:GLN:HG2	2.13	0.49
1:F:143:LYS:NZ	1:F:149:GLU:OE2	2.44	0.49
1:A:84:THR:HG23	1:A:139:VAL:HG12	1.95	0.49
1:D:143:LYS:HD2	1:D:151:TYR:CE2	2.48	0.49
1:A:137:ARG:HD2	1:A:141:ARG:HH21	1.78	0.49
1:G:153:THR:HG22	1:G:154:ASP:N	2.28	0.49
1:B:55:LYS:O	1:B:58:MET:HB2	2.13	0.48
1:F:24:GLU:HG3	1:F:103:PRO:HB2	1.93	0.48
1:E:31:ARG:HD2	4:F:321:HOH:O	2.13	0.48
1:B:15:ILE:HD12	1:B:52:PHE:HE2	1.78	0.48
1:A:91:ILE:HG21	1:A:136:LEU:HD11	1.96	0.48
1:E:56:THR:N	4:E:313:HOH:O	2.42	0.48
1:D:16:LEU:HD22	1:D:62:LEU:CD1	2.44	0.48
1:C:47:ALA:O	1:C:50:ARG:HB3	2.14	0.48
1:D:151:TYR:HE1	1:D:197:LEU:HB3	1.79	0.48
1:B:19:LEU:HD12	1:B:19:LEU:O	2.14	0.48
1:H:143:LYS:HE2	1:H:149:GLU:OE1	2.14	0.48
1:A:57:ARG:HG2	1:A:57:ARG:HH11	1.79	0.48
1:G:101:ARG:O	1:G:101:ARG:HG3	2.13	0.48
1:B:83:ASP:HB3	1:B:86:ALA:HB3	1.95	0.48
1:D:55:LYS:CG	1:D:58:MET:HE3	2.42	0.48
1:D:151:TYR:CE1	1:D:197:LEU:HB3	2.48	0.48
1:A:45:GLU:O	1:A:48:LEU:HB2	2.14	0.47
1:B:64:GLU:CG	1:B:124:ARG:HH22	2.27	0.47
1:C:49:TYR:HA	1:C:52:PHE:O	2.14	0.47
1:C:36:LYS:O	1:C:39:ALA:HB3	2.13	0.47
1:D:107:ARG:NH2	1:D:177:GLU:OE1	2.46	0.47
1:B:43:VAL:HB	1:B:47:ALA:HB3	1.96	0.47
1:G:175:ARG:HB3	1:H:126:ASN:OD1	2.14	0.47
1:D:53:PRO:HD2	1:D:57:ARG:HG3	1.96	0.47
1:A:184:ASP:O	1:A:185:ASP:HB2	2.15	0.47
1:G:189:ARG:O	1:G:192:LEU:HB2	2.14	0.47
1:G:123:GLY:O	1:G:127:GLN:HG3	2.13	0.47
1:G:57:ARG:HH11	1:G:57:ARG:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:SER:HA	1:D:21:LEU:HD12	1.96	0.47
2:T:27:DG:H2'	2:T:28:DT:H71	1.95	0.47
1:A:126:ASN:O	1:A:130:GLU:HG2	2.14	0.47
1:E:10:ASN:O	1:E:14:GLU:HB2	2.14	0.47
1:E:9:ARG:HD2	1:E:10:ASN:N	2.25	0.47
1:A:171:SER:O	1:A:175:ARG:HG3	2.15	0.47
1:E:144:ARG:NH1	4:E:323:HOH:O	2.43	0.47
1:C:191:PRO:HG3	4:C:316:HOH:O	2.15	0.47
1:A:49:TYR:HA	1:A:52:PHE:O	2.15	0.47
1:F:47:ALA:HA	1:F:50:ARG:NH1	2.29	0.47
1:B:38:ALA:HB1	1:B:43:VAL:O	2.14	0.47
1:D:11:ARG:HB3	1:D:51:HIS:CD2	2.50	0.47
1:A:37:LEU:O	1:A:41:VAL:HG23	2.14	0.47
1:F:154:ASP:OD1	1:F:156:THR:N	2.47	0.47
1:H:189:ARG:O	1:H:192:LEU:HB2	2.14	0.47
1:D:81:GLU:O	1:D:87:ARG:HD2	2.15	0.47
1:A:63:ILE:HG21	1:A:124:ARG:HD3	1.97	0.47
1:C:11:ARG:NH1	1:C:14:GLU:OE2	2.48	0.47
1:E:181:ARG:O	1:E:184:ASP:HB2	2.15	0.46
1:D:149:GLU:HG3	1:D:149:GLU:O	2.15	0.46
1:E:49:TYR:HA	1:E:52:PHE:O	2.15	0.46
1:H:126:ASN:O	1:H:130:GLU:HG2	2.15	0.46
2:Z:27:DG:C2'	2:Z:28:DT:H5''	2.45	0.46
1:A:193:ILE:HD11	1:B:161:GLN:HE22	1.80	0.46
1:E:62:LEU:CD1	3:E:201:MES:H62	2.45	0.46
1:C:161:GLN:HG2	1:D:192:LEU:HD23	1.97	0.46
1:A:57:ARG:NH1	1:A:57:ARG:HG2	2.30	0.46
1:H:12:ARG:HG3	1:H:51:HIS:HB3	1.97	0.46
1:E:137:ARG:HD2	1:E:141:ARG:NH2	2.31	0.46
1:C:153:THR:HG22	1:C:154:ASP:N	2.26	0.46
1:A:143:LYS:HD2	1:A:151:TYR:CZ	2.51	0.46
1:H:185:ASP:O	1:H:189:ARG:HG3	2.16	0.46
1:G:105:LEU:O	1:G:108:ILE:HB	2.15	0.46
1:B:66:ILE:HG22	1:B:128:LEU:HD11	1.97	0.46
1:E:117:GLU:CB	1:E:121:LEU:HD12	2.45	0.46
1:B:4:GLU:O	1:B:8:LYS:HG3	2.15	0.46
1:B:36:LYS:O	1:B:39:ALA:HB3	2.16	0.46
1:H:49:TYR:CE1	2:R:13:DC:H2'	2.51	0.45
1:B:117:GLU:HB3	1:B:121:LEU:HD12	1.98	0.45
1:C:121:LEU:O	1:C:124:ARG:HB2	2.16	0.45
1:B:33:THR:CG2	2:W:11:DC:H3'	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PHE:O	1:E:144:ARG:NH2	2.49	0.45
1:D:83:ASP:HB3	1:D:86:ALA:HB3	1.97	0.45
1:B:63:ILE:O	1:B:66:ILE:HB	2.16	0.45
1:G:41:VAL:HB	1:G:43:VAL:HG22	1.98	0.45
1:G:88:LEU:CD1	1:G:139:VAL:HG11	2.44	0.45
1:G:111:GLY:O	1:G:115:MET:HE2	2.16	0.45
1:E:161:GLN:HE22	1:F:193:ILE:HD11	1.81	0.45
1:H:74:ILE:HD12	1:H:91:ILE:HG23	1.99	0.45
1:E:137:ARG:O	1:E:141:ARG:HG3	2.17	0.45
1:F:66:ILE:HD13	1:F:105:LEU:HD13	1.97	0.45
1:C:48:LEU:O	1:C:50:ARG:N	2.50	0.45
1:E:171:SER:O	1:E:175:ARG:HG3	2.17	0.45
1:B:158:LEU:O	1:B:162:ILE:HG13	2.17	0.45
1:B:45:GLU:HB3	2:W:14:DT:H73	1.98	0.45
1:G:181:ARG:HB2	1:G:184:ASP:CG	2.37	0.45
1:H:21:LEU:HD23	1:H:21:LEU:O	2.16	0.45
1:D:121:LEU:O	1:D:124:ARG:HB2	2.17	0.45
1:E:135:GLN:NE2	1:E:135:GLN:HA	2.32	0.45
1:D:23:LEU:HD13	1:D:32:ILE:CD1	2.46	0.45
1:B:49:TYR:OH	2:W:12:DA:H2"	2.17	0.45
1:C:115:MET:CE	1:C:115:MET:HA	2.47	0.45
1:G:9:ARG:C	1:G:11:ARG:H	2.20	0.44
1:G:55:LYS:NZ	1:G:117:GLU:OE1	2.42	0.44
1:E:146:ARG:HH11	1:E:146:ARG:HG3	1.82	0.44
1:A:70:LEU:O	1:A:74:ILE:HG12	2.16	0.44
1:D:66:ILE:HD11	1:D:105:LEU:HB3	1.98	0.44
1:G:67:GLU:O	1:G:71:ILE:HG12	2.18	0.44
1:H:11:ARG:HA	1:H:14:GLU:HB2	1.99	0.44
1:G:126:ASN:OD1	1:H:175:ARG:NH1	2.50	0.44
1:G:100:GLU:OE1	1:G:183:THR:OG1	2.29	0.44
1:B:43:VAL:HB	1:B:47:ALA:CB	2.48	0.44
1:H:137:ARG:HG2	1:H:141:ARG:HH22	1.83	0.44
1:D:122:GLN:NE2	4:D:221:HOH:O	2.50	0.44
1:H:181:ARG:HB2	1:H:184:ASP:OD2	2.17	0.44
1:A:79:LYS:O	1:A:82:LYS:HE2	2.17	0.44
1:E:62:LEU:HD11	3:E:201:MES:H62	1.98	0.44
1:F:78:LEU:HD11	1:F:135:GLN:NE2	2.33	0.44
1:D:55:LYS:HA	1:D:58:MET:HE3	2.00	0.44
1:E:98:PHE:O	1:E:102:ASN:ND2	2.39	0.44
1:A:137:ARG:HD2	1:A:141:ARG:NH2	2.32	0.44
1:G:57:ARG:NH1	1:G:57:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLY:O	1:A:101:ARG:HG3	2.16	0.44
1:E:173:PHE:CD1	1:E:182:PRO:HD3	2.53	0.44
2:R:5:DA:H2"	2:R:6:DG:OP2	2.18	0.44
1:F:77:ILE:HD13	1:F:90:LEU:HB3	1.99	0.44
1:B:192:LEU:HD12	1:B:192:LEU:N	2.33	0.44
1:E:135:GLN:HE21	1:E:135:GLN:CA	2.31	0.44
1:F:49:TYR:OH	2:T:33:DA:H2"	2.17	0.43
1:A:177:GLU:O	1:A:178:PHE:HB2	2.17	0.43
2:R:2:DG:C8	2:R:3:DT:H72	2.52	0.43
1:C:85:THR:HG22	4:C:327:HOH:O	2.18	0.43
1:H:67:GLU:OE2	1:H:131:ARG:NH1	2.51	0.43
2:Z:27:DG:H2"	2:Z:28:DT:H5"	2.00	0.43
1:G:11:ARG:HE	1:G:14:GLU:CD	2.20	0.43
1:E:63:ILE:HG21	1:E:124:ARG:HD2	2.00	0.43
1:E:19:LEU:HD12	1:E:32:ILE:HG21	1.99	0.43
1:C:62:LEU:O	1:C:66:ILE:HG13	2.18	0.43
1:H:149:GLU:OE2	1:H:149:GLU:N	2.43	0.43
1:H:18:SER:O	1:H:22:MET:HG3	2.19	0.43
1:E:193:ILE:HD11	1:F:161:GLN:HE22	1.83	0.43
2:T:32:DC:H2"	2:T:33:DA:C8	2.54	0.43
1:B:177:GLU:O	1:B:178:PHE:HB2	2.18	0.43
1:D:19:LEU:O	1:D:23:LEU:HB2	2.19	0.43
1:E:181:ARG:HA	1:E:182:PRO:HD3	1.90	0.43
1:H:62:LEU:HA	1:H:62:LEU:HD12	1.80	0.43
1:G:9:ARG:HB3	1:G:12:ARG:CB	2.48	0.43
1:D:49:TYR:CE1	2:Z:34:DC:H2'	2.54	0.43
1:A:65:PHE:HB2	3:A:201:MES:O3S	2.19	0.43
1:F:176:SER:HB2	1:F:179:LYS:HB3	2.00	0.43
1:D:118:GLN:HG3	1:D:120:ARG:CG	2.48	0.43
1:B:49:TYR:CE1	2:W:13:DC:H2'	2.54	0.43
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.86	0.43
2:T:23:DG:H2"	2:T:24:DT:H71	1.99	0.43
1:D:84:THR:HG21	1:D:143:LYS:HB2	1.99	0.43
1:A:151:TYR:HD1	1:A:198:GLN:O	2.02	0.43
1:B:31:ARG:HB2	1:B:31:ARG:HH11	1.84	0.43
1:G:64:GLU:HG3	1:G:124:ARG:NH2	2.26	0.42
1:H:141:ARG:HA	1:H:155:GLU:OE1	2.19	0.42
1:A:93:LEU:HD13	1:A:186:PHE:CD2	2.54	0.42
1:C:63:ILE:HG12	1:C:125:ILE:HD11	2.00	0.42
1:B:78:LEU:HD11	1:B:135:GLN:NE2	2.34	0.42
1:A:47:ALA:O	1:A:50:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:ARG:HB2	1:H:145:MET:HE2	2.01	0.42
1:H:193:ILE:O	1:H:196:GLN:HB2	2.19	0.42
1:C:190:TRP:HB3	1:C:191:PRO:HD3	2.01	0.42
1:G:140:LEU:HB3	1:G:155:GLU:HG3	2.01	0.42
1:A:153:THR:HG21	1:B:192:LEU:HD11	2.00	0.42
1:E:60:ASP:O	1:E:64:GLU:HG2	2.18	0.42
1:F:31:ARG:NH2	1:F:116:PHE:O	2.53	0.42
1:E:131:ARG:O	1:E:134:ALA:HB3	2.19	0.42
1:E:185:ASP:CB	1:F:157:LEU:HD11	2.49	0.42
1:B:55:LYS:HA	1:B:58:MET:CE	2.49	0.42
1:F:30:GLN:HA	1:F:116:PHE:CZ	2.55	0.42
1:F:173:PHE:CD1	1:F:182:PRO:HD3	2.54	0.42
1:C:88:LEU:HD12	1:C:88:LEU:HA	1.83	0.42
1:A:190:TRP:O	1:A:193:ILE:N	2.50	0.42
1:B:109:LEU:HD23	1:B:125:ILE:HD12	2.02	0.42
1:E:143:LYS:HG3	1:E:151:TYR:CE2	2.55	0.42
1:H:149:GLU:CD	1:H:149:GLU:H	2.23	0.42
1:H:41:VAL:HG12	1:H:41:VAL:O	2.20	0.42
1:E:23:LEU:HD11	1:E:32:ILE:HG13	2.02	0.42
1:B:59:PHE:CD2	1:B:117:GLU:HG2	2.54	0.42
1:D:11:ARG:O	1:D:14:GLU:HB2	2.19	0.42
1:D:16:LEU:HD22	1:D:62:LEU:HD12	2.02	0.42
1:H:30:GLN:HG3	4:H:242:HOH:O	2.19	0.42
1:H:190:TRP:HB3	1:H:191:PRO:HD3	2.02	0.42
1:A:153:THR:HG22	1:A:154:ASP:H	1.84	0.42
1:A:154:ASP:HB3	1:A:157:LEU:HD13	2.02	0.42
1:A:45:GLU:HA	1:A:48:LEU:HD22	2.01	0.42
1:D:71:ILE:HD12	1:D:131:ARG:NH1	2.35	0.42
1:D:193:ILE:H	1:D:193:ILE:HD12	1.85	0.42
1:G:192:LEU:O	1:H:196:GLN:HG2	2.20	0.42
1:D:87:ARG:HD2	1:D:87:ARG:HH11	1.70	0.42
1:B:24:GLU:HG3	1:B:103:PRO:HB2	2.01	0.42
1:G:64:GLU:HA	1:G:67:GLU:OE2	2.20	0.42
1:B:44:SER:H	1:B:47:ALA:HB3	1.85	0.42
1:B:64:GLU:HG3	1:B:124:ARG:NH2	2.35	0.42
1:H:136:LEU:HD12	1:H:136:LEU:HA	1.86	0.42
2:W:2:DG:H2"	2:W:3:DT:OP2	2.20	0.42
1:C:145:MET:HE1	4:C:365:HOH:O	2.12	0.41
1:B:105:LEU:O	1:B:108:ILE:HB	2.20	0.41
1:C:122:GLN:NE2	4:C:360:HOH:O	2.28	0.41
1:B:15:ILE:HD12	1:B:52:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ARG:HB2	1:C:184:ASP:CG	2.40	0.41
1:B:189:ARG:O	1:B:190:TRP:C	2.59	0.41
1:C:48:LEU:C	1:C:50:ARG:N	2.74	0.41
1:C:70:LEU:HD23	1:C:132:ILE:HD11	2.02	0.41
1:E:192:LEU:N	1:E:192:LEU:HD12	2.35	0.41
1:G:9:ARG:C	1:G:11:ARG:N	2.74	0.41
1:A:24:GLU:OE2	1:A:103:PRO:HG2	2.21	0.41
1:G:141:ARG:O	1:G:144:ARG:HG3	2.20	0.41
1:H:145:MET:H	1:H:145:MET:HG2	1.39	0.41
1:B:45:GLU:HB2	2:W:14:DT:O4	2.19	0.41
1:E:153:THR:HG22	1:E:154:ASP:N	2.34	0.41
1:B:183:THR:O	1:B:183:THR:HG22	2.20	0.41
1:F:193:ILE:HD12	1:F:193:ILE:N	2.36	0.41
1:A:189:ARG:NH1	1:B:161:GLN:OE1	2.50	0.41
1:D:55:LYS:HA	1:D:58:MET:CE	2.51	0.41
1:H:12:ARG:HG2	1:H:52:PHE:CZ	2.56	0.41
2:T:28:DT:C2'	2:T:29:DA:C8	3.00	0.41
1:B:45:GLU:CD	2:W:13:DC:H41	2.24	0.41
1:G:62:LEU:HD12	1:G:62:LEU:HA	1.76	0.41
1:F:71:ILE:HG21	1:F:131:ARG:NH2	2.36	0.41
1:D:177:GLU:O	1:D:178:PHE:HB2	2.21	0.41
1:D:181:ARG:HA	1:D:182:PRO:HD3	1.83	0.41
1:E:9:ARG:NH2	1:E:11:ARG:HB2	2.22	0.41
1:G:105:LEU:HD23	1:G:105:LEU:N	2.35	0.41
1:F:12:ARG:HG3	1:F:51:HIS:HB3	2.02	0.41
1:E:65:PHE:CE1	3:E:201:MES:H31	2.56	0.41
1:H:52:PHE:HA	1:H:53:PRO:HD3	1.91	0.41
1:D:88:LEU:HD21	1:D:140:LEU:CD2	2.51	0.41
1:D:20:ALA:O	1:D:23:LEU:N	2.54	0.41
1:F:138:GLN:HE21	1:F:142:GLU:CG	2.33	0.41
1:B:93:LEU:HB2	1:B:186:PHE:CZ	2.56	0.41
1:E:52:PHE:CG	1:E:58:MET:HG2	2.56	0.41
1:H:171:SER:O	1:H:175:ARG:HG3	2.21	0.41
1:F:76:LEU:HD23	1:F:76:LEU:HA	1.89	0.41
1:D:171:SER:O	1:D:175:ARG:HG3	2.20	0.41
1:C:135:GLN:HA	1:C:135:GLN:OE1	2.20	0.41
1:C:83:ASP:HB3	1:C:86:ALA:HB3	2.03	0.41
1:E:173:PHE:HD1	1:E:180:TYR:O	2.05	0.41
1:C:19:LEU:HD13	1:C:62:LEU:HD21	2.03	0.40
1:F:66:ILE:CD1	1:F:105:LEU:HB3	2.52	0.40
1:F:33:THR:HG22	2:T:32:DC:H3'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HG2	1:A:54:SER:H	1.85	0.40
1:C:67:GLU:HG2	1:C:128:LEU:HD13	2.02	0.40
1:B:176:SER:CB	1:B:179:LYS:HB3	2.49	0.40
1:D:70:LEU:HD22	1:D:95:LEU:HD23	2.03	0.40
1:D:88:LEU:HD21	1:D:140:LEU:HD21	2.02	0.40
1:C:173:PHE:CE1	1:C:182:PRO:HD3	2.56	0.40
1:E:53:PRO:HG2	1:E:54:SER:H	1.86	0.40
1:G:57:ARG:HA	1:G:60:ASP:HB2	2.03	0.40
1:C:190:TRP:N	1:C:191:PRO:CD	2.84	0.40
1:E:60:ASP:OD2	1:E:120:ARG:NH2	2.54	0.40
1:D:138:GLN:O	1:D:142:GLU:HG3	2.21	0.40
1:G:167:GLU:OE2	1:H:172:ARG:HG2	2.21	0.40
1:G:142:GLU:CG	1:G:146:ARG:HE	2.30	0.40
1:G:76:LEU:HB2	4:G:219:HOH:O	2.20	0.40
1:E:9:ARG:C	1:E:11:ARG:H	2.23	0.40
1:B:63:ILE:HG21	1:B:124:ARG:HG2	2.04	0.40
1:B:55:LYS:HA	1:B:58:MET:HE2	2.04	0.40
1:A:164:ALA:O	1:B:168:GLY:HA3	2.21	0.40
1:F:70:LEU:HD12	1:F:70:LEU:HA	1.98	0.40
1:E:83:ASP:HB3	1:E:86:ALA:CB	2.51	0.40
1:E:55:LYS:NZ	1:E:117:GLU:OE2	2.34	0.40
1:G:50:ARG:NH1	2:R:2:DG:N7	2.70	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	188/212 (89%)	174 (93%)	14 (7%)	0	100	100
1	B	194/212 (92%)	170 (88%)	21 (11%)	3 (2%)	13	28
1	C	188/212 (89%)	178 (95%)	9 (5%)	1 (0%)	34	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	187/212 (88%)	178 (95%)	9 (5%)	0	100	100
1	E	188/212 (89%)	183 (97%)	5 (3%)	0	100	100
1	F	187/212 (88%)	180 (96%)	5 (3%)	2 (1%)	17	38
1	G	188/212 (89%)	182 (97%)	6 (3%)	0	100	100
1	H	188/212 (89%)	179 (95%)	9 (5%)	0	100	100
All	All	1508/1696 (89%)	1424 (94%)	78 (5%)	6 (0%)	39	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	197	LEU
1	B	80	ASP
1	B	197	LEU
1	C	49	TYR
1	F	118	GLN
1	B	31	ARG

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	164/183 (90%)	153 (93%)	11 (7%)	20	41
1	B	169/183 (92%)	155 (92%)	14 (8%)	14	28
1	C	165/183 (90%)	154 (93%)	11 (7%)	20	41
1	D	164/183 (90%)	150 (92%)	14 (8%)	13	27
1	E	165/183 (90%)	150 (91%)	15 (9%)	12	24
1	F	164/183 (90%)	153 (93%)	11 (7%)	20	41
1	G	165/183 (90%)	153 (93%)	12 (7%)	17	36
1	H	165/183 (90%)	146 (88%)	19 (12%)	7	14
All	All	1321/1464 (90%)	1214 (92%)	107 (8%)	15	30

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	10	ASN
1	A	23	LEU
1	A	27	ASP
1	A	48	LEU
1	A	50	ARG
1	A	62	LEU
1	A	79	LYS
1	A	122	GLN
1	A	157	LEU
1	A	158	LEU
1	B	10	ASN
1	B	21	LEU
1	B	23	LEU
1	B	26	SER
1	B	27	ASP
1	B	31	ARG
1	B	74	ILE
1	B	96	LEU
1	B	117	GLU
1	B	120	ARG
1	B	128	LEU
1	B	149	GLU
1	B	153	THR
1	B	155	GLU
1	C	19	LEU
1	C	48	LEU
1	C	50	ARG
1	C	62	LEU
1	C	67	GLU
1	C	88	LEU
1	C	124	ARG
1	C	130	GLU
1	C	145	MET
1	C	147	GLU
1	C	187	ASP
1	D	10	ASN
1	D	23	LEU
1	D	50	ARG
1	D	60	ASP
1	D	117	GLU
1	D	120	ARG

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Mol	Chain	Res	Type
1	D	128	LEU
1	D	131	ARG
1	D	136	LEU
1	D	140	LEU
1	D	145	MET
1	D	155	GLU
1	D	163	LEU
1	D	187	ASP
1	E	9	ARG
1	E	10	ASN
1	E	11	ARG
1	E	48	LEU
1	E	62	LEU
1	E	88	LEU
1	E	116	PHE
1	E	122	GLN
1	E	124	ARG
1	E	135	GLN
1	E	136	LEU
1	E	138	GLN
1	E	146	ARG
1	E	177	GLU
1	E	187	ASP
1	F	11	ARG
1	F	12	ARG
1	F	25	SER
1	F	70	LEU
1	F	96	LEU
1	F	117	GLU
1	F	120	ARG
1	F	145	MET
1	F	153	THR
1	F	157	LEU
1	F	184	ASP
1	G	19	LEU
1	G	48	LEU
1	G	62	LEU
1	G	85	THR
1	G	88	LEU
1	G	130	GLU
1	G	131	ARG
1	G	142	GLU

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Mol	Chain	Res	Type
1	G	145	MET
1	G	147	GLU
1	G	187	ASP
1	G	192	LEU
1	H	9	ARG
1	H	10	ASN
1	H	21	LEU
1	H	23	LEU
1	H	27	ASP
1	H	30	GLN
1	H	31	ARG
1	H	60	ASP
1	H	62	LEU
1	H	117	GLU
1	H	118	GLN
1	H	128	LEU
1	H	136	LEU
1	H	144	ARG
1	H	145	MET
1	H	153	THR
1	H	163	LEU
1	H	177	GLU
1	H	187	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	17	GLN
1	A	102	ASN
1	A	122	GLN
1	B	6	GLN
1	B	135	GLN
1	D	10	ASN
1	D	17	GLN
1	D	112	HIS
1	D	122	GLN
1	D	198	GLN
1	E	10	ASN
1	E	122	GLN
1	E	135	GLN
1	E	138	GLN

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Mol	Chain	Res	Type
1	F	118	GLN
1	F	135	GLN
1	F	198	GLN
1	H	30	GLN
1	H	118	GLN
1	H	122	GLN
1	H	127	GLN
1	H	198	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MES	A	201	-	11,12,12	0.87	0	14,16,16	2.44	3 (21%)
3	MES	C	201	-	11,12,12	0.92	1 (9%)	14,16,16	2.75	4 (28%)
3	MES	E	201	-	11,12,12	0.83	1 (9%)	14,16,16	2.54	4 (28%)
3	MES	F	201	-	11,12,12	0.84	0	14,16,16	2.88	4 (28%)

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	MES	A	201	-	-	0/6/14/14	0/1/1/1
3	MES	C	201	-	-	0/6/14/14	0/1/1/1
3	MES	E	201	-	-	0/6/14/14	0/1/1/1
3	MES	F	201	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	MES	C3-C2	2.04	1.58	1.50
3	E	201	MES	C3-C2	2.13	1.58	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	MES	O3S-S-O2S	-2.27	106.33	111.61
3	E	201	MES	C7-C8-S	2.07	118.91	112.51
3	F	201	MES	C7-C8-S	2.11	119.06	112.51
3	E	201	MES	C5-N4-C3	2.36	114.01	108.90
3	F	201	MES	O1S-S-C8	2.58	109.11	106.91
3	A	201	MES	O1S-S-C8	2.85	109.34	106.91
3	E	201	MES	O1S-S-C8	2.86	109.34	106.91
3	C	201	MES	O1S-S-C8	2.88	109.36	106.91
3	A	201	MES	C5-N4-C3	2.95	115.30	108.90
3	C	201	MES	C5-N4-C3	3.08	115.57	108.90
3	F	201	MES	C5-N4-C3	3.22	115.88	108.90
3	A	201	MES	O2S-S-C8	7.13	112.99	106.91
3	E	201	MES	O2S-S-C8	7.79	113.56	106.91
3	C	201	MES	O2S-S-C8	8.57	114.21	106.91
3	F	201	MES	O2S-S-C8	9.12	114.69	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	MES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	201	MES	4	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	190/212 (89%)	0.10	4 (2%) 67 66	28, 49, 99, 109	0
1	B	196/212 (92%)	0.54	19 (9%) 10 7	31, 57, 92, 112	0
1	C	190/212 (89%)	0.01	1 (0%) 91 92	18, 36, 61, 111	0
1	D	189/212 (89%)	0.12	6 (3%) 51 50	18, 38, 74, 90	0
1	E	190/212 (89%)	0.13	2 (1%) 82 82	30, 47, 72, 94	0
1	F	189/212 (89%)	0.50	19 (10%) 9 6	30, 51, 85, 97	0
1	G	190/212 (89%)	0.00	4 (2%) 67 66	27, 45, 71, 98	0
1	H	190/212 (89%)	0.24	14 (7%) 17 14	27, 45, 74, 93	0
2	R	14/14 (100%)	0.31	1 (7%) 19 16	43, 61, 85, 98	0
2	T	14/14 (100%)	0.36	1 (7%) 19 16	46, 62, 81, 96	0
2	W	14/14 (100%)	0.00	0 100 100	35, 55, 70, 92	0
2	Z	14/14 (100%)	0.08	0 100 100	34, 52, 75, 97	0
All	All	1580/1752 (90%)	0.21	71 (4%) 37 35	18, 47, 82, 112	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LYS	9.0
1	B	7	ALA	6.5
1	B	51	HIS	5.4
1	B	4	GLU	5.1
1	B	8	LYS	4.9
1	G	9	ARG	4.9
1	B	6	GLN	4.7
1	B	3	ALA	4.7
1	A	153	THR	4.4
1	C	9	ARG	4.3
1	G	10	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	10	ASN	4.3
1	H	37	LEU	4.2
1	H	10	ASN	4.1
1	A	9	ARG	3.9
1	F	16	LEU	3.8
1	D	41	VAL	3.7
1	B	48	LEU	3.6
1	H	27	ASP	3.6
1	B	50	ARG	3.6
1	H	11	ARG	3.5
1	H	28	GLY	3.5
1	F	50	ARG	3.5
1	H	15	ILE	3.5
1	B	45	GLU	3.4
1	F	48	LEU	3.4
1	D	43	VAL	3.3
1	H	48	LEU	3.3
1	F	15	ILE	3.3
1	F	53	PRO	3.2
1	B	11	ARG	3.2
1	F	11	ARG	3.0
1	F	43	VAL	3.0
1	G	11	ARG	2.9
1	B	47	ALA	2.9
1	A	143	LYS	2.8
1	B	70	LEU	2.7
1	A	151	TYR	2.7
1	D	50	ARG	2.7
1	D	11	ARG	2.7
2	R	1	DA	2.7
1	H	36	LYS	2.7
1	F	47	ALA	2.6
1	F	144	ARG	2.6
1	B	40	SER	2.6
1	B	9	ARG	2.6
1	E	11	ARG	2.5
1	B	53	PRO	2.5
1	F	118	GLN	2.5
1	H	39	ALA	2.4
1	E	10	ASN	2.4
1	D	48	LEU	2.4
1	F	64	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	44	SER	2.4
1	F	51	HIS	2.4
1	H	50	ARG	2.4
1	H	30	GLN	2.4
1	B	14	GLU	2.3
1	F	14	GLU	2.3
2	T	22	DA	2.3
1	H	40	SER	2.3
1	D	39	ALA	2.2
1	F	41	VAL	2.2
1	F	28	GLY	2.2
1	F	68	ASP	2.1
1	B	37	LEU	2.1
1	F	39	ALA	2.1
1	F	45	GLU	2.0
1	G	198	GLN	2.0
1	H	41	VAL	2.0
1	H	46	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	MES	A	201	12/12	0.91	0.36	5.19	89,94,116,117	0
3	MES	F	201	12/12	0.88	0.44	2.02	93,100,117,117	0
3	MES	E	201	12/12	0.79	0.28	0.98	80,98,111,111	0
3	MES	C	201	12/12	0.77	0.32	0.71	55,85,122,125	0

6.5 Other polymers

There are no such residues in this entry.