



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:02 AM BST

PDB ID : 4KPL
Title : Crystal structure of d-mannonate dehydratase from chromohalobacter salexigens complexed with Mg,d-mannonate and 2-keto-3-deoxy-d-gluconate
Authors : Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2013-05-13
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

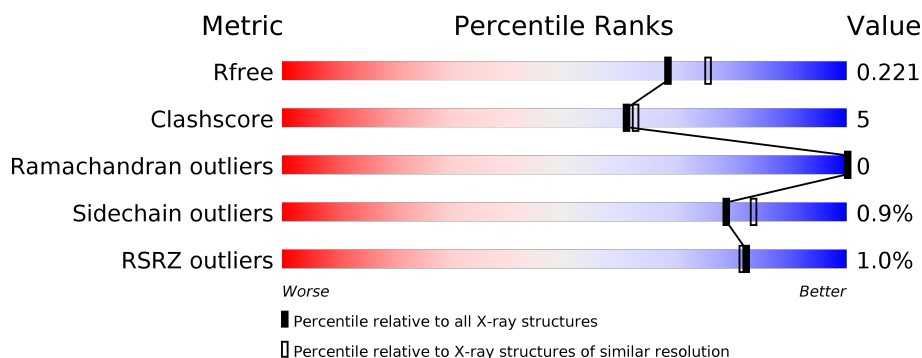
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	405	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	405	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>
1	C	405	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
1	D	405	<div> <div></div> <div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	E	405	<div> <div></div> <div> <div>86%</div> <div>9%</div> <div>•</div> </div> </div>
1	F	405	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	405	<div> <div>%</div> <div> </div> <div>83% 11% 5%</div> </div>
1	H	405	<div> <div>%</div> <div> </div> <div>83% 11% 5%</div> </div>

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
6	GOL	G	502	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 26541 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 D-mannonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	1	0
			3049	1933	545	557	14			
1	B	390	Total	C	N	O	S	0	2	0
			3100	1965	551	569	15			
1	C	385	Total	C	N	O	S	0	1	0
			3055	1936	546	559	14			
1	D	384	Total	C	N	O	S	0	0	0
			3043	1929	545	555	14			
1	E	389	Total	C	N	O	S	0	2	0
			3097	1963	551	568	15			
1	F	387	Total	C	N	O	S	0	0	0
			3068	1944	548	562	14			
1	G	383	Total	C	N	O	S	0	0	0
			3037	1926	544	553	14			
1	H	384	Total	C	N	O	S	0	0	0
			3043	1929	545	555	14			

There are 16 discrepancies between the modelled and reference sequences:

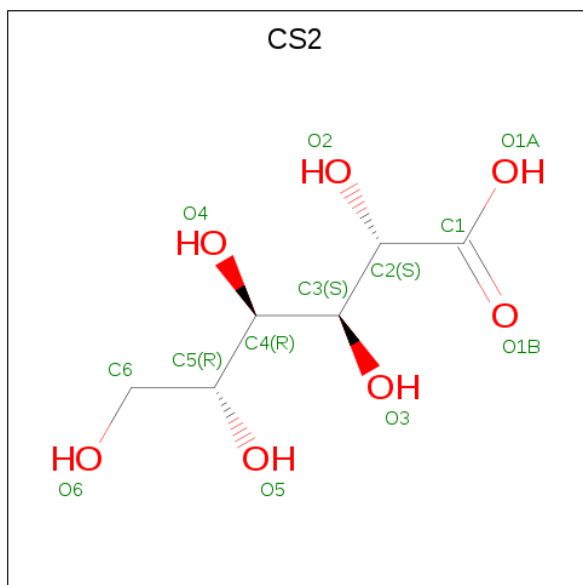
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	EXPRESSION TAG	UNP Q1QT89
A	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
B	2	SER	-	EXPRESSION TAG	UNP Q1QT89
B	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
C	2	SER	-	EXPRESSION TAG	UNP Q1QT89
C	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
D	2	SER	-	EXPRESSION TAG	UNP Q1QT89
D	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
E	2	SER	-	EXPRESSION TAG	UNP Q1QT89
E	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
F	2	SER	-	EXPRESSION TAG	UNP Q1QT89
F	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
G	2	SER	-	EXPRESSION TAG	UNP Q1QT89

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Chain	Residue	Modelled	Actual	Comment	Reference
G	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
H	2	SER	-	EXPRESSION TAG	UNP Q1QT89
H	3	LEU	-	EXPRESSION TAG	UNP Q1QT89

- Molecule 2 is D-MANNONIC ACID (three-letter code: CS2) (formula: C₆H₁₂O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0

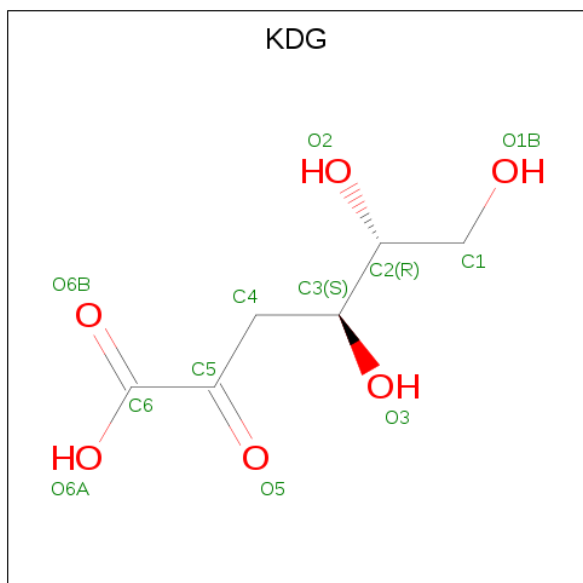
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-KETO-3-DEOXYGLUCONATE (three-letter code: KDG) (formula: C₆H₁₀O₆).



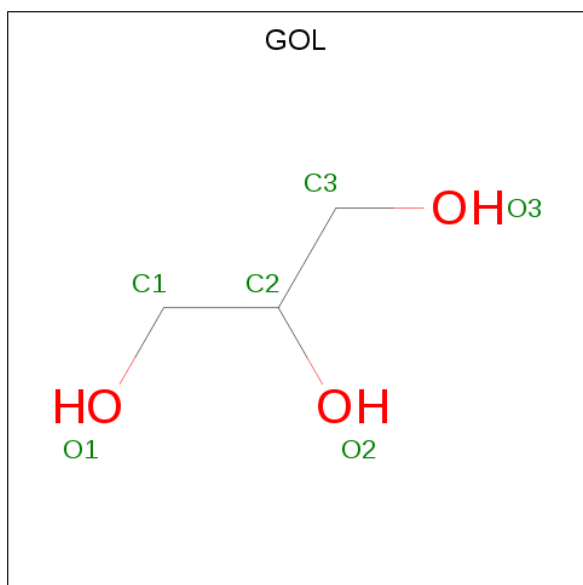
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			12	6	6		
5	D	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			12	6	6		
5	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	234	Total	O	0	2
			236	236		
7	B	242	Total	O	0	0
			242	242		
7	C	226	Total	O	0	2
			228	228		
7	D	224	Total	O	0	2
			226	226		
7	E	252	Total	O	0	1
			253	253		
7	F	244	Total	O	0	1
			245	245		

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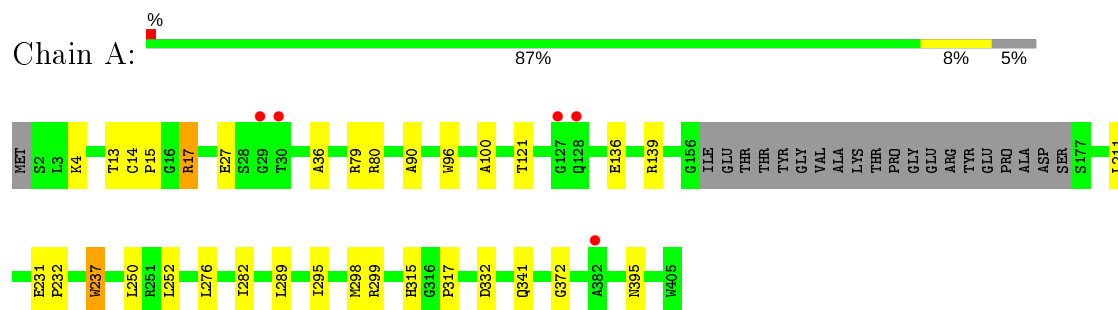
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	250	Total 251	O 251	0	1
7	H	249	Total 250	O 250	0	1

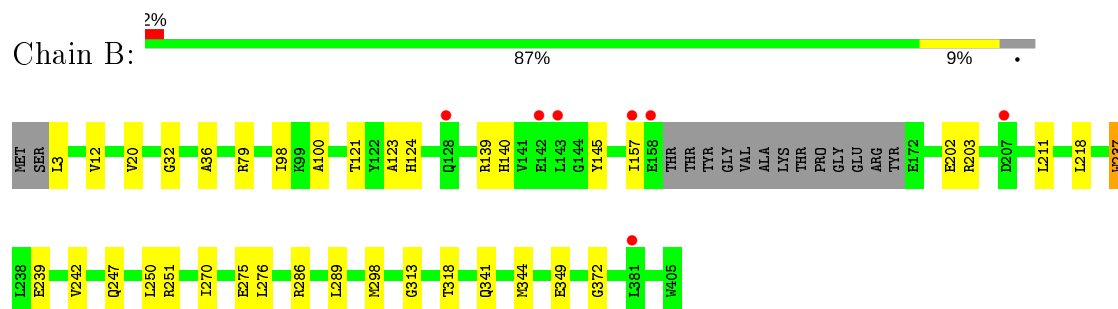
3 Residue-property plots [i](#)

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.

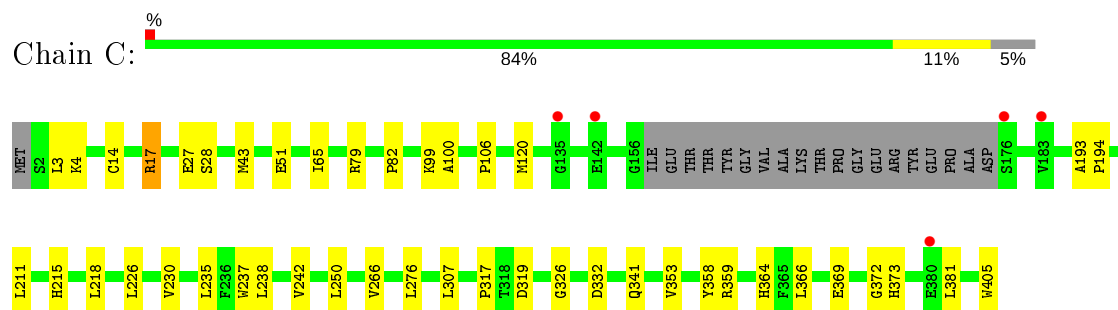
- Molecule 1: D-mannonate dehydratase



- Molecule 1: D-mannonate dehydratase

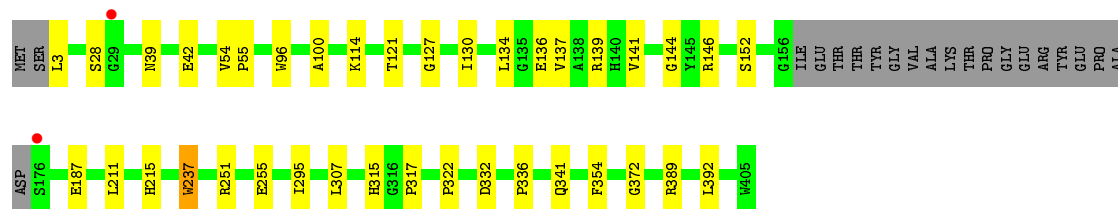


- Molecule 1: D-mannonate dehydratase



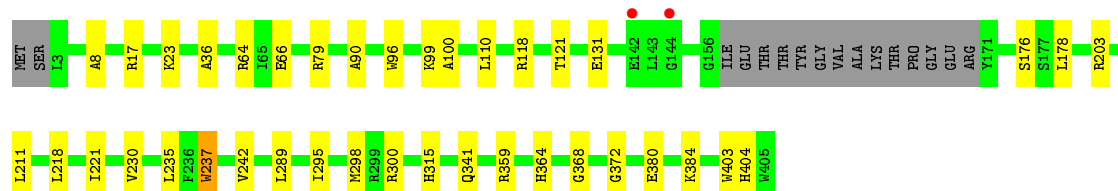
- Molecule 1: D-mannonate dehydratase





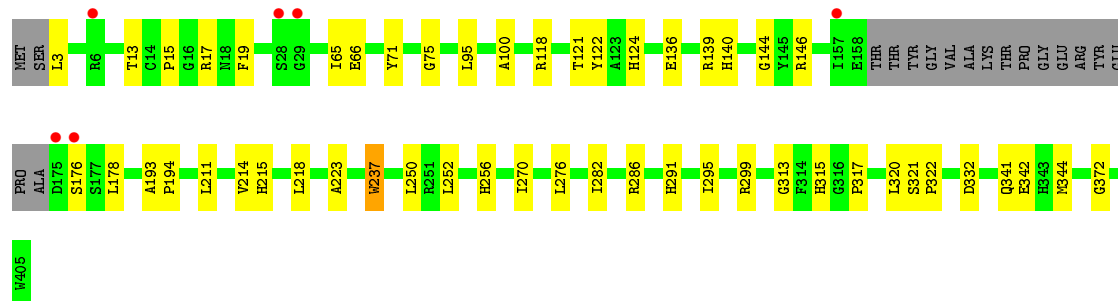
• Molecule 1: D-mannonate dehydratase

Chain E: 86% 9% •



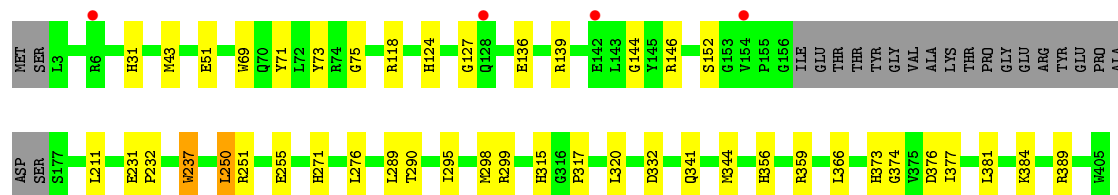
• Molecule 1: D-mannonate dehydratase

Chain F: 83% 12% •



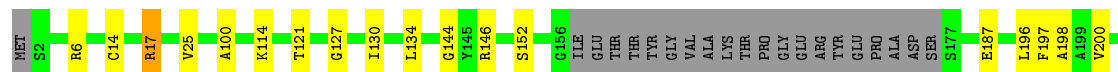
• Molecule 1: D-mannonate dehydratase

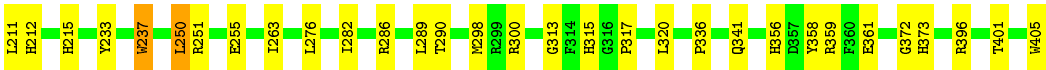
Chain G: 83% 11% 5%



• Molecule 1: D-mannonate dehydratase

Chain H: 83% 11% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.24Å 167.26Å 168.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.82 – 2.00 41.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.82-2.00) 100.0 (41.82-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.173 , 0.223 0.170 , 0.221	Depositor DCC
R_{free} test set	10558 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26541	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.00% 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: GOL, MG, KDG, CS2, CL

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	0.37	0/3137	0.53	0/4271
1	B	0.37	0/3192	0.54	0/4347
1	C	0.36	0/3143	0.52	0/4279
1	D	0.36	0/3128	0.53	0/4259
1	E	0.37	0/3187	0.53	0/4341
1	F	0.37	0/3153	0.53	0/4293
1	G	0.37	0/3122	0.52	0/4251
1	H	0.37	0/3128	0.53	0/4259
All	All	0.37	0/25190	0.53	0/34300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3049	0	2942	22	0
1	B	3100	0	2990	31	0
1	C	3055	0	2947	32	0
1	D	3043	0	2936	26	0
1	E	3097	0	2980	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3068	0	2957	31	0
1	G	3037	0	2931	34	0
1	H	3043	0	2936	28	0
2	A	13	0	10	1	0
2	B	13	0	11	0	0
2	E	13	0	11	1	0
2	F	13	0	11	1	0
3	A	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	C	12	0	9	0	0
5	D	12	0	9	0	0
5	G	12	0	9	0	0
5	H	12	0	9	0	0
6	G	6	0	8	6	0
7	A	236	0	0	2	0
7	B	242	0	0	5	0
7	C	228	0	0	4	0
7	D	226	0	0	2	0
7	E	253	0	0	3	0
7	F	245	0	0	3	0
7	G	251	0	0	3	0
7	H	250	0	0	2	0
All	All	26541	0	23706	218	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 (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:LEU:HD22	1:F:276:LEU:HD22	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:HD22	1:C:276:LEU:HD22	1.49	0.92
1:A:250:LEU:HD22	1:A:276:LEU:HD22	1.63	0.80
1:G:271:HIS:NE2	6:G:502:GOL:H11	1.94	0.80
1:B:3:LEU:HD13	7:B:724:HOH:O	1.84	0.78
1:B:318:THR:H	1:B:344[A]:MET:HE2	1.48	0.77
1:G:73:TYR:CZ	6:G:502:GOL:H2	2.23	0.73
1:G:381:LEU:HD12	1:G:384:LYS:HD2	1.74	0.69
1:B:218:LEU:O	1:B:242:VAL:HG12	1.93	0.68
1:F:214:VAL:HG11	1:F:218:LEU:HD22	1.76	0.68
1:D:389:ARG:NH1	7:D:695:HOH:O	2.28	0.65
1:C:193:ALA:HB3	1:C:194:PRO:HD3	1.77	0.65
1:F:211:LEU:HD23	1:F:237:TRP:CE2	2.33	0.64
1:B:318:THR:HG23	1:B:344[A]:MET:HE2	1.79	0.64
1:B:250:LEU:HD22	1:B:276:LEU:HD22	1.80	0.64
1:B:100:ALA:HB3	1:B:372:GLY:HA2	1.80	0.62
1:G:136:GLU:OE2	1:G:139:ARG:HD3	2.00	0.60
1:B:124:HIS:CE1	1:B:344[A]:MET:SD	2.95	0.60
1:C:359:ARG:HH11	1:C:366:LEU:HD13	1.66	0.60
1:C:3:LEU:HD21	1:C:28:SER:HB3	1.83	0.59
1:H:315:HIS:CE1	1:H:317:PRO:HG3	2.38	0.59
1:D:315:HIS:CE1	1:D:317:PRO:HG3	2.37	0.59
1:E:100:ALA:HB3	1:E:372:GLY:HA2	1.84	0.59
1:C:43:MET:HG3	1:G:51:GLU:HG3	1.85	0.58
1:A:13:THR:HG23	1:A:15:PRO:HD3	1.86	0.58
1:D:136:GLU:OE2	1:D:139:ARG:HD3	2.04	0.58
1:C:3:LEU:HD21	1:C:28:SER:H	1.69	0.58
1:D:251:ARG:O	1:D:255:GLU:HG3	2.05	0.57
1:D:211:LEU:HD23	1:D:237:TRP:CE2	2.39	0.57
1:G:359:ARG:NH2	7:G:709:HOH:O	2.38	0.57
1:H:6:ARG:HH21	1:H:25:VAL:HG11	1.71	0.56
1:C:266:VAL:HG22	7:C:668:HOH:O	2.05	0.56
1:A:100:ALA:HB3	1:A:372:GLY:HA2	1.87	0.56
1:D:100:ALA:HB3	1:D:372:GLY:HA2	1.88	0.56
1:H:127:GLY:O	1:H:152:SER:HA	2.05	0.56
1:C:4:LYS:HB2	1:C:27:GLU:HG3	1.88	0.55
1:B:203:ARG:HD3	7:B:839:HOH:O	2.05	0.55
1:C:359:ARG:NH2	7:C:771:HOH:O	2.39	0.55
1:G:118:ARG:NH2	7:G:786:HOH:O	2.39	0.55
1:G:251:ARG:O	1:G:255:GLU:HG3	2.05	0.55
1:C:218:LEU:O	1:C:242:VAL:HG12	2.05	0.55
1:G:271:HIS:NE2	6:G:502:GOL:C1	2.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:HIS:CE1	1:F:344:MET:SD	3.01	0.54
1:C:332:ASP:OD2	1:C:341:GLN:NE2	2.34	0.54
1:C:3:LEU:HD21	1:C:28:SER:CB	2.37	0.54
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.72	0.54
1:H:14:CYS:HA	1:H:17:ARG:O	2.08	0.53
1:B:211:LEU:HD23	1:B:237:TRP:CE2	2.44	0.53
1:F:250:LEU:HD22	1:F:276:LEU:CD2	2.29	0.53
1:G:315:HIS:CE1	1:G:317:PRO:HG3	2.43	0.53
1:B:123:ALA:HB2	1:B:145:TYR:CE2	2.43	0.53
1:B:289:LEU:HD23	1:B:298:MET:HG3	1.91	0.53
1:C:317:PRO:HB2	1:C:319:ASP:OD1	2.09	0.53
1:H:196:LEU:O	1:H:200:VAL:HG23	2.09	0.52
1:C:3:LEU:HD21	1:C:28:SER:N	2.24	0.52
1:G:295:ILE:O	1:G:299:ARG:HG3	2.09	0.52
1:B:237:TRP:C	1:B:237:TRP:CD1	2.83	0.52
1:D:3:LEU:HD13	1:D:28:SER:HB3	1.92	0.52
1:A:315:HIS:NE2	2:A:501:CS2:H3	2.24	0.51
1:G:250:LEU:HD13	1:G:276:LEU:HD22	1.92	0.51
1:C:79:ARG:HA	7:C:706:HOH:O	2.10	0.51
1:B:123:ALA:HB2	1:B:145:TYR:CD2	2.46	0.51
1:G:31:HIS:ND1	7:G:847:HOH:O	2.21	0.50
1:B:318:THR:HG23	1:B:344[A]:MET:CE	2.41	0.50
1:F:218:LEU:HD23	1:F:223:ALA:HA	1.93	0.50
1:G:211:LEU:HD23	1:G:237:TRP:CE2	2.46	0.50
1:E:230:VAL:HG21	1:E:235:LEU:HD22	1.92	0.50
1:E:79:ARG:HA	7:E:650:HOH:O	2.11	0.50
1:A:315:HIS:CE1	1:A:317:PRO:HG3	2.47	0.50
1:C:3:LEU:CD2	1:C:28:SER:HB3	2.42	0.50
1:G:211:LEU:N	1:G:211:LEU:HD12	2.26	0.50
1:A:36:ALA:HB2	1:A:90:ALA:HB2	1.94	0.49
1:C:211:LEU:HD12	1:C:211:LEU:N	2.27	0.49
1:C:100:ALA:HB3	1:C:372:GLY:HA2	1.94	0.49
1:F:13:THR:HG23	1:F:15:PRO:HD3	1.94	0.49
1:H:359:ARG:NH2	7:H:848:HOH:O	2.38	0.49
1:C:82:PRO:HD2	3:C:502:CL:CL	2.50	0.49
1:F:176:SER:HB2	1:F:178:LEU:O	2.13	0.49
1:E:218:LEU:O	1:E:242:VAL:HG12	2.12	0.48
1:G:290:THR:HB	1:G:320:LEU:HD22	1.94	0.48
1:E:64:ARG:HE	1:H:114:LYS:HG3	1.78	0.48
1:H:144:GLY:O	1:H:146:ARG:NH1	2.46	0.48
1:B:139:ARG:NH2	1:B:140:HIS:CE1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:776:HOH:O	1:H:300:ARG:HD3	2.13	0.48
1:D:96:TRP:CD1	1:D:295:ILE:HB	2.48	0.48
1:F:332:ASP:OD2	1:F:341:GLN:NE2	2.42	0.48
1:H:396:ARG:HA	1:H:401:THR:O	2.14	0.48
1:G:332:ASP:OD2	1:G:341:GLN:NE2	2.40	0.48
1:H:100:ALA:HB3	1:H:372:GLY:HA2	1.95	0.48
1:C:14:CYS:HA	1:C:17:ARG:O	2.13	0.47
1:D:136:GLU:HA	1:D:139:ARG:HG2	1.96	0.47
1:B:318:THR:N	1:B:344[A]:MET:HE2	2.25	0.47
1:F:140:HIS:NE2	7:F:759:HOH:O	2.35	0.47
1:F:286:ARG:HD2	1:F:313:GLY:O	2.14	0.47
1:D:130:ILE:O	1:D:134:LEU:HG	2.15	0.47
1:H:197:PHE:HZ	1:H:212:HIS:CG	2.32	0.47
1:H:251:ARG:O	1:H:255:GLU:HG3	2.15	0.47
1:C:65:ILE:HG13	1:C:99:LYS:HE3	1.97	0.47
1:C:106:PRO:HG3	1:C:369:GLU:O	2.14	0.47
1:A:121:THR:HA	1:A:341:GLN:O	2.15	0.46
1:B:247:GLN:OE1	1:B:275:GLU:HB2	2.15	0.46
1:F:315:HIS:NE2	2:F:501:CS2:H3	2.30	0.46
1:F:122:TYR:CZ	1:F:342:GLU:HB2	2.51	0.46
1:B:20:VAL:HG12	1:B:36:ALA:HB3	1.98	0.46
1:A:4:LYS:HB2	1:A:27:GLU:OE2	2.16	0.46
1:A:332:ASP:OD2	1:A:341:GLN:NE2	2.48	0.46
1:D:144:GLY:O	1:D:146:ARG:NH1	2.49	0.45
1:H:121:THR:HA	1:H:341:GLN:O	2.15	0.45
1:D:137:VAL:O	1:D:141:VAL:HG23	2.16	0.45
1:F:100:ALA:HB3	1:F:372:GLY:HA2	1.97	0.45
7:C:730:HOH:O	1:D:187:GLU:HG2	2.16	0.45
1:D:3:LEU:CD1	1:D:28:SER:HB3	2.46	0.45
1:G:69:TRP:HH2	6:G:502:GOL:HO2	1.63	0.45
1:A:289:LEU:HD23	1:A:298:MET:HG3	1.99	0.45
1:H:198:ALA:HB2	1:H:233:TYR:CZ	2.51	0.45
1:C:235:LEU:HD23	1:C:238:LEU:HD13	1.99	0.45
1:D:114:LYS:HE2	7:F:749:HOH:O	2.17	0.45
1:D:237:TRP:CD1	1:D:237:TRP:C	2.90	0.45
1:F:344:MET:HE2	1:F:344:MET:HB3	1.54	0.45
1:G:250:LEU:HD13	1:G:276:LEU:CD2	2.46	0.45
1:F:250:LEU:HD23	1:F:282:ILE:CG2	2.47	0.45
1:C:51[B]:GLU:OE2	1:G:389:ARG:HD3	2.17	0.45
1:H:237:TRP:CD1	1:H:237:TRP:C	2.90	0.45
1:E:118:ARG:HD2	1:E:364:HIS:CG	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LEU:HD21	1:F:270:ILE:HD13	1.98	0.44
1:A:237:TRP:CD1	1:A:237:TRP:C	2.90	0.44
1:A:315:HIS:CD2	1:A:317:PRO:HD3	2.52	0.44
1:E:99:LYS:HG2	1:E:110:LEU:HD21	1.99	0.44
1:G:271:HIS:CD2	6:G:502:GOL:H11	2.50	0.44
1:C:51[B]:GLU:HG2	1:G:43:MET:CG	2.48	0.44
1:F:65:ILE:HG12	1:F:95:LEU:HB3	1.99	0.44
1:G:127:GLY:O	1:G:152:SER:HA	2.17	0.44
1:A:14:CYS:HA	1:A:17:ARG:O	2.18	0.44
1:D:127:GLY:O	1:D:152:SER:HA	2.18	0.44
1:G:237:TRP:CD1	1:G:237:TRP:C	2.91	0.44
1:A:231:GLU:N	1:A:232:PRO:CD	2.81	0.44
1:A:252:LEU:HB2	7:A:633:HOH:O	2.17	0.44
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.32	0.44
1:C:226:LEU:O	1:C:230:VAL:HG13	2.18	0.44
1:F:121:THR:HA	1:F:341:GLN:O	2.17	0.44
1:B:3:LEU:HA	1:B:3:LEU:HD23	1.80	0.44
1:H:263:ILE:HG22	1:H:282:ILE:HG21	2.00	0.44
1:H:289:LEU:HD23	1:H:298:MET:HG3	2.00	0.43
1:H:215:HIS:ND1	1:H:405:TRP:OXT	2.37	0.43
1:B:121:THR:HA	1:B:341:GLN:O	2.18	0.43
1:E:211:LEU:HD23	1:E:237:TRP:CE2	2.52	0.43
1:E:315:HIS:NE2	2:E:501:CS2:H3	2.33	0.43
1:F:295:ILE:O	1:F:299:ARG:HG3	2.18	0.43
1:G:124:HIS:CE1	1:G:344:MET:SD	3.11	0.43
1:H:356:HIS:CD2	1:H:358:TYR:CZ	3.07	0.43
1:F:71:TYR:O	1:F:75:GLY:HA3	2.18	0.43
1:D:332:ASP:OD2	1:D:341:GLN:NE2	2.47	0.43
1:G:144:GLY:O	1:G:146:ARG:NH1	2.51	0.43
1:H:290:THR:HB	1:H:320:LEU:HD22	2.01	0.43
1:B:270:ILE:HD13	1:C:307:LEU:HD21	2.01	0.43
1:F:3:LEU:N	7:F:822:HOH:O	2.51	0.43
1:E:121:THR:HA	1:E:341:GLN:O	2.17	0.43
1:E:131:GLU:OE2	1:E:203:ARG:NH2	2.48	0.43
1:D:336:PRO:HG3	1:F:66:GLU:OE2	2.18	0.43
1:E:8:ALA:HA	1:E:23:LYS:O	2.19	0.43
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.78	0.42
1:A:79:ARG:O	1:A:80:ARG:HB2	2.18	0.42
1:B:349:GLU:HG2	7:B:842:HOH:O	2.19	0.42
1:C:120:MET:HA	1:C:364:HIS:CD2	2.54	0.42
1:D:39:ASN:ND2	1:D:392:LEU:HD21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:GLU:O	1:E:384:LYS:NZ	2.47	0.42
1:B:202:GLU:HB3	7:B:752:HOH:O	2.20	0.42
1:G:289:LEU:HD23	1:G:298:MET:HG3	2.00	0.42
1:A:136:GLU:HA	1:A:139:ARG:HG2	2.02	0.42
1:A:96:TRP:CD1	1:A:295:ILE:HB	2.54	0.42
1:E:237:TRP:CD1	1:E:237:TRP:C	2.93	0.42
1:A:211:LEU:HD23	1:A:237:TRP:CE2	2.55	0.42
1:E:300:ARG:HD3	7:E:735:HOH:O	2.19	0.42
1:F:315:HIS:CE1	1:F:317:PRO:HG3	2.55	0.42
1:F:291:HIS:CE1	1:F:320:LEU:HD21	2.55	0.42
1:B:237:TRP:NE1	1:B:239:GLU:HB2	2.35	0.42
1:F:19:PHE:CD1	1:F:321:SER:HB3	2.55	0.42
1:C:51[B]:GLU:HG2	1:G:43:MET:HG3	2.01	0.42
1:H:359:ARG:NE	1:H:361:GLU:OE2	2.48	0.42
1:E:176:SER:HB2	1:E:178:LEU:O	2.19	0.42
1:F:193:ALA:HB3	1:F:194:PRO:HD3	2.01	0.41
1:H:286:ARG:HD2	1:H:313:GLY:O	2.20	0.41
1:F:136:GLU:OE2	1:F:139:ARG:HD3	2.20	0.41
1:D:136:GLU:OE1	1:D:139:ARG:NH1	2.51	0.41
1:E:359:ARG:HH22	1:E:368:GLY:HA2	1.85	0.41
1:F:144:GLY:O	1:F:146:ARG:NH1	2.47	0.41
1:G:231:GLU:N	1:G:232:PRO:CD	2.84	0.41
1:A:299:ARG:NH2	7:A:693:HOH:O	2.53	0.41
1:E:96:TRP:CD1	1:E:295:ILE:HB	2.55	0.41
1:B:286:ARG:HD2	1:B:313:GLY:O	2.21	0.41
1:D:322:PRO:HG2	1:D:354:PHE:HB2	2.02	0.41
1:E:403:TRP:CG	1:E:404:HIS:N	2.87	0.41
1:G:366:LEU:N	1:G:366:LEU:HD22	2.36	0.41
1:H:130:ILE:O	1:H:134:LEU:HG	2.20	0.41
1:E:221:ILE:HA	1:E:221:ILE:HD12	1.98	0.41
1:G:69:TRP:HH2	6:G:502:GOL:H32	1.86	0.41
1:B:12:VAL:HG22	1:B:20:VAL:HG22	2.02	0.41
1:D:121:THR:HA	1:D:341:GLN:O	2.21	0.41
1:E:36:ALA:HB2	1:E:90:ALA:HB2	2.02	0.41
1:H:211:LEU:HD23	1:H:237:TRP:CE2	2.56	0.41
1:H:250:LEU:HD13	1:H:276:LEU:CD2	2.51	0.41
1:B:32:GLY:HA3	1:B:98:ILE:HG13	2.03	0.41
1:F:321:SER:HB2	1:F:322:PRO:HD2	2.03	0.41
1:F:252:LEU:O	1:F:256:HIS:HD2	2.05	0.40
1:E:66:GLU:OE2	1:H:336:PRO:HG3	2.21	0.40
1:A:250:LEU:HD23	1:A:282:ILE:CG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:VAL:N	1:D:55:PRO:CD	2.84	0.40
1:G:71:TYR:O	1:G:75:GLY:HA3	2.21	0.40
1:A:211:LEU:HD12	1:A:211:LEU:N	2.36	0.40
1:C:326:GLY:HA2	1:C:358:TYR:CD2	2.56	0.40
1:C:215:HIS:ND1	1:C:405:TRP:OXT	2.41	0.40
1:D:42:GLU:HA	7:D:655:HOH:O	2.22	0.40
1:E:289:LEU:HD23	1:E:298:MET:HG3	2.02	0.40
1:G:356:HIS:HA	1:G:374:GLY:O	2.20	0.40
1:H:187:GLU:CD	7:H:748:HOH:O	2.60	0.40
1:B:79:ARG:HA	7:B:735:HOH:O	2.21	0.40
1:C:353:VAL:HG22	1:C:381:LEU:HD22	2.03	0.40
1:G:376:ASP:CG	1:G:377:ILE:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/405 (94%)	368 (97%)	13 (3%)	0	100	100
1	B	388/405 (96%)	377 (97%)	11 (3%)	0	100	100
1	C	382/405 (94%)	374 (98%)	8 (2%)	0	100	100
1	D	380/405 (94%)	366 (96%)	14 (4%)	0	100	100
1	E	387/405 (96%)	377 (97%)	10 (3%)	0	100	100
1	F	383/405 (95%)	372 (97%)	11 (3%)	0	100	100
1	G	379/405 (94%)	368 (97%)	11 (3%)	0	100	100
1	H	380/405 (94%)	368 (97%)	12 (3%)	0	100	100
All	All	3060/3240 (94%)	2970 (97%)	90 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/332 (95%)	313 (99%)	3 (1%)	78	83
1	B	322/332 (97%)	321 (100%)	1 (0%)	92	95
1	C	317/332 (96%)	314 (99%)	3 (1%)	78	83
1	D	315/332 (95%)	313 (99%)	2 (1%)	86	90
1	E	321/332 (97%)	319 (99%)	2 (1%)	86	90
1	F	318/332 (96%)	314 (99%)	4 (1%)	69	74
1	G	314/332 (95%)	311 (99%)	3 (1%)	76	81
1	H	315/332 (95%)	311 (99%)	4 (1%)	69	74
All	All	2538/2656 (96%)	2516 (99%)	22 (1%)	78	83

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	237	TRP
1	A	395	ASN
1	B	237	TRP
1	C	17	ARG
1	C	237	TRP
1	C	373	HIS
1	D	215	HIS
1	D	237	TRP
1	E	17	ARG
1	E	237	TRP
1	F	17	ARG
1	F	118	ARG
1	F	215	HIS
1	F	237	TRP
1	G	237	TRP
1	G	250	LEU
1	G	373	HIS
1	H	17	ARG

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Mol	Chain	Res	Type
1	H	237	TRP
1	H	250	LEU
1	H	373	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	278	GLN
1	F	192	HIS
1	F	278	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 12 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	$\# Z > 2$
5	KDG	H	501	4	8,11,11	0.59	0	9,14,14	0.97	1 (11%)
2	CS2	B	501	4	9,12,12	0.46	0	12,16,16	0.94	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CS2	A	501	4	9,12,12	0.44	0	12,16,16	0.89	1 (8%)
5	KDG	D	501	4	8,11,11	0.49	0	9,14,14	1.45	1 (11%)
2	CS2	E	501	4	9,12,12	0.55	0	12,16,16	1.17	1 (8%)
5	KDG	C	501	4	8,11,11	0.49	0	9,14,14	1.53	1 (11%)
6	GOL	G	502	-	5,5,5	0.33	0	5,5,5	0.25	0
2	CS2	F	501	4	9,12,12	0.46	0	12,16,16	1.29	2 (16%)
5	KDG	G	501	4	8,11,11	0.37	0	9,14,14	1.39	2 (22%)

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
5	KDG	H	501	4	-	1/10/14/14	-
2	CS2	B	501	4	-	4/14/18/18	-
2	CS2	A	501	4	-	6/14/18/18	-
5	KDG	D	501	4	-	1/10/14/14	-
2	CS2	E	501	4	-	5/14/18/18	-
5	KDG	C	501	4	-	2/10/14/14	-
6	GOL	G	502	-	-	4/4/4/4	-
2	CS2	F	501	4	-	3/14/18/18	-
5	KDG	G	501	4	-	0/10/14/14	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	KDG	C4-C3-C2	-3.60	107.43	113.65
5	D	501	KDG	C4-C3-C2	-3.52	107.57	113.65
5	G	501	KDG	C4-C3-C2	-3.05	108.39	113.65
2	F	501	CS2	C5-C4-C3	-2.67	108.29	112.47
5	H	501	KDG	C4-C3-C2	-2.43	109.45	113.65
2	E	501	CS2	C5-C4-C3	-2.25	108.94	112.47
2	F	501	CS2	O2-C2-C3	2.13	112.22	107.39
2	B	501	CS2	O2-C2-C3	2.09	112.12	107.39
5	G	501	KDG	O1B-C1-C2	-2.06	106.59	111.07
2	A	501	CS2	C5-C4-C3	-2.04	109.28	112.47

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CS2	O4-C4-C5-C6
2	B	501	CS2	C1-C2-C3-C4
2	B	501	CS2	O2-C2-C3-C4
2	A	501	CS2	O4-C4-C5-O5
6	G	502	GOL	O2-C2-C3-O3
2	A	501	CS2	C3-C4-C5-O5
2	B	501	CS2	O2-C2-C3-O3
2	A	501	CS2	C3-C4-C5-C6
2	E	501	CS2	O2-C2-C3-C4
6	G	502	GOL	C1-C2-C3-O3
2	E	501	CS2	O5-C5-C6-O6
2	A	501	CS2	O2-C2-C3-O3
2	F	501	CS2	O2-C2-C3-O3
2	E	501	CS2	O2-C2-C3-O3
2	A	501	CS2	O2-C2-C3-C4
2	F	501	CS2	O2-C2-C3-C4
5	D	501	KDG	O1B-C1-C2-O2
2	B	501	CS2	C1-C2-C3-O3
2	E	501	CS2	C1-C2-C3-C4
2	E	501	CS2	C4-C5-C6-O6
5	C	501	KDG	O1B-C1-C2-O2
6	G	502	GOL	O1-C1-C2-C3
6	G	502	GOL	O1-C1-C2-O2
5	H	501	KDG	O1B-C1-C2-O2
5	C	501	KDG	O2-C2-C3-O3
2	F	501	CS2	O4-C4-C5-C6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CS2	1	0
2	E	501	CS2	1	0
6	G	502	GOL	6	0
2	F	501	CS2	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	384/405 (94%)	-0.19	5 (1%) 77 76	11, 18, 34, 47	0
1	B	390/405 (96%)	-0.25	7 (1%) 68 66	11, 18, 33, 71	0
1	C	385/405 (95%)	-0.20	5 (1%) 77 76	10, 19, 33, 56	0
1	D	384/405 (94%)	-0.23	2 (0%) 91 90	12, 18, 34, 50	0
1	E	389/405 (96%)	-0.35	2 (0%) 91 90	11, 17, 32, 50	0
1	F	387/405 (95%)	-0.18	6 (1%) 72 70	11, 18, 34, 56	0
1	G	383/405 (94%)	-0.16	4 (1%) 82 81	10, 18, 34, 50	0
1	H	384/405 (94%)	-0.19	0 100 100	11, 18, 32, 43	0
All	All	3086/3240 (95%)	-0.22	31 (1%) 82 81	10, 18, 34, 71	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ILE	5.1
1	B	142	GLU	3.9
1	B	158	GLU	3.3
1	C	176	SER	3.2
1	B	381	LEU	3.0
1	D	176	SER	3.0
1	F	176	SER	2.9
1	A	128	GLN	2.9
1	C	142	GLU	2.9
1	G	6	ARG	2.8
1	C	183	VAL	2.7
1	F	157	ILE	2.7
1	G	154	VAL	2.6
1	F	6	ARG	2.5
1	G	142	GLU	2.5
1	F	175	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	29	GLY	2.4
1	F	29	GLY	2.4
1	G	128	GLN	2.4
1	A	127	GLY	2.4
1	E	144	GLY	2.3
1	F	28	SER	2.3
1	B	207	ASP	2.3
1	A	30	THR	2.3
1	C	380	GLU	2.3
1	A	382	ALA	2.2
1	A	29	GLY	2.2
1	B	128	GLN	2.2
1	E	142	GLU	2.1
1	B	143	LEU	2.0
1	C	135	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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
5	KDG	G	501	12/12	0.90	0.15	19,24,30,31	0
5	KDG	D	501	12/12	0.91	0.14	16,22,30,39	0
2	CS2	F	501	13/13	0.92	0.15	15,22,37,39	0
6	GOL	G	502	6/6	0.92	0.18	22,29,33,37	0
2	CS2	E	501	13/13	0.92	0.14	15,20,35,37	0
2	CS2	B	501	13/13	0.93	0.13	13,21,30,31	0
2	CS2	A	501	13/13	0.93	0.12	17,25,36,39	0
5	KDG	H	501	12/12	0.95	0.11	8,22,28,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	KDG	C	501	12/12	0.95	0.11	10,19,24,32	0
3	CL	F	502	1/1	0.96	0.11	23,23,23,23	0
3	CL	D	502	1/1	0.97	0.06	22,22,22,22	0
4	MG	A	503	1/1	0.97	0.15	22,22,22,22	0
3	CL	A	502	1/1	0.97	0.09	22,22,22,22	0
4	MG	B	502	1/1	0.97	0.22	21,21,21,21	0
3	CL	C	502	1/1	0.97	0.13	27,27,27,27	0
4	MG	E	502	1/1	0.98	0.12	22,22,22,22	0
4	MG	H	502	1/1	0.98	0.10	17,17,17,17	0
4	MG	G	503	1/1	0.99	0.16	18,18,18,18	0
4	MG	C	503	1/1	0.99	0.08	19,19,19,19	0
4	MG	D	503	1/1	0.99	0.07	20,20,20,20	0
4	MG	F	503	1/1	0.99	0.12	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.