



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:53 PM GMT

PDB ID : 4DPW
Title : Crystal structure of Staphylococcus epidermidis D283A mevalonate diphosphate decarboxylase complexed with mevalonate diphosphate and ATPgS
Authors : Barta, M.L.; McWhorter, W.J.; Geisbrecht, B.V.
Deposited on : 2012-02-14
Resolution : 2.60 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

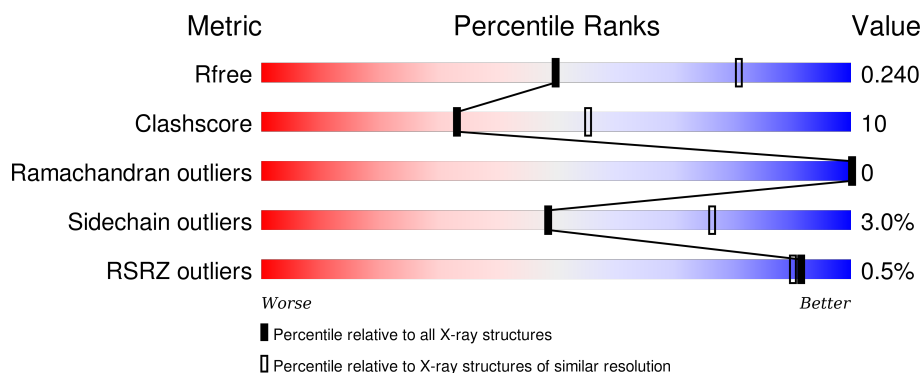
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



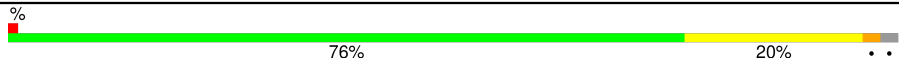


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	332	<div> <div></div> <div>76% 21% ..</div> </div>
1	B	332	<div> <div></div> <div>79% 19% ..</div> </div>
1	C	332	<div> <div></div> <div>82% 16% ..</div> </div>
1	D	332	<div> <div></div> <div>79% 18% ..</div> </div>
1	E	332	<div> <div></div> <div>81% 17% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	332	
1	G	332	
1	H	332	

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	DP6	B	402	-	-	-	X
3	DP6	C	402	-	-	-	X
3	DP6	D	402	-	-	X	X
3	DP6	E	402	-	-	X	-
3	DP6	G	402	-	-	-	X
3	DP6	H	402	-	-	-	X
4	FMT	E	404	-	-	-	X
4	FMT	H	403	-	-	-	X
5	GOL	E	403	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21044 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 Mevalonate diphosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2547	1595	441	498	13			
1	B	326	Total	C	N	O	S	0	0	0
			2547	1595	441	498	13			
1	C	326	Total	C	N	O	S	0	0	0
			2547	1595	441	498	13			
1	D	326	Total	C	N	O	S	0	0	0
			2547	1595	441	498	13			
1	E	328	Total	C	N	O	S	0	0	0
			2557	1600	443	501	13			
1	F	326	Total	C	N	O	S	0	0	0
			2547	1595	441	498	13			
1	G	326	Total	C	N	O	S	0	0	0
			2547	1595	441	498	13			
1	H	326	Total	C	N	O	S	0	0	0
			2547	1595	441	498	13			

There are 48 discrepancies between the modelled and reference sequences:

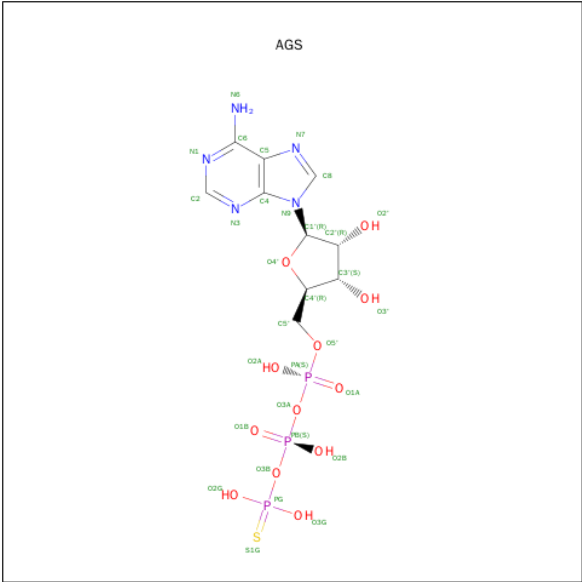
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73
A	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
A	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
A	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
A	0	SER	-	EXPRESSION TAG	UNP Q9FD73
A	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73
B	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73
B	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
B	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
B	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
B	0	SER	-	EXPRESSION TAG	UNP Q9FD73
B	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73
C	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73

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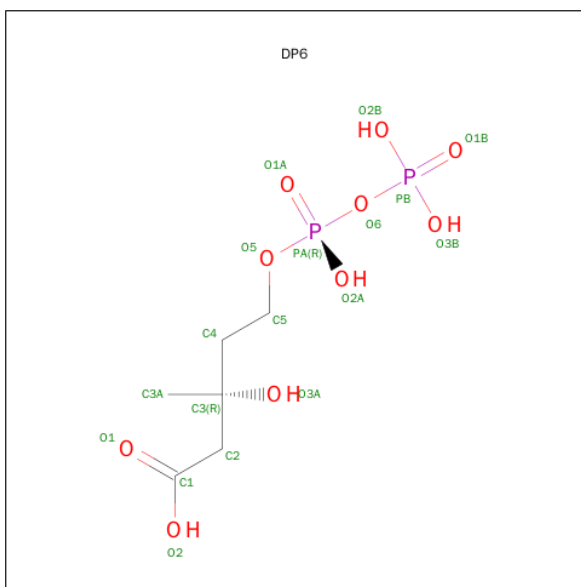
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
C	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
C	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
C	0	SER	-	EXPRESSION TAG	UNP Q9FD73
C	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73
D	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73
D	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
D	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
D	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
D	0	SER	-	EXPRESSION TAG	UNP Q9FD73
D	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73
E	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73
E	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
E	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
E	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
E	0	SER	-	EXPRESSION TAG	UNP Q9FD73
E	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73
F	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73
F	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
F	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
F	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
F	0	SER	-	EXPRESSION TAG	UNP Q9FD73
F	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73
G	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73
G	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
G	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
G	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
G	0	SER	-	EXPRESSION TAG	UNP Q9FD73
G	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73
H	-4	GLY	-	EXPRESSION TAG	UNP Q9FD73
H	-3	SER	-	EXPRESSION TAG	UNP Q9FD73
H	-2	THR	-	EXPRESSION TAG	UNP Q9FD73
H	-1	GLY	-	EXPRESSION TAG	UNP Q9FD73
H	0	SER	-	EXPRESSION TAG	UNP Q9FD73
H	283	ALA	ASP	ENGINEERED MUTATION	UNP Q9FD73

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



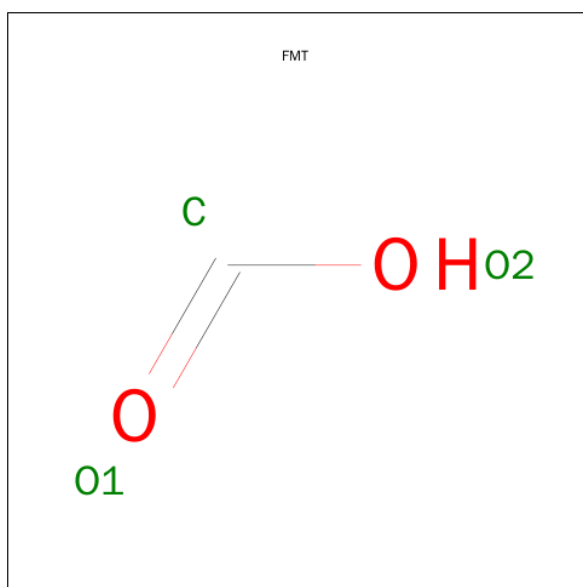
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is (3R)-3-HYDROXY-5-[[[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY]-3-METHYLPENTANOIC ACID (three-letter code: DP6) (formula: C₆H₁₄O₁₀P₂).



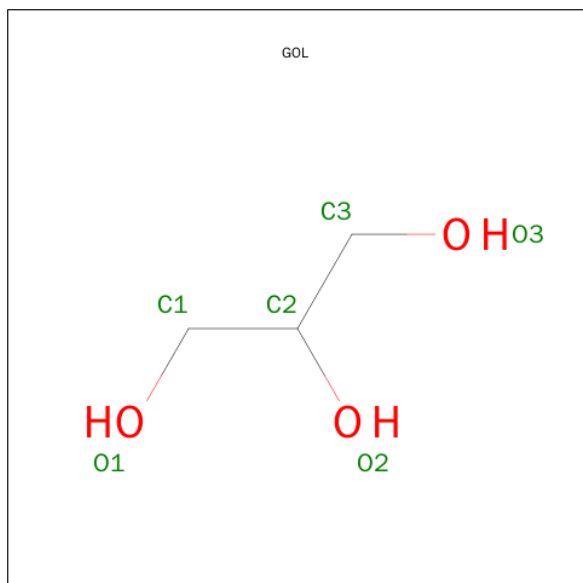
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			18	6	10	2		
3	B	1	Total	C	O	P	0	0
			18	6	10	2		
3	C	1	Total	C	O	P	0	0
			18	6	10	2		
3	D	1	Total	C	O	P	0	0
			18	6	10	2		
3	E	1	Total	C	O	P	0	0
			18	6	10	2		
3	F	1	Total	C	O	P	0	0
			18	6	10	2		
3	G	1	Total	C	O	P	0	0
			18	6	10	2		
3	H	1	Total	C	O	P	0	0
			18	6	10	2		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

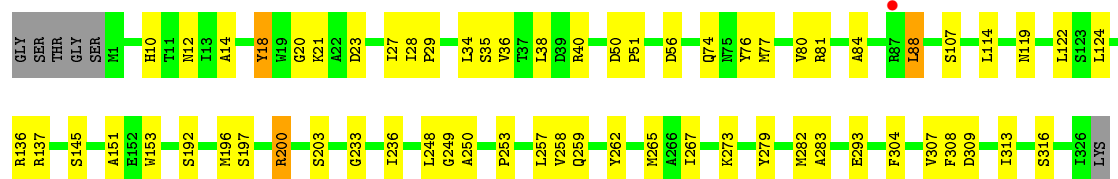


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

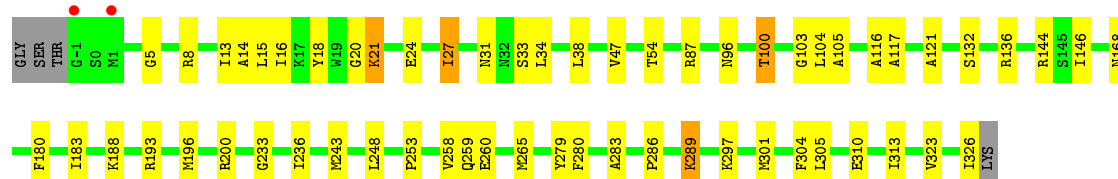
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	39	Total	O	0	0
			39	39		
6	C	28	Total	O	0	0
			28	28		
6	D	42	Total	O	0	0
			42	42		
6	E	33	Total	O	0	0
			33	33		
6	F	27	Total	O	0	0
			27	27		
6	G	42	Total	O	0	0
			42	42		
6	H	17	Total	O	0	0
			17	17		

Chain D:  79% 18% ..



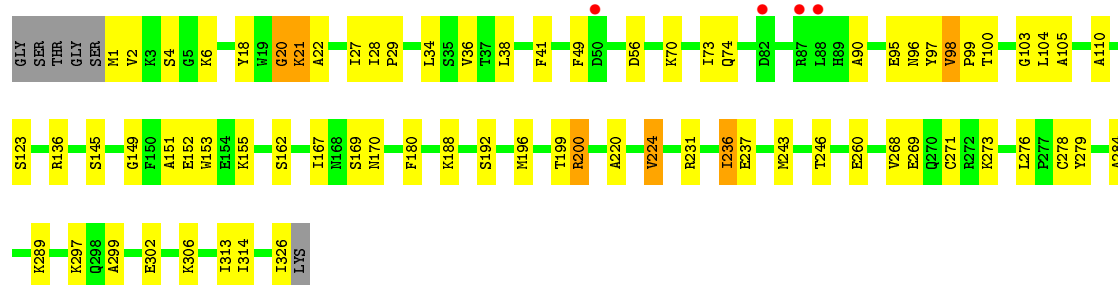
• Molecule 1: Mevalonate diphosphate decarboxylase

Chain E:  81% 17% ..



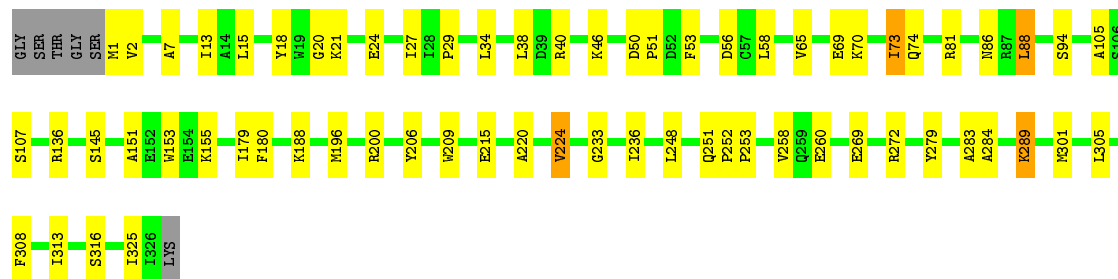
• Molecule 1: Mevalonate diphosphate decarboxylase

Chain F:  76% 20% ..



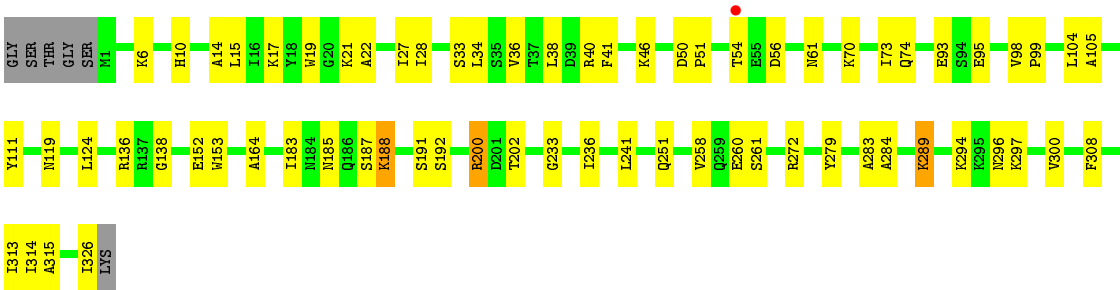
• Molecule 1: Mevalonate diphosphate decarboxylase

Chain G:  78% 19% ..



• Molecule 1: Mevalonate diphosphate decarboxylase

Chain H:  78% 20% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.46Å 99.44Å 314.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.60 46.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (46.36-2.60) 94.6 (46.55-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.199 , 0.251 0.196 , 0.240	Depositor DCC
R_{free} test set	1994 reflections (2.31%)	DCC
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.9	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 91509 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21044	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 25.18 % 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 3.3286e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, AGS, DP6

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	0.43	0/2591	0.54	0/3500
1	B	0.47	0/2591	0.56	0/3500
1	C	0.45	0/2591	0.57	1/3500 (0.0%)
1	D	0.49	0/2591	0.55	0/3500
1	E	0.47	0/2601	0.59	0/3513
1	F	0.43	0/2591	0.58	2/3500 (0.1%)
1	G	0.48	0/2591	0.57	0/3500
1	H	0.43	0/2591	0.55	0/3500
All	All	0.46	0/20738	0.56	3/28013 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	20	GLY	N-CA-C	-5.89	98.38	113.10
1	C	189	LYS	CB-CA-C	5.43	121.26	110.40
1	F	98	VAL	CB-CA-C	5.04	120.97	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2547	0	2505	52	0
1	B	2547	0	2505	45	0
1	C	2547	0	2505	45	0
1	D	2547	0	2505	55	0
1	E	2557	0	2513	55	0
1	F	2547	0	2505	61	0
1	G	2547	0	2505	48	0
1	H	2547	0	2505	44	0
2	A	31	0	12	2	0
2	B	31	0	12	6	0
2	C	31	0	12	4	0
2	D	31	0	12	4	0
2	E	31	0	12	2	0
2	F	31	0	12	4	0
2	G	31	0	12	8	0
2	H	31	0	12	4	0
3	A	18	0	10	1	0
3	B	18	0	10	6	0
3	C	18	0	10	3	0
3	D	18	0	10	8	0
3	E	18	0	10	7	0
3	F	18	0	10	3	0
3	G	18	0	10	6	0
3	H	18	0	10	6	0
4	A	3	0	1	0	0
4	D	3	0	1	0	0
4	E	3	0	1	0	0
4	H	3	0	1	0	0
5	E	6	0	8	4	0
6	A	20	0	0	1	0
6	B	39	0	0	0	0
6	C	28	0	0	2	0
6	D	42	0	0	2	0
6	E	33	0	0	1	0
6	F	27	0	0	1	0
6	G	42	0	0	2	0
6	H	17	0	0	1	0
All	All	21044	0	20236	424	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (424) 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:A:21:LYS:HZ3	1:A:196:MET:HE1	0.95	1.03
1:G:215:GLU:HG3	6:G:540:HOH:O	1.56	1.03
1:F:96:ASN:HD22	1:F:100:THR:HG22	1.19	1.03
1:A:18:TYR:O	3:A:402:DP6:H3A3	1.57	1.02
1:G:18:TYR:O	3:G:402:DP6:H3A1	1.59	1.02
1:C:18:TYR:O	3:C:402:DP6:H3A3	1.60	1.01
1:F:96:ASN:HD22	1:F:100:THR:CG2	1.75	0.99
1:F:99:PRO:HG2	1:F:104:LEU:HD22	1.40	0.98
1:H:188:LYS:HE2	1:H:284:ALA:O	1.63	0.96
1:E:20:GLY:HA2	1:E:196:MET:HG2	1.48	0.96
1:A:21:LYS:NZ	1:A:196:MET:HE1	1.78	0.95
1:E:305:LEU:HD22	1:E:310:GLU:HG2	1.46	0.95
1:A:13:ILE:HG21	1:A:289:LYS:HD2	1.48	0.93
1:G:308:PHE:HB2	1:G:313:ILE:HD11	1.48	0.93
1:F:98:VAL:HG23	1:F:99:PRO:HD2	1.51	0.91
1:H:105:ALA:HA	2:H:401:AGS:O2G	1.68	0.91
1:D:107:SER:HB3	2:D:401:AGS:H5'2	1.54	0.90
1:F:96:ASN:ND2	1:F:100:THR:HG22	1.85	0.90
1:A:21:LYS:HZ3	1:A:196:MET:CE	1.84	0.89
2:G:401:AGS:O2B	2:G:401:AGS:S1G	2.32	0.88
1:A:39:ASP:HB3	1:A:319:ILE:HB	1.56	0.88
1:H:14:ALA:HB3	3:H:402:DP6:O2	1.74	0.87
1:D:18:TYR:O	3:D:402:DP6:H3A3	1.74	0.87
1:D:27:ILE:O	1:D:136:ARG:HD3	1.75	0.86
1:C:18:TYR:O	3:C:402:DP6:C3A	2.24	0.85
1:F:18:TYR:O	3:F:402:DP6:H3A3	1.80	0.82
1:B:283:ALA:H	1:B:289:LYS:HZ3	1.27	0.81
2:A:401:AGS:S1G	2:A:401:AGS:O2B	2.39	0.81
1:C:283:ALA:H	1:C:289:LYS:HZ3	1.28	0.80
1:C:308:PHE:HB2	1:C:313:ILE:HD11	1.65	0.78
1:E:20:GLY:H	1:E:196:MET:CG	1.95	0.78
1:F:20:GLY:H	1:F:196:MET:CG	1.97	0.77
1:E:305:LEU:CD2	1:E:310:GLU:HG2	2.15	0.76
2:H:401:AGS:S1G	2:H:401:AGS:O2B	2.44	0.76
1:E:258:VAL:HG12	1:E:259:GLN:H	1.50	0.76
1:G:18:TYR:O	3:G:402:DP6:C3A	2.34	0.76
1:H:183:ILE:HG23	1:H:260:GLU:OE1	1.86	0.76
1:G:105:ALA:HA	2:G:401:AGS:S1G	2.26	0.76
1:D:283:ALA:HA	3:D:402:DP6:O2	1.86	0.76
1:D:56:ASP:HB2	1:D:74:GLN:HG2	1.67	0.75
1:G:308:PHE:CB	1:G:313:ILE:HD11	2.17	0.75
1:F:38:LEU:HD13	1:F:180:PHE:HZ	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:TYR:HA	1:D:265:MET:CE	2.16	0.75
1:C:105:ALA:HA	2:C:401:AGS:O3B	1.87	0.74
1:E:38:LEU:HD13	1:E:180:PHE:HZ	1.52	0.74
1:F:99:PRO:HG2	1:F:104:LEU:CD2	2.17	0.74
1:F:29:PRO:HD3	1:F:153:TRP:CZ2	2.23	0.74
1:D:18:TYR:O	3:D:402:DP6:C3A	2.36	0.73
1:E:283:ALA:H	1:E:289:LYS:NZ	1.87	0.73
1:B:13:ILE:HG12	1:B:38:LEU:HD11	1.71	0.72
1:B:15:LEU:HB3	1:B:236:ILE:HG21	1.70	0.72
1:E:20:GLY:N	1:E:196:MET:CG	2.53	0.72
1:E:20:GLY:N	1:E:196:MET:HG3	2.05	0.71
1:F:21:LYS:HA	1:F:29:PRO:HA	1.73	0.71
1:D:257:LEU:HD22	1:D:282:MET:CE	2.20	0.71
1:H:272:ARG:NH1	6:H:515:HOH:O	2.24	0.71
1:E:20:GLY:H	1:E:196:MET:HG3	1.55	0.71
1:F:56:ASP:HB2	1:F:74:GLN:HG2	1.74	0.69
2:D:401:AGS:O1B	2:D:401:AGS:S1G	2.50	0.69
1:B:308:PHE:HB2	1:B:313:ILE:HD11	1.73	0.68
1:A:20:GLY:H	1:A:196:MET:HG2	1.58	0.68
1:C:262:TYR:HA	1:C:265:MET:HE3	1.75	0.68
1:E:20:GLY:CA	1:E:196:MET:HG2	2.24	0.67
1:G:27:ILE:O	1:G:136:ARG:HD3	1.94	0.67
1:C:38:LEU:HD13	1:C:180:PHE:HZ	1.60	0.67
1:A:27:ILE:O	1:A:136:ARG:HD3	1.95	0.67
1:H:33:SER:HB3	1:H:153:TRP:HB3	1.76	0.67
1:G:18:TYR:HE2	3:G:402:DP6:O2A	1.79	0.66
1:E:96:ASN:HD22	1:E:100:THR:HB	1.60	0.66
1:C:289:LYS:HD2	1:C:289:LYS:N	2.11	0.66
1:D:257:LEU:HD22	1:D:282:MET:HE1	1.76	0.66
1:C:283:ALA:H	1:C:289:LYS:NZ	1.92	0.66
1:F:98:VAL:CG2	1:F:99:PRO:HD2	2.24	0.65
1:G:34:LEU:HD12	1:G:151:ALA:O	1.95	0.65
1:E:27:ILE:O	1:E:136:ARG:HD3	1.97	0.65
1:E:38:LEU:HD13	1:E:180:PHE:CZ	2.31	0.65
1:D:262:TYR:HA	1:D:265:MET:HE2	1.78	0.65
1:F:18:TYR:OH	1:F:21:LYS:HG2	1.96	0.65
1:B:107:SER:HB3	1:B:139:SER:OG	1.98	0.64
1:B:27:ILE:O	1:B:136:ARG:HD3	1.97	0.64
1:D:253:PRO:HG2	1:E:265:MET:SD	2.38	0.64
1:D:262:TYR:HA	1:D:265:MET:HE3	1.80	0.64
1:E:15:LEU:HB3	1:E:236:ILE:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:VAL:HG12	1:D:259:GLN:H	1.63	0.63
1:C:289:LYS:H	1:C:289:LYS:HD2	1.63	0.63
1:E:188:LYS:HA	5:E:403:GOL:H31	1.81	0.63
1:H:308:PHE:HB2	1:H:313:ILE:HD11	1.79	0.63
1:F:103:GLY:O	1:F:104:LEU:HD12	1.98	0.63
1:B:318:ILE:HD13	1:B:318:ILE:N	2.12	0.62
1:H:105:ALA:HA	2:H:401:AGS:PG	2.38	0.62
1:D:248:LEU:O	1:D:253:PRO:HB3	2.00	0.61
1:H:119:ASN:HA	1:H:124:LEU:HD12	1.82	0.61
1:B:105:ALA:HA	2:B:401:AGS:O3B	2.00	0.61
1:D:27:ILE:O	1:D:136:ARG:CD	2.47	0.61
1:B:283:ALA:H	1:B:289:LYS:NZ	1.98	0.61
1:H:283:ALA:H	1:H:289:LYS:NZ	1.99	0.61
1:E:146:ILE:HA	1:E:323:VAL:HG23	1.83	0.61
1:C:6:LYS:HG3	1:C:46:LYS:HB2	1.83	0.61
1:G:58:LEU:HD22	1:G:73:ILE:HD13	1.82	0.61
1:E:283:ALA:CB	3:E:402:DP6:O2	2.48	0.60
1:C:218:ASN:ND2	6:C:515:HOH:O	2.35	0.60
1:A:20:GLY:N	1:A:196:MET:HG2	2.16	0.60
1:F:99:PRO:CG	1:F:104:LEU:HD22	2.25	0.60
1:H:15:LEU:HB3	1:H:236:ILE:HG21	1.84	0.60
1:D:233:GLY:HA3	1:D:279:TYR:CD1	2.36	0.59
1:F:18:TYR:HE2	3:F:402:DP6:O1A	1.85	0.59
1:G:180:PHE:CE2	1:G:289:LYS:HG2	2.38	0.59
1:A:233:GLY:HA3	1:A:279:TYR:CD1	2.37	0.59
1:F:20:GLY:N	1:F:196:MET:CG	2.66	0.59
1:H:56:ASP:HB2	1:H:74:GLN:HG2	1.85	0.59
1:A:21:LYS:HE2	6:A:519:HOH:O	2.03	0.58
2:G:401:AGS:O3G	3:G:402:DP6:O1A	2.21	0.58
1:F:22:ALA:N	1:F:28:ILE:O	2.32	0.58
1:A:70:LYS:O	1:A:74:GLN:HG2	2.03	0.58
2:B:401:AGS:O3G	3:B:402:DP6:O2A	2.22	0.58
1:C:96:ASN:HD22	1:C:100:THR:HB	1.69	0.58
1:E:8:ARG:HB2	1:E:326:ILE:HD11	1.85	0.58
1:H:283:ALA:H	1:H:289:LYS:HZ1	1.50	0.58
1:D:233:GLY:O	1:D:236:ILE:HG13	2.04	0.58
1:E:168:ASN:ND2	6:E:532:HOH:O	2.36	0.58
1:G:70:LYS:O	1:G:73:ILE:HG22	2.04	0.58
2:H:401:AGS:O3G	3:H:402:DP6:O1A	2.21	0.58
1:E:38:LEU:CD1	1:E:180:PHE:HZ	2.16	0.58
1:F:20:GLY:HA2	1:F:196:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:SER:N	2:C:401:AGS:O1B	2.37	0.57
1:A:13:ILE:HD12	1:A:289:LYS:HD3	1.86	0.57
1:F:269:GLU:OE2	1:F:273:LYS:HE3	2.04	0.57
1:D:77:MET:CE	1:D:114:LEU:HD21	2.35	0.57
1:F:192:SER:O	1:F:196:MET:HB2	2.04	0.57
1:D:304:PHE:HB3	1:D:313:ILE:CD1	2.34	0.57
1:C:56:ASP:HB2	1:C:74:GLN:HG2	1.86	0.57
1:A:302:GLU:HA	1:A:305:LEU:HD12	1.87	0.56
1:A:13:ILE:CG2	1:A:289:LYS:HD2	2.29	0.56
1:H:19:TRP:CE3	3:H:402:DP6:H3A1	2.39	0.56
1:F:20:GLY:N	1:F:196:MET:HG2	2.19	0.56
1:E:304:PHE:HB3	1:E:313:ILE:CD1	2.35	0.56
1:A:199:THR:HG21	1:A:246:THR:OG1	2.05	0.56
1:E:286:PRO:CD	5:E:403:GOL:H12	2.35	0.56
1:C:233:GLY:HA3	1:C:279:TYR:CD1	2.41	0.56
1:F:105:ALA:HA	2:F:401:AGS:PG	2.45	0.56
1:E:305:LEU:HD22	1:E:310:GLU:CG	2.28	0.56
1:A:188:LYS:HE3	2:A:401:AGS:O3A	2.05	0.56
1:F:20:GLY:CA	1:F:196:MET:HG2	2.37	0.55
1:F:6:LYS:HG2	1:F:326:ILE:HG13	1.89	0.55
2:D:401:AGS:O1A	2:D:401:AGS:O3G	2.24	0.55
1:D:192:SER:O	1:D:196:MET:HB2	2.07	0.55
1:B:248:LEU:O	1:B:253:PRO:HB3	2.06	0.55
1:E:193:ARG:HH21	3:E:402:DP6:PB	2.29	0.54
1:G:283:ALA:H	1:G:289:LYS:NZ	2.05	0.54
1:D:283:ALA:CA	3:D:402:DP6:O2	2.55	0.54
1:D:262:TYR:CD1	1:D:265:MET:CE	2.90	0.54
1:E:96:ASN:ND2	1:E:100:THR:HB	2.22	0.54
1:E:258:VAL:HG12	1:E:259:GLN:N	2.21	0.54
1:G:81:ARG:HD3	1:G:88:LEU:O	2.07	0.54
1:D:23:ASP:HB3	1:D:28:ILE:HG12	1.88	0.54
1:H:10:HIS:HB3	1:H:38:LEU:O	2.07	0.54
1:A:86:ASN:ND2	1:A:88:LEU:HD12	2.22	0.54
1:F:70:LYS:O	1:F:74:GLN:HG3	2.06	0.54
1:D:77:MET:HE1	1:D:114:LEU:HD21	1.89	0.54
1:E:14:ALA:HB3	3:E:402:DP6:O1	2.08	0.54
1:C:119:ASN:HA	1:C:124:LEU:HD12	1.88	0.54
1:E:21:LYS:HD3	1:E:27:ILE:HG23	1.88	0.54
1:G:179:ILE:HD13	1:G:301:MET:HG3	1.90	0.54
1:E:20:GLY:CA	1:E:196:MET:CG	2.85	0.53
1:G:94:SER:OG	2:G:401:AGS:N6	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HD3	1:A:153:TRP:CZ2	2.43	0.53
1:D:81:ARG:HD3	1:D:88:LEU:O	2.09	0.53
1:G:50:ASP:HB3	1:G:53:PHE:CE2	2.43	0.53
1:C:73:ILE:O	1:C:77:MET:HG2	2.09	0.53
1:D:293:GLU:HB2	6:D:512:HOH:O	2.09	0.52
1:G:21:LYS:NZ	3:G:402:DP6:O2B	2.29	0.52
1:B:297:LYS:HE3	1:B:301:MET:HE1	1.92	0.52
1:G:18:TYR:CE2	3:G:402:DP6:O2A	2.60	0.52
1:D:34:LEU:HD12	1:D:151:ALA:O	2.09	0.52
1:A:172:TRP:CG	1:A:227:GLN:HG2	2.44	0.52
1:E:13:ILE:HG12	1:E:38:LEU:HD11	1.92	0.52
1:E:304:PHE:HB3	1:E:313:ILE:HD11	1.91	0.52
1:A:13:ILE:HD12	1:A:289:LYS:CD	2.40	0.52
1:B:223:ALA:HB2	1:B:231:ARG:HG2	1.92	0.52
1:F:38:LEU:HD13	1:F:180:PHE:CZ	2.36	0.51
1:B:33:SER:HB3	1:B:153:TRP:HB3	1.92	0.51
1:G:29:PRO:HD3	1:G:153:TRP:CZ2	2.45	0.51
1:H:233:GLY:HA3	1:H:279:TYR:CD1	2.45	0.51
1:F:199:THR:HG21	1:F:246:THR:OG1	2.09	0.51
1:B:15:LEU:HB3	1:B:236:ILE:CG2	2.39	0.51
1:D:304:PHE:HB3	1:D:313:ILE:HD13	1.93	0.51
1:D:308:PHE:HB2	1:D:313:ILE:HD11	1.91	0.51
1:G:7:ALA:HB2	1:G:325:ILE:HD13	1.92	0.51
1:H:15:LEU:HD22	1:H:236:ILE:HD12	1.91	0.51
1:C:188:LYS:NZ	2:C:401:AGS:O2A	2.32	0.51
1:B:258:VAL:CG1	1:B:259:GLN:N	2.72	0.51
1:F:1:MET:HG2	1:F:2:VAL:H	1.75	0.51
1:C:188:LYS:HE2	1:C:284:ALA:O	2.10	0.51
1:G:29:PRO:HG2	1:G:155:LYS:CB	2.41	0.51
1:H:202:THR:HB	1:H:251:GLN:HB3	1.93	0.51
1:B:189:LYS:O	1:B:189:LYS:HG3	2.10	0.51
1:D:21:LYS:NZ	3:D:402:DP6:O1B	2.42	0.50
1:A:119:ASN:OD1	1:A:124:LEU:HB2	2.11	0.50
1:E:283:ALA:H	1:E:289:LYS:HZ2	1.58	0.50
1:G:1:MET:HG2	1:G:2:VAL:H	1.75	0.50
1:F:49:PHE:CE2	1:F:90:ALA:HB2	2.47	0.50
1:B:264:ALA:HA	1:B:267:ILE:HD12	1.92	0.50
1:A:13:ILE:CD1	1:A:289:LYS:HD3	2.42	0.50
2:E:401:AGS:S1G	2:E:401:AGS:O1B	2.70	0.50
1:G:65:VAL:HB	1:G:69:GLU:HB2	1.94	0.50
2:C:401:AGS:O2A	2:C:401:AGS:O2B	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:O	1:C:27:ILE:HG22	2.12	0.49
1:G:40:ARG:HB3	1:G:316:SER:HB2	1.94	0.49
1:F:70:LYS:O	1:F:73:ILE:HG22	2.13	0.49
1:A:36:VAL:HB	1:A:318:ILE:HD12	1.93	0.49
1:H:21:LYS:HD3	1:H:27:ILE:HA	1.95	0.49
1:F:21:LYS:HE3	1:F:27:ILE:HG23	1.95	0.49
1:C:27:ILE:O	1:C:136:ARG:HD3	2.11	0.49
1:F:152:GLU:HB2	1:F:167:ILE:HD11	1.93	0.49
1:C:168:ASN:O	6:C:524:HOH:O	2.20	0.49
1:B:86:ASN:ND2	1:B:88:LEU:HD12	2.27	0.49
1:F:98:VAL:CG2	1:F:99:PRO:CD	2.91	0.49
1:A:6:LYS:HD3	1:A:326:ILE:HG13	1.93	0.49
1:F:220:ALA:O	1:F:224:VAL:HG13	2.12	0.49
1:F:278:CYS:C	1:F:279:TYR:CD1	2.85	0.48
2:G:401:AGS:O1A	2:G:401:AGS:O3B	2.30	0.48
1:D:20:GLY:N	1:D:196:MET:HG2	2.27	0.48
1:C:49:PHE:HB3	1:C:88:LEU:HB3	1.95	0.48
1:A:10:HIS:CD2	1:A:39:ASP:HA	2.49	0.48
1:E:283:ALA:HB2	3:E:402:DP6:O2	2.13	0.48
1:A:20:GLY:H	1:A:196:MET:CG	2.25	0.48
1:B:105:ALA:HA	2:B:401:AGS:PG	2.54	0.48
1:H:6:LYS:HD3	1:H:326:ILE:HG13	1.94	0.48
1:F:27:ILE:O	1:F:136:ARG:HD3	2.14	0.48
1:B:50:ASP:HB3	1:B:53:PHE:CD2	2.48	0.48
1:H:19:TRP:HE3	3:H:402:DP6:H3A1	1.77	0.48
1:F:70:LYS:HA	1:F:73:ILE:HG22	1.96	0.48
1:D:258:VAL:HG12	1:D:259:GLN:N	2.27	0.48
1:C:237:GLU:OE1	1:C:272:ARG:NH2	2.47	0.48
1:G:188:LYS:HZ3	1:G:284:ALA:HB3	1.77	0.48
1:D:283:ALA:CB	3:D:402:DP6:O2	2.62	0.48
1:G:38:LEU:HD13	1:G:180:PHE:HZ	1.78	0.48
1:A:221:LYS:O	1:A:224:VAL:HG22	2.14	0.47
1:G:15:LEU:HB3	1:G:236:ILE:HG21	1.96	0.47
1:A:136:ARG:NH2	1:A:159:ASP:O	2.46	0.47
1:G:248:LEU:O	1:G:253:PRO:HB3	2.15	0.47
1:A:196:MET:HE3	1:A:196:MET:HB3	1.73	0.47
2:B:401:AGS:O1B	2:B:401:AGS:O2A	2.33	0.47
1:H:27:ILE:O	1:H:136:ARG:HD3	2.14	0.47
1:D:119:ASN:OD1	1:D:124:LEU:HB2	2.14	0.47
1:H:241:LEU:HD23	1:H:241:LEU:HA	1.77	0.47
1:D:262:TYR:CD1	1:D:265:MET:HE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:SER:OG	3:B:402:DP6:O1A	2.21	0.47
1:G:13:ILE:HG12	1:G:38:LEU:HD11	1.96	0.47
1:C:111:TYR:CD1	1:C:138:GLY:HA3	2.50	0.47
1:E:183:ILE:HD13	1:E:260:GLU:HB3	1.97	0.47
1:D:137:ARG:NH1	6:D:520:HOH:O	2.48	0.46
1:H:111:TYR:CD1	1:H:138:GLY:HA3	2.51	0.46
1:D:20:GLY:H	1:D:196:MET:CG	2.28	0.46
1:C:77:MET:CE	1:C:114:LEU:HD21	2.45	0.46
1:B:70:LYS:O	1:B:74:GLN:HG3	2.16	0.46
1:F:236:ILE:HG13	1:F:237:GLU:N	2.29	0.46
1:B:96:ASN:HD22	1:B:100:THR:HB	1.80	0.46
1:C:49:PHE:CD1	1:C:122:LEU:HD21	2.51	0.46
1:H:40:ARG:CZ	1:H:314:ILE:HG23	2.46	0.46
1:A:10:HIS:CD2	1:A:42:TYR:HB3	2.50	0.46
1:E:103:GLY:O	1:E:104:LEU:HD23	2.15	0.46
1:A:46:LYS:HE3	1:A:48:THR:CG2	2.46	0.46
1:F:34:LEU:HD12	1:F:151:ALA:O	2.15	0.46
1:H:61:ASN:HA	1:H:95:GLU:OE1	2.16	0.46
1:C:18:TYR:O	3:C:402:DP6:H3A2	2.14	0.46
1:E:297:LYS:HG2	1:E:301:MET:HE2	1.97	0.46
1:H:188:LYS:HE3	1:H:188:LYS:HB3	1.56	0.46
1:C:273:LYS:HD3	1:C:273:LYS:HA	1.74	0.46
1:F:95:GLU:HB3	1:F:97:TYR:CE1	2.51	0.46
1:B:174:LYS:HE3	1:B:320:SER:OG	2.15	0.46
3:B:402:DP6:O2A	3:B:402:DP6:O2B	2.34	0.46
1:D:50:ASP:OD1	1:D:51:PRO:HD2	2.16	0.46
1:G:252:PRO:O	6:G:536:HOH:O	2.20	0.46
1:E:105:ALA:HA	2:E:401:AGS:PG	2.56	0.46
1:D:273:LYS:HD3	1:D:273:LYS:HA	1.64	0.46
1:B:13:ILE:HG12	1:B:38:LEU:CD1	2.44	0.45
1:H:297:LYS:HE3	1:H:315:ALA:HB1	1.98	0.45
1:H:296:ASN:O	1:H:300:VAL:HG23	2.16	0.45
1:A:21:LYS:HD3	1:A:27:ILE:HA	1.99	0.45
1:G:40:ARG:CB	1:G:316:SER:HB2	2.47	0.45
1:D:262:TYR:CD1	1:D:265:MET:HE1	2.52	0.45
1:E:5:GLY:N	1:E:121:ALA:HB2	2.32	0.45
1:B:20:GLY:H	1:B:196:MET:CG	2.30	0.45
1:H:70:LYS:O	1:H:74:GLN:HG3	2.16	0.45
1:F:188:LYS:HE3	2:F:401:AGS:O3A	2.15	0.45
1:G:251:GLN:HA	1:G:252:PRO:HA	1.87	0.45
1:G:56:ASP:HB2	1:G:74:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:SER:HB3	2:G:401:AGS:H5'2	1.98	0.45
1:A:319:ILE:HG12	1:A:321:SER:H	1.81	0.45
1:B:18:TYR:O	3:B:402:DP6:H3A3	2.16	0.45
1:F:36:VAL:HA	1:F:149:GLY:O	2.17	0.45
1:A:206:TYR:CE2	1:A:210:LEU:HD11	2.52	0.45
1:B:206:TYR:O	1:B:209:TRP:HB3	2.16	0.45
1:F:18:TYR:OH	1:F:21:LYS:HE3	2.16	0.45
1:E:15:LEU:HB3	1:E:236:ILE:CG2	2.47	0.45
1:B:20:GLY:N	1:B:196:MET:HG3	2.32	0.45
2:D:401:AGS:O3G	3:D:402:DP6:O2A	2.34	0.45
1:D:29:PRO:HD3	1:D:153:TRP:CZ2	2.52	0.45
1:D:12:ASN:HB2	1:D:36:VAL:O	2.17	0.45
1:E:33:SER:OG	1:E:144:ARG:NH1	2.50	0.45
1:B:199:THR:HG21	1:B:246:THR:OG1	2.16	0.44
1:F:96:ASN:ND2	1:F:100:THR:CG2	2.56	0.44
1:G:107:SER:OG	2:G:401:AGS:O2G	2.32	0.44
1:C:13:ILE:HG12	1:C:38:LEU:HD11	1.98	0.44
1:E:146:ILE:HA	1:E:323:VAL:CG2	2.45	0.44
1:F:231:ARG:O	6:F:510:HOH:O	2.21	0.44
1:A:49:PHE:CE2	1:A:90:ALA:HB2	2.52	0.44
1:F:98:VAL:HG23	1:F:99:PRO:CD	2.36	0.44
1:F:49:PHE:CD2	1:F:90:ALA:HB2	2.53	0.44
1:A:15:LEU:HD21	1:A:36:VAL:HG22	2.00	0.44
1:H:21:LYS:O	1:H:200:ARG:HD3	2.16	0.44
1:D:10:HIS:HB3	1:D:38:LEU:O	2.18	0.44
1:G:233:GLY:HA3	1:G:279:TYR:CG	2.53	0.44
1:H:73:ILE:HA	1:H:73:ILE:HD12	1.77	0.44
1:D:257:LEU:HD22	1:D:282:MET:HE2	1.99	0.44
1:F:268:VAL:O	1:F:271:CYS:HB2	2.17	0.44
1:A:31:ASN:ND2	1:A:213:VAL:HG21	2.33	0.44
1:F:155:LYS:O	1:F:162:SER:HB2	2.18	0.44
1:H:41:PHE:HB3	1:H:98:VAL:HB	2.00	0.44
1:H:289:LYS:HE3	1:H:289:LYS:H	1.83	0.44
1:C:38:LEU:CD1	1:C:180:PHE:HZ	2.28	0.44
2:B:401:AGS:S1G	3:B:402:DP6:H21	2.58	0.43
1:D:233:GLY:HA3	1:D:279:TYR:CG	2.53	0.43
1:B:178:MET:HG2	1:B:180:PHE:CE1	2.53	0.43
1:F:200:ARG:O	1:F:200:ARG:HD2	2.19	0.43
1:F:18:TYR:CE2	3:F:402:DP6:O1A	2.68	0.43
1:B:292:VAL:HG22	1:B:293:GLU:O	2.18	0.43
1:C:77:MET:HE1	1:C:114:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:SER:HA	1:D:249:GLY:O	2.19	0.43
1:A:107:SER:HB3	1:A:139:SER:OG	2.18	0.43
1:B:86:ASN:HD22	1:B:88:LEU:HD12	1.84	0.43
1:C:14:ALA:HA	1:C:35:SER:HB3	2.01	0.43
1:H:15:LEU:HD11	1:H:36:VAL:HG13	2.00	0.43
1:G:180:PHE:CD2	1:G:289:LYS:HG2	2.52	0.43
1:F:110:ALA:HB1	2:F:401:AGS:C6	2.49	0.43
1:C:269:GLU:OE2	1:C:273:LYS:HE3	2.18	0.43
1:A:206:TYR:O	1:A:209:TRP:HB3	2.18	0.43
1:A:111:TYR:CD1	1:A:138:GLY:HA3	2.53	0.43
1:B:218:ASN:O	1:B:222:GLU:HG3	2.19	0.43
1:C:129:THR:O	1:C:133:ARG:HG3	2.17	0.43
1:G:258:VAL:HG12	1:G:260:GLU:H	1.84	0.43
1:H:98:VAL:HG22	1:H:99:PRO:O	2.19	0.43
1:G:269:GLU:OE1	1:G:272:ARG:NH1	2.52	0.43
1:E:248:LEU:O	1:E:253:PRO:HB3	2.18	0.43
1:F:188:LYS:NZ	1:F:284:ALA:O	2.44	0.43
1:E:233:GLY:HA3	1:E:279:TYR:CD1	2.54	0.43
1:B:99:PRO:HG2	1:B:104:LEU:HD12	2.01	0.43
1:C:26:TYR:O	1:C:27:ILE:HB	2.19	0.42
1:B:188:LYS:HZ3	1:B:192:SER:HB3	1.84	0.42
1:B:73:ILE:HD12	1:B:73:ILE:HA	1.89	0.42
1:A:76:TYR:CE2	1:A:114:LEU:HD23	2.54	0.42
1:A:16:ILE:HA	1:A:239:ASN:OD1	2.18	0.42
1:D:267:ILE:HD11	1:D:307:VAL:HG21	1.99	0.42
1:G:50:ASP:HA	1:G:51:PRO:HD3	1.77	0.42
1:B:147:PHE:CZ	1:B:165:HIS:HA	2.54	0.42
1:A:185:ASN:HB3	1:A:186:GLN:OE1	2.20	0.42
1:G:206:TYR:O	1:G:209:TRP:HB3	2.19	0.42
1:F:41:PHE:HB3	1:F:98:VAL:HB	2.02	0.42
1:C:10:HIS:ND1	1:C:38:LEU:O	2.53	0.42
2:F:401:AGS:O1B	2:F:401:AGS:S1G	2.78	0.42
1:H:22:ALA:N	1:H:28:ILE:O	2.41	0.42
1:H:191:SER:O	1:H:192:SER:C	2.58	0.42
1:A:218:ASN:O	1:A:222:GLU:HG2	2.19	0.42
1:A:32:ASN:OD1	1:A:155:LYS:HD3	2.20	0.42
1:F:273:LYS:HD3	1:F:273:LYS:HA	1.62	0.42
1:B:81:ARG:HD3	1:B:88:LEU:O	2.20	0.42
1:G:94:SER:CB	2:G:401:AGS:HN62	2.33	0.42
1:B:258:VAL:HG12	1:B:260:GLU:H	1.85	0.42
1:B:258:VAL:HG12	1:B:259:GLN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ALA:HA	1:D:35:SER:HB3	2.02	0.42
1:E:47:VAL:HG12	1:E:117:ALA:HB1	2.02	0.42
1:B:289:LYS:N	1:B:289:LYS:HD2	2.35	0.42
1:E:286:PRO:HG3	5:E:403:GOL:H12	2.02	0.42
2:B:401:AGS:O1A	2:B:401:AGS:O3G	2.37	0.41
1:A:192:SER:O	1:A:196:MET:HB2	2.20	0.41
1:H:40:ARG:NH2	1:H:314:ILE:HG23	2.35	0.41
1:A:108:ALA:HB2	1:A:141:SER:HB2	2.02	0.41
3:E:402:DP6:O3B	3:E:402:DP6:O2A	2.39	0.41
1:G:220:ALA:O	1:G:224:VAL:HG13	2.20	0.41
1:E:286:PRO:CG	5:E:403:GOL:H12	2.51	0.41
1:C:10:HIS:CE1	1:C:39:ASP:O	2.74	0.41
1:G:86:ASN:ND2	1:G:88:LEU:HD12	2.35	0.41
1:D:203:SER:HA	1:D:250:ALA:HA	2.02	0.41
1:F:313:ILE:C	1:F:314:ILE:HD12	2.41	0.41
1:H:50:ASP:HA	1:H:51:PRO:HD3	1.91	0.41
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.79	0.41
1:A:191:SER:O	1:A:192:SER:C	2.59	0.41
1:F:38:LEU:CD1	1:F:180:PHE:HZ	2.28	0.41
1:E:265:MET:HG2	1:E:280:PHE:CE1	2.56	0.41
1:F:276:LEU:HD21	1:F:299:ALA:HB1	2.03	0.41
1:E:16:ILE:HB	1:E:34:LEU:HB3	2.03	0.41
1:E:116:ALA:CB	1:E:323:VAL:HG11	2.50	0.41
1:H:15:LEU:N	1:H:34:LEU:O	2.47	0.41
1:E:304:PHE:HB3	1:E:313:ILE:HD13	2.02	0.41
1:H:17:LYS:CD	3:H:402:DP6:O2	2.69	0.41
1:C:188:LYS:HG3	1:C:188:LYS:H	1.59	0.41
1:C:262:TYR:HA	1:C:265:MET:CE	2.48	0.41
1:C:38:LEU:HD13	1:C:180:PHE:CZ	2.48	0.41
1:D:84:ALA:CB	1:D:122:LEU:HD13	2.50	0.41
1:A:295:LYS:HG2	1:A:295:LYS:H	1.58	0.41
1:D:84:ALA:HB2	1:D:122:LEU:HD13	2.01	0.41
1:H:46:LYS:HB3	1:H:93:GLU:HB3	2.02	0.41
1:G:20:GLY:HA2	1:G:196:MET:HG2	2.03	0.41
1:F:169:SER:O	1:F:170:ASN:HB2	2.21	0.41
1:B:305:LEU:HD23	1:B:313:ILE:HD13	2.02	0.40
1:H:152:GLU:O	1:H:164:ALA:HA	2.21	0.40
1:G:305:LEU:HA	1:G:305:LEU:HD23	1.92	0.40
1:E:21:LYS:NZ	3:E:402:DP6:O2B	2.50	0.40
1:B:188:LYS:HD3	1:B:190:VAL:O	2.21	0.40
1:A:251:GLN:HA	1:A:252:PRO:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:VAL:HG12	1:C:117:ALA:HB1	2.02	0.40
3:H:402:DP6:O1	3:H:402:DP6:O3A	2.34	0.40
1:C:262:TYR:CD1	1:C:265:MET:HE3	2.56	0.40
3:B:402:DP6:H52	3:B:402:DP6:H21	1.63	0.40
1:E:116:ALA:HB2	1:E:323:VAL:HG11	2.03	0.40
1:G:196:MET:HE2	1:G:196:MET:HB2	1.92	0.40
1:C:15:LEU:HB3	1:C:236:ILE:HG21	2.04	0.40
1:D:40:ARG:HB3	1:D:316:SER:HB2	2.03	0.40
1:D:18:TYR:HE2	3:D:402:DP6:O6	2.04	0.40
1:E:193:ARG:NH2	3:E:402:DP6:O3B	2.54	0.40
1:B:209:TRP:CZ3	1:B:243:MET:HB2	2.57	0.40
1:D:76:TYR:O	1:D:80:VAL:HG23	2.22	0.40
1:D:200:ARG:HH11	1:D:200:ARG:HD2	1.75	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	324/332 (98%)	307 (95%)	17 (5%)	0	100	100
1	B	324/332 (98%)	315 (97%)	9 (3%)	0	100	100
1	C	324/332 (98%)	314 (97%)	10 (3%)	0	100	100
1	D	324/332 (98%)	315 (97%)	9 (3%)	0	100	100
1	E	326/332 (98%)	312 (96%)	14 (4%)	0	100	100
1	F	324/332 (98%)	316 (98%)	8 (2%)	0	100	100
1	G	324/332 (98%)	314 (97%)	10 (3%)	0	100	100
1	H	324/332 (98%)	314 (97%)	10 (3%)	0	100	100
All	All	2594/2656 (98%)	2507 (97%)	87 (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	274/278 (99%)	266 (97%)	8 (3%)	50	77
1	B	274/278 (99%)	271 (99%)	3 (1%)	80	93
1	C	274/278 (99%)	269 (98%)	5 (2%)	66	87
1	D	274/278 (99%)	268 (98%)	6 (2%)	60	83
1	E	275/278 (99%)	263 (96%)	12 (4%)	35	63
1	F	274/278 (99%)	261 (95%)	13 (5%)	32	59
1	G	274/278 (99%)	266 (97%)	8 (3%)	50	77
1	H	274/278 (99%)	264 (96%)	10 (4%)	42	71
All	All	2193/2224 (99%)	2128 (97%)	65 (3%)	48	76

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	54	THR
1	A	55	GLU
1	A	83	LEU
1	A	131	LEU
1	A	196	MET
1	A	200	ARG
1	A	295	LYS
1	B	38	LEU
1	B	200	ARG
1	B	231	ARG
1	C	63	ASN
1	C	188	LYS
1	C	200	ARG
1	C	224	VAL
1	C	236	ILE

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Mol	Chain	Res	Type
1	D	18	TYR
1	D	88	LEU
1	D	145	SER
1	D	197	SER
1	D	200	ARG
1	D	309	ASP
1	E	18	TYR
1	E	21	LYS
1	E	24	GLU
1	E	27	ILE
1	E	31	ASN
1	E	54	THR
1	E	87	ARG
1	E	100	THR
1	E	132	SER
1	E	200	ARG
1	E	243	MET
1	E	289	LYS
1	F	4	SER
1	F	21	LYS
1	F	123	SER
1	F	145	SER
1	F	200	ARG
1	F	224	VAL
1	F	236	ILE
1	F	243	MET
1	F	260	GLU
1	F	289	LYS
1	F	297	LYS
1	F	302	GLU
1	F	306	LYS
1	G	24	GLU
1	G	46	LYS
1	G	73	ILE
1	G	88	LEU
1	G	145	SER
1	G	200	ARG
1	G	224	VAL
1	G	289	LYS
1	H	54	THR
1	H	104	LEU
1	H	185	ASN

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Mol	Chain	Res	Type
1	H	187	SER
1	H	188	LYS
1	H	200	ARG
1	H	258	VAL
1	H	261	SER
1	H	289	LYS
1	H	294	LYS

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

Mol	Chain	Res	Type
1	A	10	HIS
1	F	303	GLN
1	G	74	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](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	A	401	-	24,33,33	2.16	6 (25%)	28,52,52	2.75	7 (25%)
3	DP6	A	402	-	11,17,17	1.65	2 (18%)	14,26,26	1.45	3 (21%)
4	FMT	A	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AGS	B	401	-	24,33,33	2.16	6 (25%)	28,52,52	2.76	7 (25%)
3	DP6	B	402	-	11,17,17	1.75	2 (18%)	14,26,26	1.34	3 (21%)
2	AGS	C	401	-	24,33,33	2.14	6 (25%)	28,52,52	2.68	6 (21%)
3	DP6	C	402	-	11,17,17	1.65	2 (18%)	14,26,26	1.44	3 (21%)
2	AGS	D	401	-	24,33,33	2.17	6 (25%)	28,52,52	2.68	6 (21%)
3	DP6	D	402	-	11,17,17	1.65	2 (18%)	14,26,26	1.46	3 (21%)
4	FMT	D	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AGS	E	401	-	24,33,33	2.16	6 (25%)	28,52,52	2.76	7 (25%)
3	DP6	E	402	-	11,17,17	1.65	2 (18%)	14,26,26	1.46	3 (21%)
5	GOL	E	403	-	5,5,5	0.34	0	5,5,5	0.24	0
4	FMT	E	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AGS	F	401	-	24,33,33	2.16	6 (25%)	28,52,52	2.77	7 (25%)
3	DP6	F	402	-	11,17,17	1.69	2 (18%)	14,26,26	1.49	3 (21%)
2	AGS	G	401	-	24,33,33	2.13	6 (25%)	28,52,52	2.76	8 (28%)
3	DP6	G	402	-	11,17,17	1.79	2 (18%)	14,26,26	1.47	3 (21%)
2	AGS	H	401	-	24,33,33	2.17	6 (25%)	28,52,52	2.75	7 (25%)
3	DP6	H	402	-	11,17,17	1.67	2 (18%)	14,26,26	1.45	3 (21%)
4	FMT	H	403	-	0,2,2	0.00	-	0,1,1	0.00	-

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	AGS	A	401	-	-	0/15/38/38	0/3/3/3
3	DP6	A	402	-	-	0/17/19/19	0/0/0/0
4	FMT	A	403	-	-	0/0/0/0	0/0/0/0
2	AGS	B	401	-	-	0/15/38/38	0/3/3/3
3	DP6	B	402	-	-	0/17/19/19	0/0/0/0
2	AGS	C	401	-	-	0/15/38/38	0/3/3/3
3	DP6	C	402	-	-	0/17/19/19	0/0/0/0
2	AGS	D	401	-	-	0/15/38/38	0/3/3/3
3	DP6	D	402	-	-	0/17/19/19	0/0/0/0
4	FMT	D	403	-	-	0/0/0/0	0/0/0/0
2	AGS	E	401	-	-	0/15/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DP6	E	402	-	-	0/17/19/19	0/0/0/0
5	GOL	E	403	-	-	0/4/4/4	0/0/0/0
4	FMT	E	404	-	-	0/0/0/0	0/0/0/0
2	AGS	F	401	-	-	0/15/38/38	0/3/3/3
3	DP6	F	402	-	-	0/17/19/19	0/0/0/0
2	AGS	G	401	-	-	0/15/38/38	0/3/3/3
3	DP6	G	402	-	-	0/17/19/19	0/0/0/0
2	AGS	H	401	-	-	0/15/38/38	0/3/3/3
3	DP6	H	402	-	-	0/17/19/19	0/0/0/0
4	FMT	H	403	-	-	0/0/0/0	0/0/0/0

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	AGS	C2'-C3'	-4.36	1.41	1.53
2	C	401	AGS	C2'-C3'	-4.30	1.41	1.53
2	F	401	AGS	C2'-C3'	-4.18	1.42	1.53
2	E	401	AGS	C2'-C3'	-4.18	1.42	1.53
2	B	401	AGS	C2'-C3'	-4.18	1.42	1.53
2	H	401	AGS	C2'-C3'	-4.17	1.42	1.53
2	G	401	AGS	C2'-C3'	-4.16	1.42	1.53
2	A	401	AGS	C2'-C3'	-4.16	1.42	1.53
3	G	402	DP6	O3A-C3	-4.14	1.37	1.44
3	B	402	DP6	O3A-C3	-4.13	1.37	1.44
3	F	402	DP6	O3A-C3	-4.02	1.37	1.44
3	C	402	DP6	O3A-C3	-3.94	1.38	1.44
3	H	402	DP6	O3A-C3	-3.94	1.38	1.44
3	E	402	DP6	O3A-C3	-3.93	1.38	1.44
3	A	402	DP6	O3A-C3	-3.92	1.38	1.44
3	D	402	DP6	O3A-C3	-3.92	1.38	1.44
3	G	402	DP6	C3A-C3	-3.20	1.49	1.52
3	B	402	DP6	C3A-C3	-2.96	1.49	1.52
3	H	402	DP6	C3A-C3	-2.84	1.49	1.52
3	F	402	DP6	C3A-C3	-2.82	1.49	1.52
3	E	402	DP6	C3A-C3	-2.79	1.49	1.52
3	A	402	DP6	C3A-C3	-2.79	1.49	1.52
3	D	402	DP6	C3A-C3	-2.78	1.49	1.52
3	C	402	DP6	C3A-C3	-2.75	1.49	1.52
2	G	401	AGS	O4'-C4'	-2.64	1.38	1.45
2	B	401	AGS	O4'-C4'	-2.64	1.38	1.45
2	E	401	AGS	O4'-C4'	-2.63	1.38	1.45
2	A	401	AGS	O4'-C4'	-2.62	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	AGS	O4'-C4'	-2.61	1.39	1.45
2	F	401	AGS	O4'-C4'	-2.60	1.39	1.45
2	D	401	AGS	O4'-C4'	-2.54	1.39	1.45
2	C	401	AGS	O4'-C4'	-2.54	1.39	1.45
2	D	401	AGS	C3'-C4'	-2.21	1.47	1.53
2	C	401	AGS	C3'-C4'	-2.20	1.47	1.53
2	H	401	AGS	PG-O3G	-2.14	1.47	1.55
2	F	401	AGS	PG-O3G	-2.13	1.47	1.55
2	C	401	AGS	PG-O3G	-2.12	1.47	1.55
2	H	401	AGS	C3'-C4'	-2.12	1.47	1.53
2	E	401	AGS	PG-O3G	-2.12	1.47	1.55
2	B	401	AGS	PG-O3G	-2.12	1.47	1.55
2	G	401	AGS	PG-O3G	-2.11	1.47	1.55
2	A	401	AGS	C3'-C4'	-2.11	1.47	1.53
2	D	401	AGS	PG-O3G	-2.11	1.47	1.55
2	A	401	AGS	PG-O3G	-2.10	1.47	1.55
2	G	401	AGS	C3'-C4'	-2.09	1.47	1.53
2	F	401	AGS	C3'-C4'	-2.09	1.47	1.53
2	E	401	AGS	C3'-C4'	-2.08	1.47	1.53
2	B	401	AGS	C3'-C4'	-2.07	1.47	1.53
2	D	401	AGS	C6-N6	2.34	1.42	1.34
2	C	401	AGS	C6-N6	2.35	1.42	1.34
2	G	401	AGS	C6-N6	2.36	1.42	1.34
2	B	401	AGS	C6-N6	2.36	1.42	1.34
2	A	401	AGS	C6-N6	2.37	1.42	1.34
2	H	401	AGS	C6-N6	2.37	1.42	1.34
2	F	401	AGS	C6-N6	2.37	1.42	1.34
2	E	401	AGS	C6-N6	2.38	1.42	1.34
2	C	401	AGS	PG-S1G	7.21	2.04	1.90
2	G	401	AGS	PG-S1G	7.21	2.04	1.90
2	E	401	AGS	PG-S1G	7.22	2.04	1.90
2	D	401	AGS	PG-S1G	7.23	2.04	1.90
2	B	401	AGS	PG-S1G	7.24	2.04	1.90
2	A	401	AGS	PG-S1G	7.25	2.04	1.90
2	F	401	AGS	PG-S1G	7.26	2.04	1.90
2	H	401	AGS	PG-S1G	7.30	2.04	1.90

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	AGS	N3-C2-N1	-11.40	120.17	128.89
2	G	401	AGS	N3-C2-N1	-11.40	120.17	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	AGS	N3-C2-N1	-11.39	120.18	128.89
2	B	401	AGS	N3-C2-N1	-11.34	120.21	128.89
2	H	401	AGS	N3-C2-N1	-11.33	120.22	128.89
2	A	401	AGS	N3-C2-N1	-11.32	120.23	128.89
2	C	401	AGS	N3-C2-N1	-11.32	120.23	128.89
2	D	401	AGS	N3-C2-N1	-11.31	120.24	128.89
2	A	401	AGS	PA-O3A-PB	-4.67	119.63	132.73
2	E	401	AGS	PA-O3A-PB	-4.65	119.66	132.73
2	F	401	AGS	PA-O3A-PB	-4.65	119.68	132.73
2	H	401	AGS	PA-O3A-PB	-4.65	119.68	132.73
2	B	401	AGS	PA-O3A-PB	-4.64	119.70	132.73
2	G	401	AGS	PA-O3A-PB	-4.64	119.71	132.73
2	D	401	AGS	PA-O3A-PB	-4.62	119.76	132.73
2	C	401	AGS	PA-O3A-PB	-4.40	120.38	132.73
3	F	402	DP6	PA-O6-PB	-4.15	118.74	132.67
2	C	401	AGS	PB-O3B-PG	-4.01	119.21	132.67
2	A	401	AGS	PB-O3B-PG	-3.96	119.39	132.67
3	G	402	DP6	PA-O6-PB	-3.95	119.42	132.67
2	B	401	AGS	PB-O3B-PG	-3.95	119.42	132.67
2	H	401	AGS	PB-O3B-PG	-3.95	119.43	132.67
2	E	401	AGS	PB-O3B-PG	-3.95	119.43	132.67
2	F	401	AGS	PB-O3B-PG	-3.95	119.43	132.67
2	G	401	AGS	PB-O3B-PG	-3.94	119.45	132.67
3	D	402	DP6	PA-O6-PB	-3.90	119.59	132.67
3	E	402	DP6	PA-O6-PB	-3.89	119.61	132.67
3	A	402	DP6	PA-O6-PB	-3.87	119.68	132.67
3	H	402	DP6	PA-O6-PB	-3.83	119.81	132.67
2	D	401	AGS	PB-O3B-PG	-3.83	119.84	132.67
3	C	402	DP6	PA-O6-PB	-3.79	119.97	132.67
2	B	401	AGS	C4'-O4'-C1'	-3.11	106.30	109.72
2	H	401	AGS	C4'-O4'-C1'	-3.11	106.30	109.72
3	B	402	DP6	PA-O6-PB	-3.11	122.25	132.67
2	A	401	AGS	C4'-O4'-C1'	-3.09	106.32	109.72
2	F	401	AGS	C4'-O4'-C1'	-3.09	106.33	109.72
2	E	401	AGS	C4'-O4'-C1'	-3.09	106.33	109.72
2	G	401	AGS	C4'-O4'-C1'	-3.06	106.36	109.72
2	B	401	AGS	C4-C5-N7	-2.24	107.42	109.48
2	C	401	AGS	C4-C5-N7	-2.23	107.43	109.48
2	G	401	AGS	C4-C5-N7	-2.22	107.43	109.48
2	A	401	AGS	C4-C5-N7	-2.22	107.44	109.48
2	F	401	AGS	C4-C5-N7	-2.20	107.45	109.48
2	E	401	AGS	C4-C5-N7	-2.19	107.46	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	AGS	C4-C5-N7	-2.19	107.47	109.48
2	H	401	AGS	C4-C5-N7	-2.17	107.48	109.48
2	G	401	AGS	C2-N1-C6	2.01	122.36	118.77
3	G	402	DP6	O5-C5-C4	2.10	117.16	109.01
3	F	402	DP6	O5-C5-C4	2.15	117.34	109.01
3	A	402	DP6	O5-C5-C4	2.15	117.36	109.01
3	H	402	DP6	O5-C5-C4	2.17	117.43	109.01
3	B	402	DP6	O5-C5-C4	2.17	117.44	109.01
3	B	402	DP6	O6-PA-O5	2.18	108.72	102.94
3	C	402	DP6	O5-C5-C4	2.18	117.46	109.01
3	E	402	DP6	O5-C5-C4	2.19	117.52	109.01
3	D	402	DP6	O5-C5-C4	2.20	117.55	109.01
2	D	401	AGS	O5'-C5'-C4'	2.23	117.34	109.12
2	E	401	AGS	O5'-C5'-C4'	2.24	117.38	109.12
2	G	401	AGS	O5'-C5'-C4'	2.24	117.38	109.12
2	B	401	AGS	O5'-C5'-C4'	2.24	117.39	109.12
2	F	401	AGS	O5'-C5'-C4'	2.25	117.40	109.12
2	H	401	AGS	O5'-C5'-C4'	2.25	117.40	109.12
2	A	401	AGS	O5'-C5'-C4'	2.25	117.42	109.12
2	C	401	AGS	O5'-C5'-C4'	2.27	117.48	109.12
3	F	402	DP6	O6-PA-O5	2.31	109.07	102.94
2	C	401	AGS	O3A-PA-O5'	2.35	109.17	102.94
3	C	402	DP6	O6-PA-O5	2.42	109.35	102.94
3	G	402	DP6	O6-PA-O5	2.42	109.37	102.94
3	A	402	DP6	O6-PA-O5	2.43	109.37	102.94
2	H	401	AGS	O3A-PA-O5'	2.43	109.38	102.94
2	D	401	AGS	O3A-PA-O5'	2.43	109.39	102.94
3	D	402	DP6	O6-PA-O5	2.44	109.40	102.94
2	E	401	AGS	O3A-PA-O5'	2.44	109.41	102.94
3	E	402	DP6	O6-PA-O5	2.44	109.42	102.94
2	F	401	AGS	O3A-PA-O5'	2.44	109.42	102.94
3	H	402	DP6	O6-PA-O5	2.44	109.42	102.94
2	A	401	AGS	O3A-PA-O5'	2.45	109.43	102.94
2	B	401	AGS	O3A-PA-O5'	2.45	109.44	102.94
2	G	401	AGS	O3A-PA-O5'	2.46	109.45	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	AGS	2	0
3	A	402	DP6	1	0
2	B	401	AGS	6	0
3	B	402	DP6	6	0
2	C	401	AGS	4	0
3	C	402	DP6	3	0
2	D	401	AGS	4	0
3	D	402	DP6	8	0
2	E	401	AGS	2	0
3	E	402	DP6	7	0
5	E	403	GOL	4	0
2	F	401	AGS	4	0
3	F	402	DP6	3	0
2	G	401	AGS	8	0
3	G	402	DP6	6	0
2	H	401	AGS	4	0
3	H	402	DP6	6	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	326/332 (98%)	-0.20	3 (0%) 85 83	38, 54, 77, 96	0
1	B	326/332 (98%)	-0.36	0 100 100	34, 46, 62, 77	0
1	C	326/332 (98%)	-0.34	1 (0%) 94 93	36, 49, 69, 97	0
1	D	326/332 (98%)	-0.40	1 (0%) 94 93	35, 45, 65, 86	0
1	E	328/332 (98%)	-0.29	2 (0%) 90 88	34, 47, 67, 96	0
1	F	326/332 (98%)	-0.34	4 (1%) 81 77	36, 49, 70, 88	0
1	G	326/332 (98%)	-0.37	0 100 100	32, 44, 63, 88	0
1	H	326/332 (98%)	-0.16	1 (0%) 94 93	36, 56, 74, 87	0
All	All	2610/2656 (98%)	-0.31	12 (0%) 91 90	32, 49, 70, 97	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	88	LEU	2.9
1	D	87	ARG	2.7
1	C	87	ARG	2.7
1	F	50	ASP	2.7
1	A	87	ARG	2.4
1	A	57	CYS	2.4
1	H	54	THR	2.4
1	F	87	ARG	2.1
1	A	52	ASP	2.1
1	F	82	ASP	2.1
1	E	-1	GLY	2.0
1	E	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
5	GOL	E	403	6/6	0.72	0.34	9.38	57,59,61,63	0
4	FMT	H	403	3/3	0.77	0.24	6.91	59,59,62,64	0
3	DP6	G	402	18/18	0.94	0.22	4.31	37,44,64,74	0
4	FMT	E	404	3/3	0.82	0.31	4.26	66,66,67,68	0
3	DP6	C	402	18/18	0.96	0.19	3.25	40,48,58,63	18
3	DP6	B	402	18/18	0.95	0.20	2.95	38,48,67,67	0
3	DP6	D	402	18/18	0.96	0.20	2.65	36,50,66,66	0
3	DP6	H	402	18/18	0.96	0.21	2.09	42,54,71,71	0
2	AGS	B	401	31/31	0.92	0.20	1.86	37,44,57,77	0
3	DP6	E	402	18/18	0.96	0.19	1.31	31,40,56,63	0
2	AGS	G	401	31/31	0.93	0.20	1.23	34,41,57,83	0
2	AGS	A	401	31/31	0.89	0.20	1.12	41,51,70,79	0
2	AGS	E	401	31/31	0.93	0.18	1.00	34,46,66,68	0
4	FMT	D	403	3/3	0.94	0.17	0.93	54,54,62,65	0
2	AGS	H	401	31/31	0.93	0.18	0.79	45,60,72,80	0
2	AGS	F	401	31/31	0.93	0.18	0.69	35,53,68,82	0
2	AGS	C	401	31/31	0.92	0.16	0.64	37,52,60,80	0
3	DP6	F	402	18/18	0.96	0.18	0.57	39,51,66,76	0
2	AGS	D	401	31/31	0.94	0.16	0.10	36,44,53,68	0
3	DP6	A	402	18/18	0.97	0.13	-0.88	38,47,57,57	0
4	FMT	A	403	3/3	0.84	0.21	-	68,68,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.