Full wwPDB X-ray Structure Validation Report (i)

Jun 20, 2016 – 04:57 AM EDT

PDB ID	:	5EJ4
Title	:	EcMenD-ThDP-Mn2+ complex soaked with 2-ketoglutarate for 15 min
Authors	:	Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.
Deposited on	:	2015-11-01
Resolution	:	1.77 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

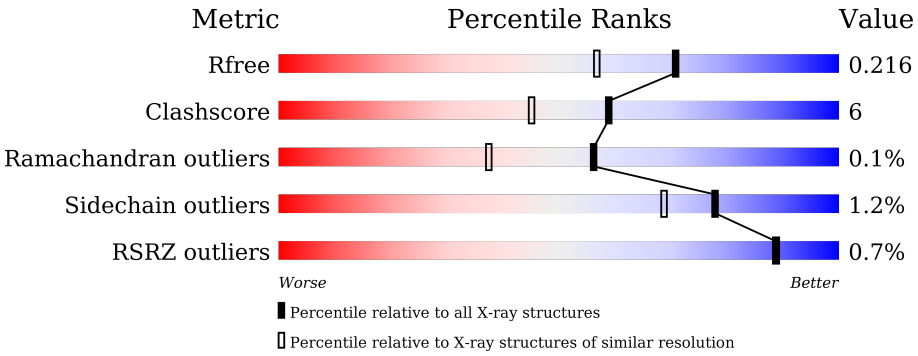
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.77 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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 <=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	556	89% 10%
1	B	556	90% 9%
1	C	556	90% 9%
1	D	556	89% 11%
1	E	556	91% 9%
1	F	556	89% 11%

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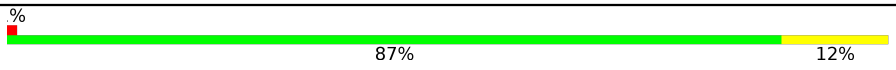
Mol	Chain	Length	Quality of chain
1	G	556	
1	H	556	

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
4	GOL	A	604	-	-	-	X
4	GOL	B	605	-	-	-	X
4	GOL	C	604	-	-	-	X
4	GOL	D	605	-	-	-	X
4	GOL	E	604	-	-	-	X
4	GOL	F	605	-	-	-	X
4	GOL	G	604	-	-	X	X
4	GOL	H	604	-	-	-	X
4	GOL	H	605	-	-	-	X
5	FMT	D	601	-	-	X	-
5	FMT	F	601	-	-	X	X
5	FMT	G	605	-	-	-	X
5	FMT	H	601	-	-	-	X

2 Entry composition

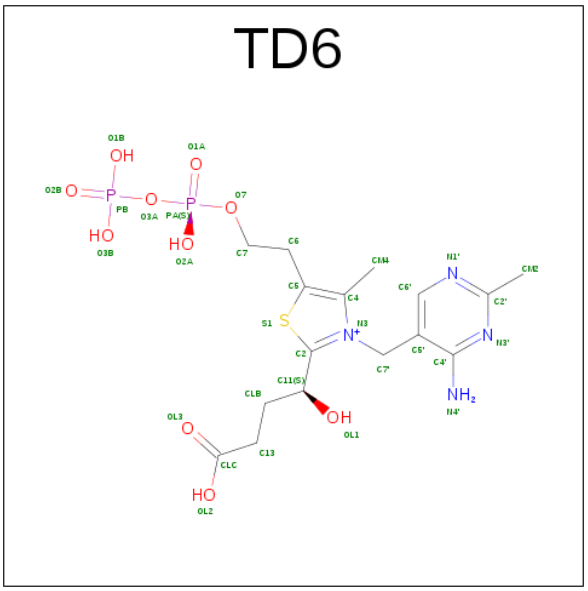
There are 6 unique types of molecules in this entry. The entry contains 39804 atoms, of which 304 are hydrogens and 0 are deuteriums.

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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxyl ate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	11	0
			4402	2793	794	799	16			
1	B	556	Total	C	N	O	S	0	3	0
			4337	2753	778	791	15			
1	C	556	Total	C	N	O	S	0	2	0
			4321	2742	776	788	15			
1	D	556	Total	C	N	O	S	0	2	0
			4321	2740	778	787	16			
1	E	556	Total	C	N	O	S	0	6	0
			4357	2764	786	791	16			
1	F	556	Total	C	N	O	S	0	4	0
			4329	2743	777	793	16			
1	G	556	Total	C	N	O	S	0	4	0
			4355	2760	784	796	15			
1	H	556	Total	C	N	O	S	0	3	0
			4329	2747	775	793	14			

- Molecule 2 is (4S)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3lambda 5 -thiazol-2-yl}-4-hydroxybutanoic acid (three-letter code: TD6) (formula: $C_{16}H_{25}N_4O_{10}P_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		

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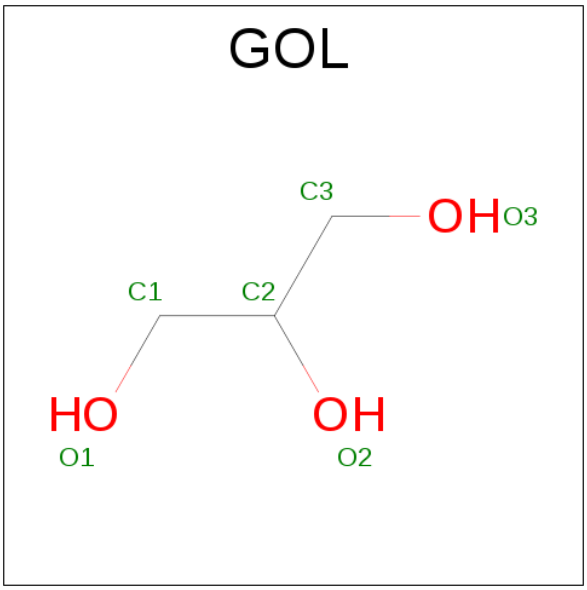
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0
4	C	1	Total C H O 14 3 8 3	0	0
4	D	1	Total C H O 14 3 8 3	0	0

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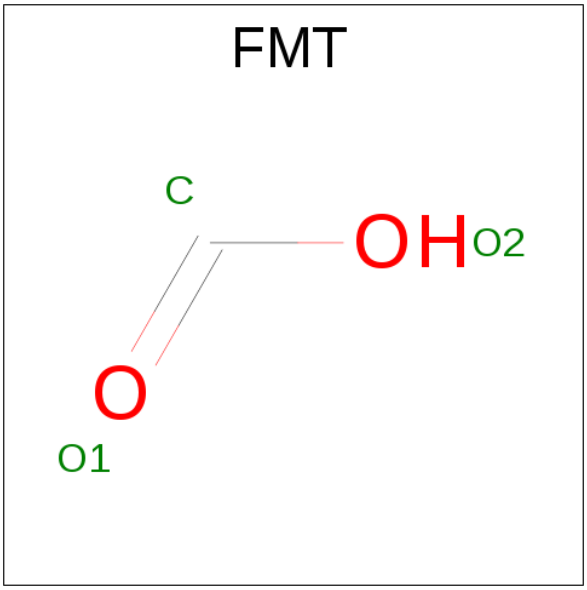
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			5	1	2	2		
5	B	1	Total	C	H	O	0	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			5	1	2	2		
5	D	1	Total	C	H	O	0	0
			5	1	2	2		
5	E	1	Total	C	H	O	0	0
			5	1	2	2		
5	F	1	Total	C	H	O	0	0
			5	1	2	2		
5	G	1	Total	C	H	O	0	0
			5	1	2	2		
5	H	1	Total	C	H	O	0	0
			5	1	2	2		

- Molecule 6 is water.

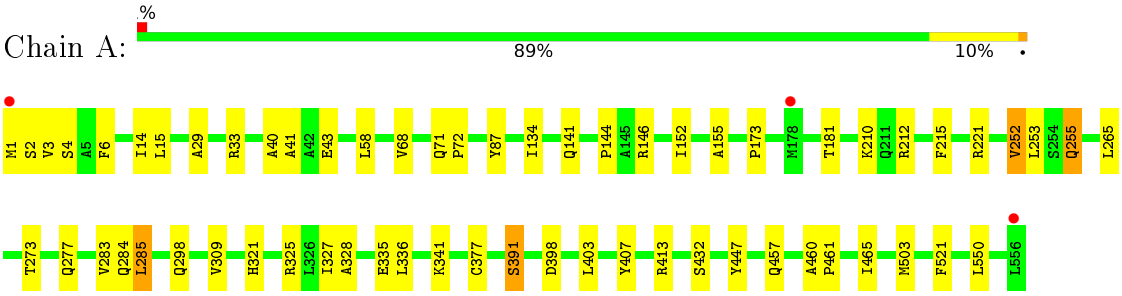
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	574	Total	O	0	0
			574	574		
6	B	556	Total	O	0	0
			556	556		
6	C	578	Total	O	0	0
			578	578		
6	D	501	Total	O	0	0
			501	501		
6	E	481	Total	O	0	0
			481	481		
6	F	535	Total	O	0	0
			535	535		
6	G	585	Total	O	0	0
			585	585		
6	H	547	Total	O	0	0
			547	547		

3 Residue-property plots (i)

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.

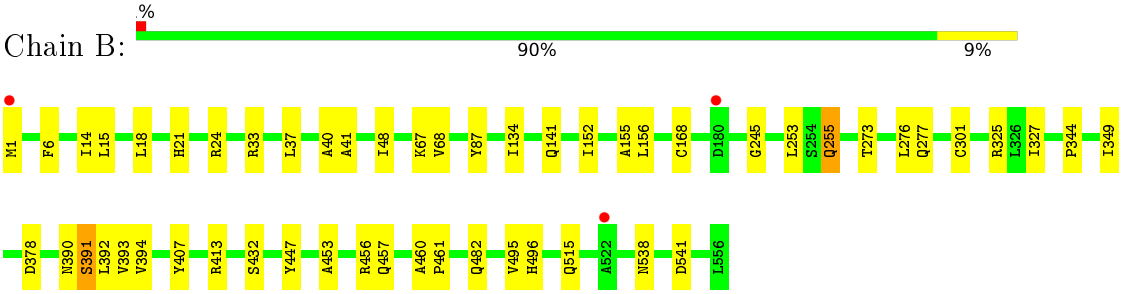
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain A:



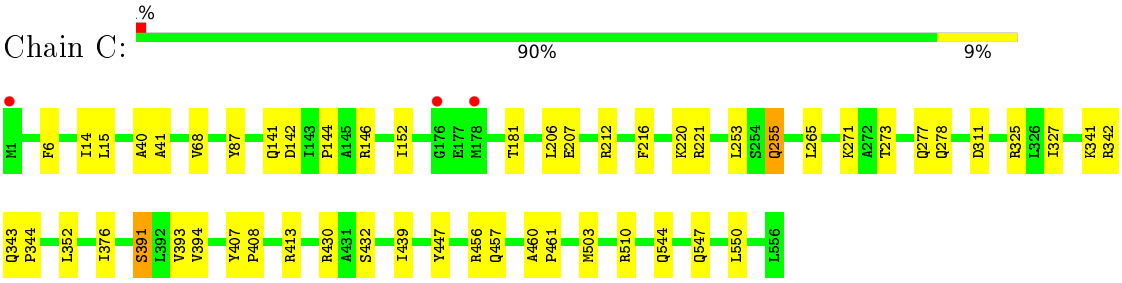
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain B:



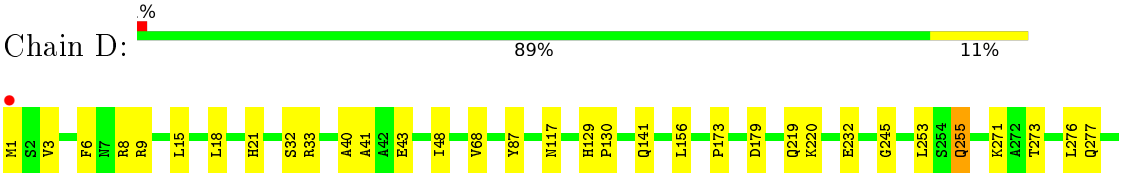
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain C:



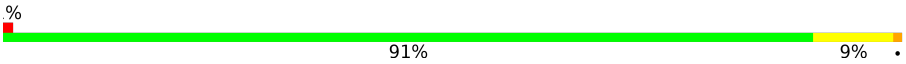
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

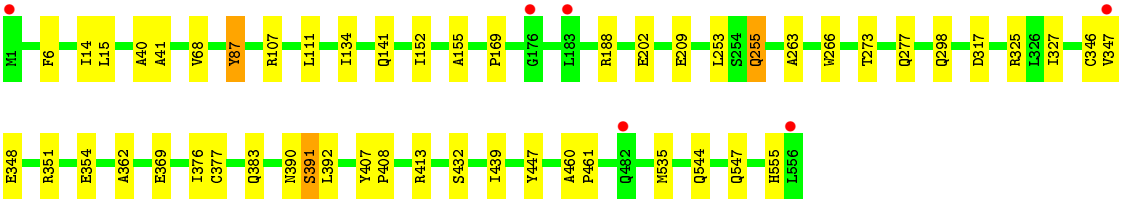
Chain D:



• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

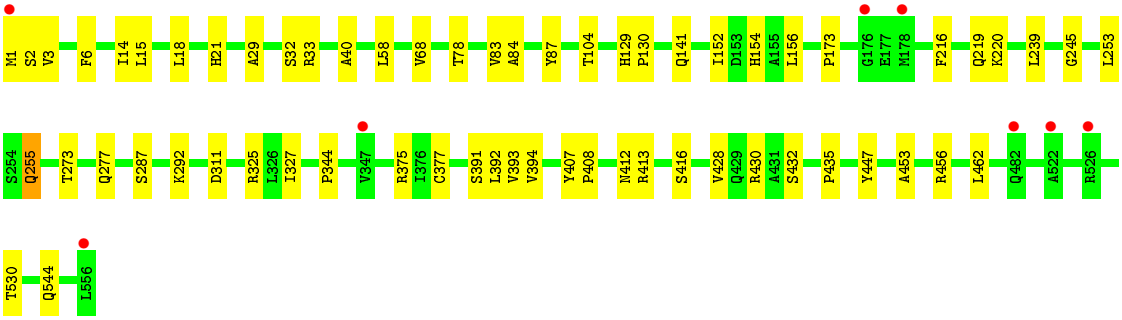
Chain E:





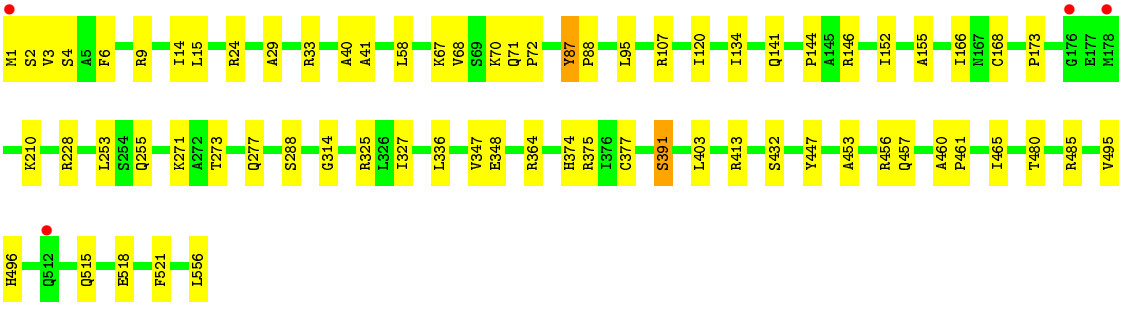
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain F:



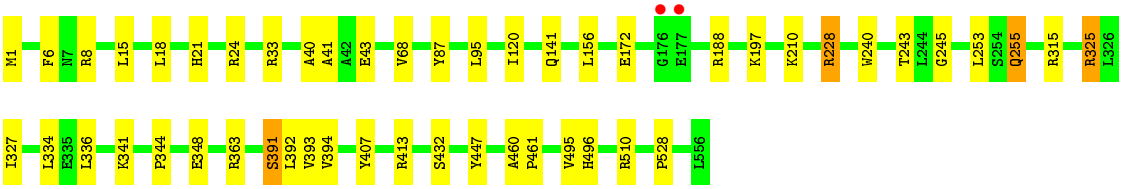
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain G:



• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.79Å 90.77Å 169.56Å 83.27° 76.01° 64.30°	Depositor
Resolution (Å)	41.82 – 1.77 45.26 – 1.77	Depositor EDS
% Data completeness (in resolution range)	96.6 (41.82-1.77) 92.6 (45.26-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 1.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.176 , 0.217 0.176 , 0.216	Depositor DCC
R_{free} test set	20988 reflections (4.92%)	DCC
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.050 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	39804	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, MN, TD6

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	0/4511	0.53	0/6153
1	B	0.35	0/4443	0.53	0/6062
1	C	0.36	0/4429	0.53	0/6044
1	D	0.34	0/4427	0.52	0/6041
1	E	0.34	0/4463	0.51	0/6088
1	F	0.36	0/4437	0.53	0/6058
1	G	0.36	0/4463	0.54	0/6088
1	H	0.36	0/4437	0.52	1/6056 (0.0%)
All	All	0.35	0/35610	0.52	1/48590 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	228	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	4402	0	4358	60	0
1	B	4337	0	4291	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4321	0	4265	41	0
1	D	4321	0	4263	58	0
1	E	4357	0	4314	50	0
1	F	4329	0	4255	50	0
1	G	4355	0	4309	51	0
1	H	4329	0	4266	44	0
2	A	33	20	21	2	0
2	B	33	20	21	3	0
2	C	33	20	21	2	0
2	D	33	20	21	4	0
2	E	33	20	21	3	0
2	F	33	20	21	3	0
2	G	33	20	21	2	0
2	H	33	20	21	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	16	16	0	0
4	B	12	16	16	1	0
4	C	12	16	16	1	0
4	D	12	16	16	0	0
4	E	12	16	16	0	0
4	F	12	16	16	2	0
4	G	12	16	16	4	0
4	H	12	16	16	0	0
5	A	3	2	1	1	0
5	B	3	2	1	1	0
5	C	3	2	1	0	0
5	D	3	2	1	5	0
5	E	3	2	1	0	0
5	F	3	2	1	4	0
5	G	3	2	1	1	0
5	H	3	2	1	1	0
6	A	574	0	0	13	4
6	B	556	0	0	8	1
6	C	578	0	0	16	0
6	D	501	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	481	0	0	14	0
6	F	535	0	0	13	4
6	G	585	0	0	10	1
6	H	547	0	0	13	2
All	All	39500	304	34625	402	6

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 6.

All (402) 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:252[A]:VAL:HG23	1:A:398:ASP:HA	1.41	1.02
1:A:285[A]:LEU:HD12	1:A:309:VAL:HB	1.49	0.90
1:C:503:MET:SD	6:D:1151:HOH:O	2.30	0.90
1:F:453:ALA:HA	1:F:456:ARG:HD2	1.53	0.88
1:A:146[B]:ARG:HH21	1:A:146[B]:ARG:HG2	1.38	0.88
1:B:515:GLN:NE2	1:B:515:GLN:CG	2.41	0.83
1:G:15:LEU:HD12	1:G:40:ALA:HB3	1.61	0.82
1:E:377[B]:CYS:SG	6:E:1131:HOH:O	2.38	0.82
1:E:535:MET:SD	6:E:1057:HOH:O	2.38	0.81
1:A:15[A]:LEU:HD12	1:A:40:ALA:HB3	1.61	0.81
1:D:515:GLN:NE2	1:D:515:GLN:CG	2.43	0.80
1:B:168:CYS:SG	6:B:1246:HOH:O	2.39	0.79
1:E:351[B]:ARG:HA	1:E:351[B]:ARG:NE	1.98	0.77
1:A:146[A]:ARG:NH2	6:A:703:HOH:O	2.18	0.77
1:B:33:ARG:H	5:B:601:FMT:H	1.50	0.77
1:D:15:LEU:HD12	1:D:40:ALA:HB3	1.66	0.77
1:G:166:ILE:HG22	6:G:707:HOH:O	1.83	0.77
1:D:219:GLN:OE1	1:D:342:ARG:NH1	2.19	0.75
1:D:9:ARG:NH1	6:D:703:HOH:O	2.19	0.75
1:C:15:LEU:HD12	1:C:40:ALA:HB3	1.68	0.74
1:G:33:ARG:H	5:G:605:FMT:H	1.52	0.74
1:E:351[B]:ARG:NH1	1:E:354:GLU:OE1	2.21	0.74
1:B:37:LEU:HD21	6:B:1246:HOH:O	1.88	0.74
1:A:212:ARG:O	6:A:701:HOH:O	2.05	0.73
1:E:209:GLU:OE1	1:E:209:GLU:CG	2.37	0.72
1:E:209:GLU:CG	1:E:209:GLU:OE2	2.37	0.72
1:E:317:ASP:OD1	6:E:701:HOH:O	2.06	0.72
2:D:602:TD6:HN4A	2:D:602:TD6:H11	1.53	0.72
1:A:1:MET:HG3	1:A:2:SER:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:ARG:NH1	6:G:705:HOH:O	2.23	0.72
1:F:1:MET:SD	6:F:1226:HOH:O	2.49	0.71
1:B:515:GLN:OE1	1:B:515:GLN:NE2	2.24	0.71
1:A:146[B]:ARG:NH2	6:A:703:HOH:O	2.24	0.71
1:A:1:MET:HG3	1:A:2:SER:N	2.05	0.71
1:B:515:GLN:OE1	1:B:515:GLN:CG	2.39	0.70
1:D:515:GLN:OE1	1:D:515:GLN:CG	2.39	0.70
1:E:15[B]:LEU:HD12	1:E:40:ALA:HB3	1.71	0.70
1:D:515:GLN:OE1	1:D:515:GLN:NE2	2.24	0.70
1:D:449:LEU:HD21	6:D:1151:HOH:O	1.92	0.70
1:C:547:GLN:NE2	6:C:704:HOH:O	2.21	0.70
2:A:601:TD6:H11	2:A:601:TD6:HN4A	1.56	0.69
2:C:601:TD6:H11	2:C:601:TD6:HN4A	1.57	0.69
2:G:601:TD6:HN4A	2:G:601:TD6:H11	1.57	0.69
2:F:602:TD6:HN4A	2:F:602:TD6:H11	1.58	0.69
1:G:15:LEU:HD12	1:G:40:ALA:CB	2.22	0.69
1:F:1:MET:HG3	1:F:2:SER:N	2.08	0.69
1:E:369:GLU:OE1	6:E:702:HOH:O	2.11	0.68
1:F:33:ARG:H	5:F:601:FMT:H	1.59	0.68
1:F:15:LEU:HD12	1:F:40:ALA:HB3	1.76	0.67
1:A:252[A]:VAL:CG2	1:A:398:ASP:HA	2.21	0.67
1:D:33:ARG:H	5:D:601:FMT:H	1.58	0.67
1:G:210:LYS:HG2	1:G:336:LEU:HD13	1.77	0.67
2:B:602:TD6:HN4A	2:B:602:TD6:H11	1.59	0.66
1:C:544:GLN:HG2	6:C:704:HOH:O	1.95	0.66
1:H:315:ARG:NH2	6:H:705:HOH:O	2.28	0.66
2:E:601:TD6:H11	2:E:601:TD6:HN4A	1.61	0.66
1:B:453:ALA:HA	1:B:456:ARG:HD2	1.78	0.66
1:H:43:GLU:HG3	6:H:953:HOH:O	1.95	0.66
1:H:15[A]:LEU:HD12	1:H:40:ALA:HB3	1.77	0.65
1:D:15:LEU:HD12	1:D:40:ALA:CB	2.26	0.65
2:H:602:TD6:H11	2:H:602:TD6:HN4A	1.60	0.65
1:H:528:PRO:O	6:H:701:HOH:O	2.14	0.65
1:A:15[A]:LEU:HD12	1:A:40:ALA:CB	2.27	0.65
1:D:311:ASP:OD2	6:D:701:HOH:O	2.15	0.64
1:C:311:ASP:OD2	6:C:701:HOH:O	2.15	0.64
1:B:15:LEU:HD12	1:B:40:ALA:HB3	1.80	0.63
1:C:273:THR:O	1:C:277:GLN:HG3	1.98	0.63
1:C:15:LEU:HD12	1:C:40:ALA:CB	2.28	0.63
1:D:383:GLN:NE2	1:E:544:GLN:OE1	2.25	0.63
1:G:347:VAL:HG23	1:G:348:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:NH1	6:B:708:HOH:O	2.32	0.62
1:C:253:LEU:HD11	1:C:413:ARG:HG3	1.81	0.62
1:D:18:LEU:HD22	1:D:156:LEU:HD21	1.82	0.62
1:D:32:SER:H	5:D:601:FMT:C	2.12	0.62
1:F:1:MET:HG3	1:F:2:SER:H	1.65	0.62
1:H:6:PHE:CE1	1:H:141:GLN:HG2	2.34	0.61
1:F:311:ASP:HB3	6:F:1082:HOH:O	2.00	0.61
1:A:43:GLU:HG3	6:A:776:HOH:O	2.00	0.61
1:C:278:GLN:HG2	6:C:1204:HOH:O	2.00	0.61
1:G:6:PHE:CE1	1:G:141:GLN:HG2	2.36	0.61
1:B:253:LEU:HD11	1:B:413:ARG:HG3	1.83	0.61
1:B:495[B]:VAL:HG12	1:B:496:HIS:O	2.01	0.61
1:D:32:SER:H	5:D:601:FMT:H	1.66	0.60
1:D:347:VAL:O	6:D:702:HOH:O	2.16	0.60
1:E:209:GLU:OE1	1:E:209:GLU:OE2	2.20	0.60
1:H:188:ARG:NH1	6:H:710:HOH:O	2.33	0.60
1:A:181:THR:O	6:A:702:HOH:O	2.17	0.60
1:A:252[A]:VAL:HG23	1:A:398:ASP:CA	2.26	0.60
1:D:117:ASN:ND2	6:D:709:HOH:O	2.32	0.60
1:H:243:THR:HG23	1:H:341:LYS:HG2	1.83	0.60
1:C:181:THR:O	6:C:702:HOH:O	2.16	0.60
1:G:375:ARG:HA	4:G:604:GOL:H11	1.81	0.60
1:F:253:LEU:HD11	1:F:413:ARG:HG3	1.84	0.59
1:G:3:VAL:HB	1:G:173:PRO:HD2	1.84	0.59
1:D:21:HIS:HB2	1:D:156:LEU:HD23	1.84	0.59
1:F:32:SER:H	5:F:601:FMT:C	2.16	0.59
1:A:457:GLN:HG3	6:A:939:HOH:O	2.02	0.59
1:G:253:LEU:HD11	1:G:413:ARG:HG3	1.83	0.59
1:H:1:MET:N	6:H:711:HOH:O	2.35	0.59
1:A:253:LEU:HD11	1:A:413:ARG:HG3	1.84	0.58
1:F:435:PRO:HG3	6:F:1185:HOH:O	2.03	0.58
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.37	0.58
1:C:14:ILE:HG12	1:C:152:ILE:HD11	1.85	0.58
1:G:24:ARG:NH1	6:G:710:HOH:O	2.29	0.58
1:C:206:LEU:O	6:C:703:HOH:O	2.17	0.58
1:C:457:GLN:HG3	6:C:926:HOH:O	2.03	0.58
1:B:273:THR:O	1:B:277:GLN:HG3	2.03	0.58
1:E:253:LEU:HD11	1:E:413:ARG:HG3	1.86	0.57
1:A:146[B]:ARG:HG2	6:A:824:HOH:O	2.03	0.57
1:E:15[B]:LEU:HD12	1:E:40:ALA:CB	2.35	0.57
1:A:465:ILE:HD11	1:A:521:PHE:HZ	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE2	6:B:1136:HOH:O	2.05	0.57
1:F:219[B]:GLN:NE2	6:F:715:HOH:O	2.37	0.57
1:H:33:ARG:NH2	1:H:172:GLU:OE1	2.37	0.57
1:H:363:ARG:HA	6:H:1121:HOH:O	2.05	0.57
2:D:602:TD6:HN4A	2:D:602:TD6:C11	2.18	0.56
1:E:14:ILE:HG12	1:E:152:ILE:HD11	1.86	0.56
1:G:374:HIS:NE2	4:G:604:GOL:H32	2.20	0.56
1:A:14:ILE:HG12	1:A:152:ILE:HD11	1.88	0.56
2:F:602:TD6:HN4A	2:F:602:TD6:C11	2.19	0.56
1:G:14:ILE:HG12	1:G:152:ILE:HD11	1.88	0.56
1:F:311:ASP:OD2	6:F:701:HOH:O	2.18	0.56
1:D:253:LEU:HD11	1:D:413:ARG:HG3	1.87	0.56
1:E:273:THR:O	1:E:277:GLN:HG3	2.05	0.56
1:G:168:CYS:SG	6:G:707:HOH:O	2.58	0.56
1:C:327:ILE:N	1:C:327:ILE:HD12	2.21	0.56
1:D:528:PRO:HG2	1:E:555:HIS:CE1	2.41	0.56
1:D:219:GLN:NE2	1:D:340:GLU:OE1	2.39	0.55
1:H:24:ARG:NH2	6:H:714:HOH:O	2.39	0.55
1:B:482:GLN:HG3	6:B:1086:HOH:O	2.05	0.55
1:G:465:ILE:HD11	1:G:521:PHE:HZ	1.71	0.55
1:A:210:LYS:HD3	1:A:336:LEU:HD22	1.89	0.55
1:E:351[B]:ARG:HH21	1:E:351[B]:ARG:HG2	1.72	0.55
1:C:277:GLN:HG2	6:C:1181:HOH:O	2.06	0.55
1:F:68:VAL:HG11	1:F:432:SER:HB3	1.87	0.55
1:G:518:GLU:OE1	6:G:701:HOH:O	2.18	0.55
2:G:601:TD6:HN4A	2:G:601:TD6:C11	2.18	0.55
1:H:253:LEU:HD11	1:H:413:ARG:HG3	1.89	0.55
2:C:601:TD6:HN4A	2:C:601:TD6:C11	2.20	0.55
1:A:212:ARG:NH1	6:A:719:HOH:O	2.38	0.55
1:D:507:LYS:HD3	6:D:769:HOH:O	2.07	0.55
1:G:453:ALA:HA	1:G:456:ARG:HD2	1.87	0.55
1:H:68:VAL:HG11	1:H:432:SER:HB3	1.88	0.55
2:B:602:TD6:HN4A	2:B:602:TD6:C11	2.20	0.54
1:A:15[B]:LEU:HD23	1:A:41:ALA:HA	1.88	0.54
1:F:375:ARG:HD3	6:F:882:HOH:O	2.07	0.54
1:D:271:LYS:NZ	1:D:556:LEU:OXT	2.35	0.54
1:H:21:HIS:HB2	1:H:156:LEU:HD23	1.89	0.54
1:E:134:ILE:HD11	1:E:155:ALA:HB2	1.88	0.54
1:G:15:LEU:HD13	1:G:41:ALA:N	2.23	0.54
1:E:460:ALA:HB1	1:E:461:PRO:HD2	1.90	0.53
1:F:216:PHE:CZ	1:F:220:LYS:HE3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:CZ	1:B:48:ILE:HD11	2.39	0.53
1:F:311:ASP:HB3	6:F:1130:HOH:O	2.07	0.53
1:B:18:LEU:HD22	1:B:156:LEU:HD21	1.91	0.53
1:F:377[B]:CYS:SG	4:F:605:GOL:O1	2.55	0.53
1:B:495[B]:VAL:HG12	1:B:496:HIS:N	2.23	0.53
1:F:216:PHE:O	1:F:219[A]:GLN:HG2	2.08	0.53
2:A:601:TD6:C11	2:A:601:TD6:HN4A	2.21	0.53
1:C:216:PHE:CZ	1:C:220:LYS:HE3	2.44	0.53
2:H:602:TD6:C11	2:H:602:TD6:HN4A	2.21	0.53
1:A:68:VAL:HG11	1:A:432:SER:HB3	1.90	0.52
1:H:18:LEU:HD22	1:H:156:LEU:HD21	1.90	0.52
1:B:378:ASP:OD2	4:B:605:GOL:O2	2.27	0.52
1:A:134:ILE:HD11	1:A:155:ALA:HB2	1.91	0.52
1:E:298:GLN:HG2	6:E:701:HOH:O	2.10	0.52
1:E:68:VAL:HG11	1:E:432:SER:HB3	1.90	0.52
1:A:146[B]:ARG:HH21	1:A:146[B]:ARG:CG	2.16	0.52
1:A:215:PHE:HD2	6:A:701:HOH:O	1.92	0.52
1:H:15[B]:LEU:CD2	1:H:41:ALA:HB2	2.40	0.52
1:H:255:GLN:HG2	1:H:407:TYR:O	2.10	0.52
1:G:24:ARG:HD3	6:G:710:HOH:O	2.08	0.51
1:D:15:LEU:HD13	1:D:41:ALA:N	2.25	0.51
1:D:495:VAL:HG12	1:D:496:HIS:N	2.26	0.51
1:F:15:LEU:HD12	1:F:40:ALA:CB	2.39	0.51
1:A:15[A]:LEU:HD13	1:A:41:ALA:N	2.25	0.51
1:F:14:ILE:HG12	1:F:152:ILE:HD11	1.93	0.51
1:G:377:CYS:SG	1:G:403:LEU:HD23	2.50	0.51
1:H:15[A]:LEU:HD12	1:H:40:ALA:CB	2.39	0.51
1:D:347:VAL:HG23	1:D:348:GLU:HG2	1.93	0.51
1:D:48:ILE:HD11	1:E:362:ALA:HB1	1.91	0.51
1:D:18:LEU:CD2	1:D:156:LEU:HD21	2.41	0.51
2:E:601:TD6:C11	2:E:601:TD6:HN4A	2.22	0.51
1:A:284:GLN:C	1:A:285[A]:LEU:HD13	2.31	0.51
1:C:207:GLU:HG2	6:C:956:HOH:O	2.11	0.51
1:B:15:LEU:HD12	1:B:40:ALA:CB	2.41	0.51
1:G:327:ILE:N	1:G:327:ILE:HD12	2.26	0.51
1:F:6:PHE:CE1	1:F:141:GLN:HG2	2.45	0.51
1:G:68:VAL:HG11	1:G:432:SER:HB3	1.93	0.51
1:A:273:THR:O	1:A:277:GLN:HG3	2.11	0.50
1:D:495:VAL:HG12	1:D:496:HIS:O	2.10	0.50
1:B:301:CYS:HB2	6:B:1101:HOH:O	2.10	0.50
1:A:14:ILE:HA	1:A:152:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HB	1:A:173:PRO:HD2	1.94	0.50
1:B:14:ILE:HG12	1:B:152[A]:ILE:HD11	1.93	0.50
1:A:210:LYS:HG2	1:A:336:LEU:HD13	1.93	0.50
1:F:21:HIS:HB2	1:F:156:LEU:HD23	1.94	0.50
1:C:6:PHE:CE1	1:C:141:GLN:HG2	2.47	0.50
1:E:351[B]:ARG:NH2	1:E:351[B]:ARG:HG2	2.26	0.50
1:C:255:GLN:HG2	1:C:407:TYR:O	2.11	0.49
1:D:8:ARG:NH2	1:D:43:GLU:OE2	2.44	0.49
1:D:33:ARG:H	5:D:601:FMT:C	2.25	0.49
1:G:375:ARG:HG2	4:G:604:GOL:H31	1.94	0.49
1:A:283:VAL:HG12	1:A:285[B]:LEU:CD2	2.43	0.49
1:D:3:VAL:HB	1:D:173:PRO:HD2	1.94	0.49
1:E:263:ALA:HA	1:E:266:TRP:NE1	2.28	0.49
1:E:376:ILE:HD11	1:E:439:ILE:HD11	1.93	0.49
1:G:9:ARG:NE	6:G:702:HOH:O	2.22	0.49
1:A:6:PHE:CE1	1:A:141:GLN:HG2	2.48	0.49
1:E:347:VAL:HG23	1:E:348:GLU:HG2	1.94	0.49
1:A:15[A]:LEU:CD1	1:A:40:ALA:HB3	2.37	0.49
1:C:456:ARG:NH2	6:C:706:HOH:O	2.24	0.49
1:B:21:HIS:HB2	1:B:156:LEU:HD23	1.93	0.49
1:E:547:GLN:NE2	6:E:715:HOH:O	2.37	0.49
1:F:292:LYS:NZ	6:F:707:HOH:O	2.28	0.49
1:G:457:GLN:HG2	6:G:1101:HOH:O	2.12	0.49
1:A:265:LEU:HD23	1:A:550:LEU:HD23	1.94	0.49
1:G:210:LYS:HD3	1:G:336:LEU:HD22	1.93	0.49
1:H:510:ARG:NH2	6:H:726:HOH:O	2.46	0.49
1:A:15[B]:LEU:HD23	1:A:41:ALA:CA	2.43	0.48
1:A:460:ALA:HB1	1:A:461:PRO:HD2	1.94	0.48
1:F:327:ILE:N	1:F:327:ILE:HD12	2.27	0.48
1:H:327:ILE:HD12	1:H:327:ILE:N	2.29	0.48
1:A:327:ILE:HD12	1:A:327:ILE:N	2.28	0.48
1:B:393:VAL:HG13	1:B:394:VAL:N	2.28	0.48
1:C:460:ALA:HB1	1:C:461:PRO:HD2	1.96	0.48
1:E:169:PRO:HD2	6:E:987:HOH:O	2.14	0.48
1:G:134:ILE:HD11	1:G:155:ALA:HB2	1.96	0.48
1:H:15[A]:LEU:HD13	1:H:41:ALA:N	2.28	0.48
1:F:216:PHE:CE1	1:F:220:LYS:HE3	2.49	0.48
1:H:15[B]:LEU:HD23	1:H:41:ALA:HA	1.96	0.48
1:C:503:MET:CE	1:D:495:VAL:HG11	2.43	0.48
1:D:220:LYS:HE3	1:D:280:GLN:NE2	2.29	0.47
1:H:228:ARG:HD2	6:H:1176:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:LEU:CD1	1:G:40:ALA:HB3	2.37	0.47
1:B:24:ARG:NE	1:B:48:ILE:HD11	2.29	0.47
1:D:255:GLN:HG2	1:D:407:TYR:O	2.14	0.47
1:D:528:PRO:HG2	1:E:555:HIS:NE2	2.28	0.47
1:D:68:VAL:HG11	1:D:432:SER:HB3	1.95	0.47
1:E:255:GLN:HG2	1:E:407:TYR:O	2.14	0.47
1:B:392:LEU:HB2	2:B:602:TD6:O2B	2.15	0.47
1:H:495:VAL:HG22	1:H:496:HIS:N	2.29	0.47
1:A:33:ARG:H	5:A:605:FMT:C	2.28	0.47
1:B:495[A]:VAL:HG22	1:B:496:HIS:O	2.14	0.47
1:D:273:THR:O	1:D:277:GLN:HG3	2.15	0.47
1:D:327:ILE:N	1:D:327:ILE:HD12	2.30	0.46
1:D:6:PHE:CE1	1:D:141:GLN:HG2	2.51	0.46
1:F:255:GLN:HG2	1:F:407:TYR:O	2.14	0.46
1:G:271:LYS:NZ	1:G:556:LEU:O	2.47	0.46
1:B:457:GLN:HG3	6:B:1030:HOH:O	2.14	0.46
1:F:245:GLY:O	1:F:344:PRO:HA	2.16	0.46
1:G:210:LYS:CG	1:G:336:LEU:HD13	2.43	0.46
1:H:460:ALA:HB1	1:H:461:PRO:HD2	1.97	0.46
1:H:495:VAL:HG22	1:H:496:HIS:O	2.16	0.46
1:B:495[A]:VAL:HG22	1:B:496:HIS:N	2.30	0.46
1:F:393:VAL:HG13	1:F:394:VAL:N	2.30	0.46
1:F:544:GLN:NE2	6:F:726:HOH:O	2.48	0.46
1:C:144:PRO:HB2	1:C:146:ARG:HG2	1.97	0.46
1:E:327:ILE:HD12	1:E:327:ILE:N	2.31	0.46
1:A:377[A]:CYS:SG	1:A:403:LEU:HD23	2.56	0.46
1:H:15[A]:LEU:HD13	1:H:41:ALA:CA	2.46	0.46
1:F:430:ARG:NH2	4:F:604:GOL:O1	2.45	0.46
1:G:67:LYS:O	1:G:70:LYS:NZ	2.49	0.46
1:A:335:GLU:OE1	6:A:704:HOH:O	2.21	0.45
1:C:15:LEU:HD13	1:C:41:ALA:N	2.31	0.45
1:A:255:GLN:HG2	1:A:407:TYR:O	2.16	0.45
1:D:245:GLY:O	1:D:344:PRO:HA	2.17	0.45
1:D:515:GLN:NE2	1:D:518:GLU:OE1	2.50	0.45
1:E:40:ALA:HB2	6:E:823:HOH:O	2.15	0.45
1:F:273:THR:O	1:F:277:GLN:HG3	2.16	0.45
1:B:327:ILE:N	1:B:327:ILE:HD12	2.31	0.45
1:D:377[B]:CYS:SG	6:D:996:HOH:O	2.60	0.45
1:D:518:GLU:HG3	6:D:920:HOH:O	2.15	0.45
1:E:188:ARG:HD3	6:E:1119:HOH:O	2.15	0.45
1:H:15[B]:LEU:HD21	1:H:41:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:VAL:HG11	1:C:432:SER:HB3	1.99	0.45
1:A:40:ALA:HB2	6:A:981:HOH:O	2.14	0.45
1:C:271:LYS:HE3	1:C:352:LEU:HD21	1.98	0.45
1:C:265:LEU:HD23	1:C:550:LEU:HD23	1.98	0.45
1:D:495:VAL:CG1	1:D:496:HIS:N	2.79	0.45
1:D:21:HIS:CB	1:D:156:LEU:HD23	2.46	0.45
1:F:18:LEU:HD22	1:F:156:LEU:HD21	1.98	0.45
1:G:71[B]:GLN:HB3	1:G:72:PRO:HD2	1.98	0.45
1:C:142:ASP:HA	6:C:744:HOH:O	2.16	0.45
1:D:68:VAL:HG21	1:D:428:VAL:HG13	1.99	0.45
1:H:8:ARG:NH2	1:H:43:GLU:OE2	2.48	0.45
1:B:15:LEU:HD13	1:B:41:ALA:N	2.32	0.44
1:E:107:ARG:HG3	6:E:756:HOH:O	2.17	0.44
1:E:6:PHE:CE1	1:E:141:GLN:HG2	2.52	0.44
1:G:495:VAL:HG22	1:G:496:HIS:O	2.18	0.44
1:H:210:LYS:HE3	1:H:336:LEU:HD11	1.98	0.44
1:E:392:LEU:HB2	2:E:601:TD6:O2B	2.17	0.44
1:B:134:ILE:HD11	1:B:155:ALA:HB2	1.99	0.44
1:B:453:ALA:O	1:B:456:ARG:HD3	2.18	0.44
1:C:503:MET:HE2	1:D:495:VAL:HG11	1.97	0.44
1:F:29:ALA:HB2	1:F:58:LEU:HD22	2.00	0.44
1:D:382:GLU:HG3	1:D:383:GLN:HG2	1.99	0.44
1:E:15[B]:LEU:HD13	1:E:41:ALA:CA	2.48	0.44
1:H:528:PRO:HB2	6:H:1110:HOH:O	2.18	0.44
1:E:383:GLN:NE2	6:E:728:HOH:O	2.50	0.44
1:H:33:ARG:H	5:H:601:FMT:C	2.31	0.44
1:A:15[B]:LEU:HD21	1:A:41:ALA:HB2	2.00	0.44
1:C:221:ARG:NH1	6:C:730:HOH:O	2.50	0.44
1:C:547:GLN:OE1	6:C:705:HOH:O	2.21	0.44
1:G:29:ALA:HB2	1:G:58:LEU:HD22	1.99	0.44
1:H:348:GLU:OE1	6:H:702:HOH:O	2.21	0.44
1:C:376:ILE:HD11	1:C:439:ILE:HD11	1.99	0.44
1:A:29:ALA:HB2	1:A:58:LEU:HD22	2.00	0.44
1:F:129:HIS:N	1:F:130:PRO:HD2	2.32	0.44
1:C:510:ARG:NH2	6:C:731:HOH:O	2.50	0.44
1:F:239:LEU:HD12	6:F:872:HOH:O	2.16	0.44
1:H:141:GLN:HG3	6:H:1021:HOH:O	2.17	0.44
1:H:15[B]:LEU:HD23	1:H:41:ALA:CA	2.48	0.44
1:D:129:HIS:N	1:D:130:PRO:HD2	2.33	0.43
1:F:83:VAL:HG13	1:F:104:THR:HG21	2.00	0.43
1:F:462:LEU:O	1:F:530:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLN:O	1:A:285[A]:LEU:HD13	2.19	0.43
1:D:232:GLU:HG2	6:D:982:HOH:O	2.18	0.43
1:E:390:ASN:OD1	1:E:413:ARG:HD2	2.18	0.43
1:G:495:VAL:HG22	1:G:496:HIS:N	2.33	0.43
1:B:67:LYS:NZ	6:B:728:HOH:O	2.51	0.43
1:C:343:GLN:HA	1:C:344:PRO:HD3	1.92	0.43
1:G:460:ALA:HB1	1:G:461:PRO:HD2	2.00	0.43
1:A:503:MET:CE	1:B:495[B]:VAL:HG11	2.48	0.43
1:G:228:ARG:NH2	1:G:288:SER:OG	2.51	0.43
1:C:343:GLN:H	1:C:343:GLN:CD	2.20	0.43
1:D:15:LEU:HD13	1:D:41:ALA:CA	2.49	0.43
1:F:407:TYR:HA	1:F:408:PRO:HD3	1.92	0.43
1:G:14:ILE:HA	1:G:152:ILE:HD13	2.01	0.43
1:D:460:ALA:HB1	1:D:461:PRO:HD2	2.01	0.43
1:A:4[A]:SER:OG	1:A:173:PRO:HB2	2.19	0.43
1:A:14:ILE:HA	1:A:152:ILE:CD1	2.48	0.43
1:D:500:ALA:HB2	6:D:1151:HOH:O	2.19	0.43
1:F:1:MET:N	6:F:720:HOH:O	2.44	0.43
1:G:515:GLN:NE2	6:G:704:HOH:O	2.23	0.43
1:B:460:ALA:HB1	1:B:461:PRO:HD2	2.01	0.42
1:A:144:PRO:HB2	1:A:146[A]:ARG:HG2	2.00	0.42
1:B:255:GLN:HG2	1:B:407:TYR:O	2.19	0.42
1:F:154:HIS:CE1	1:G:314:GLY:HA2	2.55	0.42
1:E:351[A]:ARG:HD2	1:E:351[A]:ARG:O	2.19	0.42
1:F:68:VAL:CG2	1:F:428:VAL:HG13	2.50	0.42
1:B:276:LEU:HG	1:B:349:ILE:HD11	2.01	0.42
1:D:1:MET:HE3	1:D:179:ASP:OD2	2.19	0.42
2:D:602:TD6:H6	2:D:602:TD6:HM4	1.93	0.42
1:G:95:LEU:HD11	1:H:120:ILE:HG22	2.01	0.42
1:A:298:GLN:O	1:A:321:HIS:HE1	2.02	0.42
1:D:392:LEU:HB2	2:D:602:TD6:O2B	2.19	0.42
1:E:346:CYS:HB2	6:E:895:HOH:O	2.19	0.42
1:E:87:TYR:HB3	1:F:84:ALA:HB1	2.01	0.42
1:F:456:ARG:NH2	6:F:730:HOH:O	2.49	0.42
1:G:273:THR:O	1:G:277:GLN:HG3	2.19	0.42
1:A:146[B]:ARG:NH2	1:A:146[B]:ARG:HG2	2.17	0.42
1:A:71[B]:GLN:HB3	1:A:72:PRO:HD2	2.02	0.42
1:B:15:LEU:HD13	1:B:41:ALA:CA	2.50	0.42
1:C:393:VAL:HG13	1:C:394:VAL:N	2.35	0.42
1:D:32:SER:N	5:D:601:FMT:H	2.34	0.42
1:E:351[B]:ARG:CZ	1:E:351[B]:ARG:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ALA:HA	1:E:266:TRP:CD1	2.55	0.42
1:B:538:ASN:HB2	1:B:541:ASP:OD2	2.19	0.41
1:F:3:VAL:HB	1:F:173:PRO:HD2	2.02	0.41
1:F:412:ASN:O	1:F:416:SER:HA	2.20	0.41
1:G:144:PRO:HB2	1:G:146:ARG:HG2	2.01	0.41
1:G:480:THR:O	1:G:485:ARG:NH2	2.49	0.41
1:B:68:VAL:HG11	1:B:432:SER:HB3	2.01	0.41
1:C:407:TYR:HA	1:C:408:PRO:HD3	1.96	0.41
1:F:392:LEU:HB2	2:F:602:TD6:O2B	2.21	0.41
1:H:393:VAL:HG13	1:H:394:VAL:N	2.36	0.41
1:A:252[A]:VAL:CG2	1:A:398:ASP:CA	2.90	0.41
1:B:245:GLY:O	1:B:344:PRO:HA	2.21	0.41
1:D:276:LEU:HD23	1:D:276:LEU:HA	1.94	0.41
1:G:1:MET:HG3	1:G:2:SER:N	2.35	0.41
1:H:18:LEU:CD2	1:H:156:LEU:HD21	2.50	0.41
1:H:197:LYS:HD3	6:H:742:HOH:O	2.20	0.41
1:A:377[A]:CYS:SG	1:A:403:LEU:HA	2.60	0.41
1:E:346:CYS:HB2	6:E:1089:HOH:O	2.21	0.41
1:G:364:ARG:HE	4:G:604:GOL:C3	2.34	0.41
1:B:390:ASN:OD1	1:B:413:ARG:HD2	2.21	0.41
1:A:221:ARG:HD3	6:A:1010:HOH:O	2.21	0.41
1:C:212:ARG:NH2	6:C:736:HOH:O	2.53	0.41
1:H:245:GLY:O	1:H:344:PRO:HA	2.20	0.41
1:A:328:ALA:HB2	6:A:902:HOH:O	2.21	0.41
1:C:342:ARG:NH1	6:C:715:HOH:O	2.41	0.41
1:F:33:ARG:H	5:F:601:FMT:C	2.30	0.41
1:G:4[A]:SER:OG	1:G:173:PRO:HB2	2.20	0.41
1:C:430:ARG:NH2	4:C:603:GOL:O1	2.49	0.41
1:E:111:LEU:HD13	6:E:756:HOH:O	2.20	0.41
1:A:15[B]:LEU:CD2	1:A:41:ALA:N	2.84	0.40
1:A:285[B]:LEU:HD13	1:A:309:VAL:HB	2.03	0.40
1:E:347:VAL:HG23	1:E:348:GLU:N	2.36	0.40
1:E:15[A]:LEU:CD2	1:E:41:ALA:HB2	2.51	0.40
1:G:87:TYR:HB3	1:G:88:PRO:HD3	2.04	0.40
1:E:202:GLU:HB2	1:H:325:ARG:HB3	2.03	0.40
1:E:407:TYR:HA	1:E:408:PRO:HD3	1.93	0.40
1:F:78:THR:OG1	5:F:601:FMT:H	2.21	0.40
1:F:68:VAL:HG21	1:F:428:VAL:HG13	2.03	0.40
1:H:240:TRP:CG	1:H:334:LEU:HD22	2.56	0.40
1:C:15:LEU:CD1	1:C:40:ALA:HB3	2.45	0.40
1:G:120:ILE:HG22	1:H:95:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:ARG:HB3	6:G:716:HOH:O	2.20	0.40
1:D:276:LEU:HG	1:D:349:ILE:HD11	2.03	0.40
1:H:392:LEU:HB2	2:H:602:TD6:O2B	2.21	0.40
1:F:287:SER:HB2	6:F:946:HOH:O	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1118:HOH:O	6:F:777:HOH:O[1_456]	2.04	0.16
6:A:701:HOH:O	6:B:916:HOH:O[1_455]	2.10	0.10
6:A:811:HOH:O	6:G:1148:HOH:O[1_456]	2.14	0.06
6:F:1103:HOH:O	6:H:1194:HOH:O[1_645]	2.15	0.05
6:F:1227:HOH:O	6:H:1222:HOH:O[1_645]	2.16	0.04
6:A:951:HOH:O	6:F:952:HOH:O[1_456]	2.18	0.02

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	565/556 (102%)	554 (98%)	10 (2%)	1 (0%)	52	34
1	B	557/556 (100%)	545 (98%)	11 (2%)	1 (0%)	52	34
1	C	556/556 (100%)	546 (98%)	9 (2%)	1 (0%)	52	34
1	D	556/556 (100%)	546 (98%)	10 (2%)	0	100	100
1	E	560/556 (101%)	550 (98%)	9 (2%)	1 (0%)	52	34
1	F	558/556 (100%)	549 (98%)	9 (2%)	0	100	100
1	G	558/556 (100%)	547 (98%)	10 (2%)	1 (0%)	52	34
1	H	557/556 (100%)	547 (98%)	9 (2%)	1 (0%)	52	34
All	All	4467/4448 (100%)	4384 (98%)	77 (2%)	6 (0%)	56	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	391	SER
1	E	391	SER
1	G	391	SER
1	H	391	SER
1	A	391	SER
1	B	391	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	459/452 (102%)	449 (98%)	10 (2%)	60	42
1	B	451/452 (100%)	446 (99%)	5 (1%)	80	72
1	C	448/452 (99%)	442 (99%)	6 (1%)	76	66
1	D	447/452 (99%)	443 (99%)	4 (1%)	84	78
1	E	452/452 (100%)	447 (99%)	5 (1%)	80	72
1	F	449/452 (99%)	444 (99%)	5 (1%)	80	72
1	G	454/452 (100%)	448 (99%)	6 (1%)	76	66
1	H	449/452 (99%)	444 (99%)	5 (1%)	80	72
All	All	3609/3616 (100%)	3563 (99%)	46 (1%)	78	66

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

Mol	Chain	Res	Type
1	A	87	TYR
1	A	252[A]	VAL
1	A	252[B]	VAL
1	A	255	GLN
1	A	285[A]	LEU
1	A	285[B]	LEU
1	A	325	ARG
1	A	341	LYS

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Mol	Chain	Res	Type
1	A	391	SER
1	A	447	TYR
1	B	87	TYR
1	B	255	GLN
1	B	325	ARG
1	B	391	SER
1	B	447	TYR
1	C	87	TYR
1	C	255	GLN
1	C	325	ARG
1	C	341	LYS
1	C	391	SER
1	C	447	TYR
1	D	87	TYR
1	D	255	GLN
1	D	325	ARG
1	D	447	TYR
1	E	87	TYR
1	E	255	GLN
1	E	325	ARG
1	E	391	SER
1	E	447	TYR
1	F	87	TYR
1	F	255	GLN
1	F	325	ARG
1	F	391	SER
1	F	447	TYR
1	G	87	TYR
1	G	107	ARG
1	G	255	GLN
1	G	325	ARG
1	G	391	SER
1	G	447	TYR
1	H	87	TYR
1	H	255	GLN
1	H	325	ARG
1	H	391	SER
1	H	447	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	547	GLN
1	H	141	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
2	TD6	A	601	3	24,34,34	1.31	3 (12%)	32,50,50	1.76	8 (25%)
4	GOL	A	603	-	5,5,5	0.40	0	5,5,5	0.43	0
4	GOL	A	604	-	5,5,5	0.43	0	5,5,5	0.34	0
5	FMT	A	605	-	2,2,2	0.71	0	1,1,1	0.49	0
5	FMT	B	601	-	2,2,2	0.74	0	1,1,1	0.47	0
2	TD6	B	602	3	24,34,34	1.37	4 (16%)	32,50,50	1.95	9 (28%)
4	GOL	B	604	-	5,5,5	0.34	0	5,5,5	0.50	0
4	GOL	B	605	-	5,5,5	0.42	0	5,5,5	0.46	0
2	TD6	C	601	3	24,34,34	1.34	4 (16%)	32,50,50	1.75	6 (18%)
4	GOL	C	603	-	5,5,5	0.39	0	5,5,5	0.16	0
4	GOL	C	604	-	5,5,5	0.32	0	5,5,5	0.48	0
5	FMT	C	605	-	2,2,2	0.62	0	1,1,1	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	D	601	-	2,2,2	0.70	0	1,1,1	0.31	0
2	TD6	D	602	3	24,34,34	1.38	5 (20%)	32,50,50	1.97	7 (21%)
4	GOL	D	604	-	5,5,5	0.36	0	5,5,5	0.29	0
4	GOL	D	605	-	5,5,5	0.39	0	5,5,5	0.31	0
2	TD6	E	601	3	24,34,34	1.30	4 (16%)	32,50,50	1.95	9 (28%)
4	GOL	E	603	-	5,5,5	0.31	0	5,5,5	0.35	0
4	GOL	E	604	-	5,5,5	0.32	0	5,5,5	0.47	0
5	FMT	E	605	-	2,2,2	0.66	0	1,1,1	0.41	0
5	FMT	F	601	-	2,2,2	0.67	0	1,1,1	0.46	0
2	TD6	F	602	3	24,34,34	1.33	5 (20%)	32,50,50	1.86	8 (25%)
4	GOL	F	604	-	5,5,5	0.45	0	5,5,5	0.30	0
4	GOL	F	605	-	5,5,5	0.35	0	5,5,5	0.66	0
2	TD6	G	601	3	24,34,34	1.34	4 (16%)	32,50,50	1.80	8 (25%)
4	GOL	G	603	-	5,5,5	0.33	0	5,5,5	0.46	0
4	GOL	G	604	-	5,5,5	0.48	0	5,5,5	0.22	0
5	FMT	G	605	-	2,2,2	0.71	0	1,1,1	0.31	0
5	FMT	H	601	-	2,2,2	0.74	0	1,1,1	0.63	0
2	TD6	H	602	3	24,34,34	1.34	4 (16%)	32,50,50	2.03	9 (28%)
4	GOL	H	604	-	5,5,5	0.29	0	5,5,5	0.55	0
4	GOL	H	605	-	5,5,5	0.34	0	5,5,5	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TD6	A	601	3	-	0/19/26/26	0/2/2/2
4	GOL	A	603	-	-	0/4/4/4	0/0/0/0
4	GOL	A	604	-	-	0/4/4/4	0/0/0/0
5	FMT	A	605	-	-	0/0/0/0	0/0/0/0
5	FMT	B	601	-	-	0/0/0/0	0/0/0/0
2	TD6	B	602	3	-	0/19/26/26	0/2/2/2
4	GOL	B	604	-	-	0/4/4/4	0/0/0/0
4	GOL	B	605	-	-	0/4/4/4	0/0/0/0
2	TD6	C	601	3	-	0/19/26/26	0/2/2/2
4	GOL	C	603	-	-	0/4/4/4	0/0/0/0
4	GOL	C	604	-	-	0/4/4/4	0/0/0/0
5	FMT	C	605	-	-	0/0/0/0	0/0/0/0
5	FMT	D	601	-	-	0/0/0/0	0/0/0/0
2	TD6	D	602	3	-	0/19/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	604	-	-	0/4/4/4	0/0/0/0
4	GOL	D	605	-	-	0/4/4/4	0/0/0/0
2	TD6	E	601	3	-	0/19/26/26	0/2/2/2
4	GOL	E	603	-	-	0/4/4/4	0/0/0/0
4	GOL	E	604	-	-	0/4/4/4	0/0/0/0
5	FMT	E	605	-	-	0/0/0/0	0/0/0/0
5	FMT	F	601	-	-	0/0/0/0	0/0/0/0
2	TD6	F	602	3	-	0/19/26/26	0/2/2/2
4	GOL	F	604	-	-	0/4/4/4	0/0/0/0
4	GOL	F	605	-	-	0/4/4/4	0/0/0/0
2	TD6	G	601	3	-	0/19/26/26	0/2/2/2
4	GOL	G	603	-	-	0/4/4/4	0/0/0/0
4	GOL	G	604	-	-	0/4/4/4	0/0/0/0
5	FMT	G	605	-	-	0/0/0/0	0/0/0/0
5	FMT	H	601	-	-	0/0/0/0	0/0/0/0
2	TD6	H	602	3	-	0/19/26/26	0/2/2/2
4	GOL	H	604	-	-	0/4/4/4	0/0/0/0
4	GOL	H	605	-	-	0/4/4/4	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	TD6	C5'-C4'	-2.20	1.39	1.42
2	F	602	TD6	C5'-C4'	-2.00	1.39	1.42
2	E	601	TD6	C7'-C5'	2.01	1.55	1.51
2	G	601	TD6	C6-C7	2.11	1.57	1.50
2	D	602	TD6	C7'-C5'	2.14	1.55	1.51
2	E	601	TD6	C6-C7	2.21	1.57	1.50
2	D	602	TD6	C6-C7	2.23	1.57	1.50
2	F	602	TD6	C6-C7	2.25	1.57	1.50
2	B	602	TD6	C6-C7	2.25	1.57	1.50
2	F	602	TD6	C7'-C5'	2.28	1.56	1.51
2	C	601	TD6	C6-C7	2.29	1.57	1.50
2	A	601	TD6	C6-C7	2.31	1.57	1.50
2	H	602	TD6	C6-C7	2.33	1.58	1.50
2	C	601	TD6	CM2-C2'	2.45	1.57	1.49
2	F	602	TD6	CM2-C2'	2.48	1.57	1.49
2	A	601	TD6	CM2-C2'	2.50	1.57	1.49
2	D	602	TD6	CM2-C2'	2.54	1.57	1.49
2	C	601	TD6	C7'-C5'	2.54	1.56	1.51
2	B	602	TD6	CM2-C2'	2.55	1.57	1.49
2	G	601	TD6	C7'-C5'	2.56	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	TD6	CM2-C2'	2.60	1.57	1.49
2	H	602	TD6	C7'-C5'	2.61	1.56	1.51
2	E	601	TD6	CM2-C2'	2.62	1.57	1.49
2	B	602	TD6	C7'-C5'	2.70	1.56	1.51
2	H	602	TD6	CM2-C2'	2.75	1.58	1.49
2	H	602	TD6	CM4-C4	2.76	1.55	1.49
2	E	601	TD6	CM4-C4	3.01	1.56	1.49
2	C	601	TD6	CM4-C4	3.04	1.56	1.49
2	G	601	TD6	CM4-C4	3.10	1.56	1.49
2	F	602	TD6	CM4-C4	3.11	1.56	1.49
2	B	602	TD6	CM4-C4	3.12	1.56	1.49
2	D	602	TD6	CM4-C4	3.17	1.56	1.49
2	A	601	TD6	CM4-C4	3.17	1.56	1.49

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	602	TD6	CM4-C4-C5	-4.05	120.33	128.91
2	A	601	TD6	CM4-C4-C5	-4.03	120.37	128.91
2	D	602	TD6	CM4-C4-C5	-3.94	120.56	128.91
2	E	601	TD6	CM4-C4-C5	-3.94	120.56	128.91
2	H	602	TD6	CM4-C4-C5	-3.85	120.75	128.91
2	B	602	TD6	CM4-C4-C5	-3.82	120.81	128.91
2	C	601	TD6	CM4-C4-C5	-3.82	120.83	128.91
2	G	601	TD6	CM4-C4-C5	-3.62	121.23	128.91
2	H	602	TD6	C13-CLB-C11	-3.49	110.63	114.74
2	H	602	TD6	C5'-C6'-N1'	-3.22	118.24	123.86
2	A	601	TD6	C5'-C6'-N1'	-3.14	118.37	123.86
2	C	601	TD6	C5'-C6'-N1'	-3.11	118.43	123.86
2	H	602	TD6	N1'-C2'-N3'	-3.07	119.75	125.50
2	F	602	TD6	N1'-C2'-N3'	-3.07	119.75	125.50
2	G	601	TD6	C5'-C6'-N1'	-3.04	118.55	123.86
2	D	602	TD6	N1'-C2'-N3'	-3.03	119.81	125.50
2	E	601	TD6	N1'-C2'-N3'	-3.00	119.86	125.50
2	E	601	TD6	C13-CLB-C11	-2.99	111.22	114.74
2	B	602	TD6	C5'-C6'-N1'	-2.98	118.65	123.86
2	B	602	TD6	N1'-C2'-N3'	-2.96	119.94	125.50
2	D	602	TD6	C5'-C6'-N1'	-2.77	119.02	123.86
2	F	602	TD6	C5'-C6'-N1'	-2.65	119.22	123.86
2	E	601	TD6	C5'-C6'-N1'	-2.61	119.29	123.86
2	F	602	TD6	C13-CLB-C11	-2.59	111.68	114.74
2	B	602	TD6	C5'-C7'-N3	-2.59	108.82	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	601	TD6	N1'-C2'-N3'	-2.59	120.64	125.50
2	A	601	TD6	N1'-C2'-N3'	-2.58	120.66	125.50
2	B	602	TD6	C13-CLB-C11	-2.58	111.70	114.74
2	A	601	TD6	C13-CLB-C11	-2.56	111.72	114.74
2	C	601	TD6	N1'-C2'-N3'	-2.49	120.83	125.50
2	G	601	TD6	C13-CLB-C11	-2.07	112.30	114.74
2	B	602	TD6	CM2-C2'-N3'	2.06	120.72	117.20
2	E	601	TD6	O2A-PA-O3A	2.20	114.70	105.27
2	H	602	TD6	O2A-PA-O3A	2.22	114.78	105.27
2	H	602	TD6	CM2-C2'-N1'	2.44	120.06	117.05
2	A	601	TD6	CM2-C2'-N1'	2.74	120.43	117.05
2	E	601	TD6	CM2-C2'-N1'	2.86	120.58	117.05
2	F	602	TD6	CM2-C2'-N1'	2.90	120.63	117.05
2	E	601	TD6	C6'-N1'-C2'	2.97	121.57	115.92
2	D	602	TD6	C6'-N1'-C2'	3.24	122.08	115.92
2	C	601	TD6	C6'-N1'-C2'	3.25	122.09	115.92
2	G	601	TD6	C6'-N1'-C2'	3.26	122.11	115.92
2	G	601	TD6	C5-C4-N3	3.26	115.55	107.94
2	A	601	TD6	C5-C4-N3	3.27	115.58	107.94
2	F	602	TD6	C6'-N1'-C2'	3.30	122.19	115.92
2	C	601	TD6	C5-C4-N3	3.30	115.65	107.94
2	G	601	TD6	CM2-C2'-N1'	3.33	121.16	117.05
2	E	601	TD6	C5-C4-N3	3.34	115.74	107.94
2	F	602	TD6	C5-C4-N3	3.38	115.83	107.94
2	B	602	TD6	C5-C4-N3	3.39	115.86	107.94
2	D	602	TD6	C5-C4-N3	3.41	115.92	107.94
2	A	601	TD6	C6'-N1'-C2'	3.44	122.47	115.92
2	A	601	TD6	C6-C5-S1	3.49	125.12	120.24
2	G	601	TD6	C6-C5-S1	3.61	125.29	120.24
2	H	602	TD6	C5-C4-N3	3.61	116.37	107.94
2	D	602	TD6	CM2-C2'-N1'	3.74	121.67	117.05
2	B	602	TD6	C6'-N1'-C2'	3.84	123.22	115.92
2	H	602	TD6	C6'-N1'-C2'	3.92	123.37	115.92
2	C	601	TD6	C6-C5-S1	4.27	126.22	120.24
2	F	602	TD6	C6-C5-S1	4.50	126.53	120.24
2	E	601	TD6	C6-C5-S1	4.52	126.56	120.24
2	B	602	TD6	C6-C5-S1	4.82	126.98	120.24
2	H	602	TD6	C6-C5-S1	5.03	127.28	120.24
2	D	602	TD6	C6-C5-S1	5.35	127.73	120.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TD6	2	0
5	A	605	FMT	1	0
5	B	601	FMT	1	0
2	B	602	TD6	3	0
4	B	605	GOL	1	0
2	C	601	TD6	2	0
4	C	603	GOL	1	0
5	D	601	FMT	5	0
2	D	602	TD6	4	0
2	E	601	TD6	3	0
5	F	601	FMT	4	0
2	F	602	TD6	3	0
4	F	604	GOL	1	0
4	F	605	GOL	1	0
2	G	601	TD6	2	0
4	G	604	GOL	4	0
5	G	605	FMT	1	0
5	H	601	FMT	1	0
2	H	602	TD6	3	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	556/556 (100%)	-0.19	3 (0%)	91	91	9, 14, 27, 55	5 (0%)
1	B	556/556 (100%)	-0.16	3 (0%)	91	91	10, 16, 27, 43	2 (0%)
1	C	556/556 (100%)	-0.12	3 (0%)	91	91	9, 15, 28, 49	3 (0%)
1	D	556/556 (100%)	-0.06	4 (0%)	89	89	9, 18, 33, 46	3 (0%)
1	E	556/556 (100%)	-0.10	6 (1%)	82	82	10, 18, 32, 52	4 (0%)
1	F	556/556 (100%)	-0.07	8 (1%)	78	77	9, 16, 29, 50	0
1	G	556/556 (100%)	-0.15	4 (0%)	89	89	8, 15, 29, 58	5 (0%)
1	H	556/556 (100%)	-0.19	2 (0%)	93	92	9, 16, 27, 46	3 (0%)
All	All	4448/4448 (100%)	-0.13	33 (0%)	89	89	8, 16, 30, 58	25 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.0
1	G	1	MET	5.3
1	F	1	MET	3.9
1	F	176	GLY	3.5
1	D	1	MET	3.5
1	D	347	VAL	3.4
1	G	176	GLY	3.0
1	B	1	MET	3.0
1	C	1	MET	2.9
1	H	177	GLU	2.9
1	G	178	MET	2.8
1	E	347	VAL	2.6
1	F	347	VAL	2.6
1	F	556	LEU	2.6
1	E	1	MET	2.4
1	H	176	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	178	MET	2.4
1	E	556	LEU	2.3
1	A	178	MET	2.3
1	D	556	LEU	2.3
1	E	183	LEU	2.3
1	E	482	GLN	2.2
1	F	526	ARG	2.2
1	E	176	GLY	2.2
1	F	482	GLN	2.1
1	C	178	MET	2.1
1	B	180	ASP	2.1
1	B	522	ALA	2.1
1	C	176	GLY	2.1
1	G	512	GLN	2.0
1	D	555	HIS	2.0
1	F	522	ALA	2.0
1	A	556	LEU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	E	604	6/6	0.95	0.19	10.23	20,36,45,47	0
4	GOL	F	605	6/6	0.86	0.23	9.82	22,34,42,44	0
4	GOL	C	604	6/6	0.89	0.16	8.20	20,34,39,43	0
4	GOL	H	605	6/6	0.71	0.23	5.58	26,46,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	604	6/6	0.94	0.16	4.88	20,37,46,46	0
4	GOL	B	605	6/6	0.87	0.18	4.65	27,40,52,62	0
4	GOL	D	605	6/6	0.90	0.15	3.78	28,39,48,52	0
4	GOL	G	604	6/6	0.88	0.14	3.07	26,43,51,54	0
4	GOL	H	604	6/6	0.94	0.13	2.56	22,30,37,39	0
5	FMT	F	601	3/3	0.95	0.13	2.28	26,26,31,37	0
5	FMT	G	605	3/3	0.83	0.12	2.11	26,31,37,45	0
5	FMT	H	601	3/3	0.90	0.14	2.02	26,27,33,40	0
4	GOL	G	603	6/6	0.95	0.11	0.95	15,28,41,41	0
5	FMT	C	605	3/3	0.96	0.10	0.74	25,25,30,31	0
4	GOL	A	603	6/6	0.95	0.09	0.73	13,25,34,34	0
4	GOL	B	604	6/6	0.94	0.09	0.51	18,23,35,35	0
4	GOL	F	604	6/6	0.97	0.10	0.50	18,30,35,36	0
4	GOL	C	603	6/6	0.96	0.08	0.37	16,32,39,39	0
4	GOL	E	603	6/6	0.94	0.09	0.22	21,29,41,41	0
5	FMT	B	601	3/3	0.94	0.09	0.19	26,29,33,39	0
5	FMT	A	605	3/3	0.97	0.09	0.11	23,25,30,35	0
4	GOL	D	604	6/6	0.95	0.09	-0.12	19,29,35,36	0
2	TD6	D	602	33/33	0.98	0.08	-0.45	10,18,29,35	0
2	TD6	H	602	33/33	0.98	0.08	-0.51	10,18,38,46	0
2	TD6	G	601	33/33	0.98	0.09	-0.55	8,15,29,35	0
5	FMT	E	605	3/3	0.97	0.08	-0.68	29,30,35,36	0
2	TD6	C	601	33/33	0.97	0.08	-0.84	8,16,35,41	0
5	FMT	D	601	3/3	0.95	0.08	-0.89	25,30,34,37	0
2	TD6	A	601	33/33	0.98	0.08	-0.90	8,15,31,38	0
2	TD6	E	601	33/33	0.98	0.07	-1.02	11,19,33,44	0
2	TD6	B	602	33/33	0.98	0.07	-1.04	9,17,29,40	0
2	TD6	F	602	33/33	0.98	0.07	-1.19	10,16,30,37	0
3	MN	H	603	1/1	0.99	0.03	-1.95	21,21,21,21	0
3	MN	A	602	1/1	1.00	0.03	-3.08	19,19,19,19	0
3	MN	B	603	1/1	0.99	0.03	-3.30	20,20,20,20	0
3	MN	C	602	1/1	1.00	0.04	-4.07	19,19,19,19	0
3	MN	E	602	1/1	0.99	0.03	-4.10	23,23,23,23	0
3	MN	D	603	1/1	1.00	0.03	-4.21	20,20,20,20	0
3	MN	G	602	1/1	1.00	0.03	-4.37	19,19,19,19	0
3	MN	F	603	1/1	1.00	0.01	-5.76	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.