Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:14 PM GMT

PDB ID	:	4HN1
Title	:	Crystal Structure of H60N/Y130F double mutant of ChmJ, a 3'-monoepimerase from Streptomyces bikiniensis in complex with dTDP
Authors	:	Holden, H.M.; Kubiak, R.L.
Deposited on	:	2012-10-18
Resolution	:	1.60 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 (i) symbol.

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

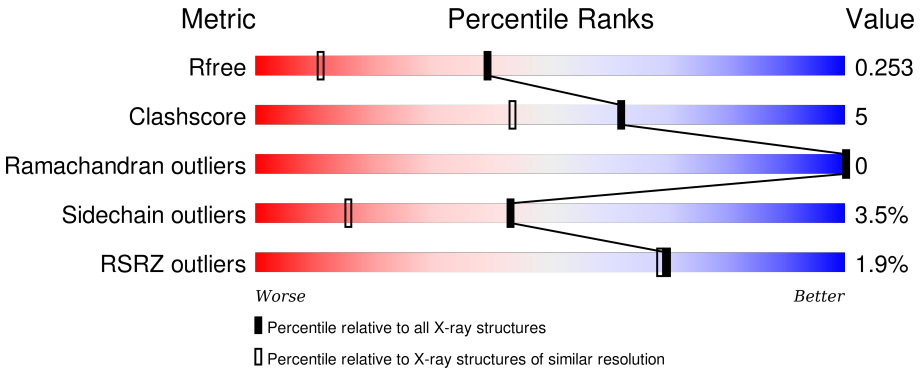
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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 <=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	201	88% 9%
1	B	201	89% 9%
1	C	201	83% 14%
1	D	201	85% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	302	-	-	-	X
2	EDO	A	304	-	-	-	X
2	EDO	B	303	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6909 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 Putative 3-epimerase in D-allose pathway.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	4	0
			1568	986	281	297	4			
1	B	199	Total	C	N	O	S	0	5	0
			1576	991	284	297	4			
1	C	201	Total	C	N	O	S	0	2	0
			1585	996	287	298	4			
1	D	200	Total	C	N	O	S	0	1	0
			1565	984	284	293	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	HIS	ENGINEERED MUTATION	UNP Q5SFD1
A	130	PHE	TYR	ENGINEERED MUTATION	UNP Q5SFD1
A	197	LEU	-	EXPRESSION TAG	UNP Q5SFD1
A	198	GLU	-	EXPRESSION TAG	UNP Q5SFD1
A	199	HIS	-	EXPRESSION TAG	UNP Q5SFD1
A	200	HIS	-	EXPRESSION TAG	UNP Q5SFD1
A	201	HIS	-	EXPRESSION TAG	UNP Q5SFD1
B	60	ASN	HIS	ENGINEERED MUTATION	UNP Q5SFD1
B	130	PHE	TYR	ENGINEERED MUTATION	UNP Q5SFD1
B	197	LEU	-	EXPRESSION TAG	UNP Q5SFD1
B	198	GLU	-	EXPRESSION TAG	UNP Q5SFD1
B	199	HIS	-	EXPRESSION TAG	UNP Q5SFD1
B	200	HIS	-	EXPRESSION TAG	UNP Q5SFD1
B	201	HIS	-	EXPRESSION TAG	UNP Q5SFD1
C	60	ASN	HIS	ENGINEERED MUTATION	UNP Q5SFD1
C	130	PHE	TYR	ENGINEERED MUTATION	UNP Q5SFD1
C	197	LEU	-	EXPRESSION TAG	UNP Q5SFD1
C	198	GLU	-	EXPRESSION TAG	UNP Q5SFD1
C	199	HIS	-	EXPRESSION TAG	UNP Q5SFD1
C	200	HIS	-	EXPRESSION TAG	UNP Q5SFD1
C	201	HIS	-	EXPRESSION TAG	UNP Q5SFD1

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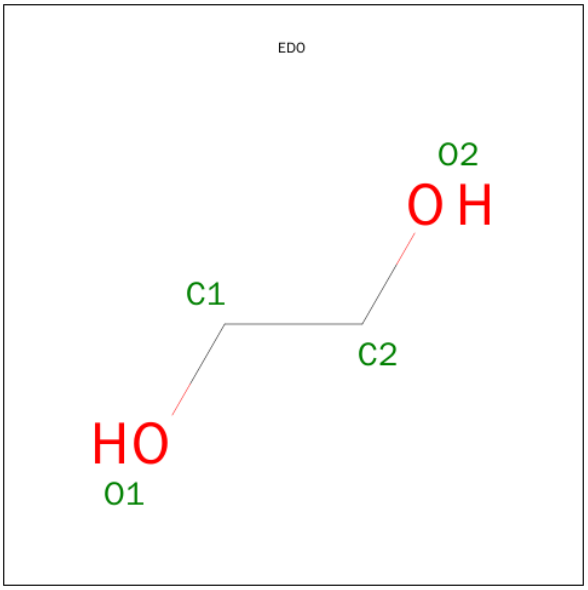
Chain	Residue	Modelled	Actual	Comment	Reference
D	60	ASN	HIS	ENGINEERED MUTATION	UNP Q5SFD1
D	130	PHE	TYR	ENGINEERED MUTATION	UNP Q5SFD1
D	197	LEU	-	EXPRESSION TAG	UNP Q5SFD1
D	198	GLU	-	EXPRESSION TAG	UNP Q5SFD1
D	199	HIS	-	EXPRESSION TAG	UNP Q5SFD1
D	200	HIS	-	EXPRESSION TAG	UNP Q5SFD1
D	201	HIS	-	EXPRESSION TAG	UNP Q5SFD1

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



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

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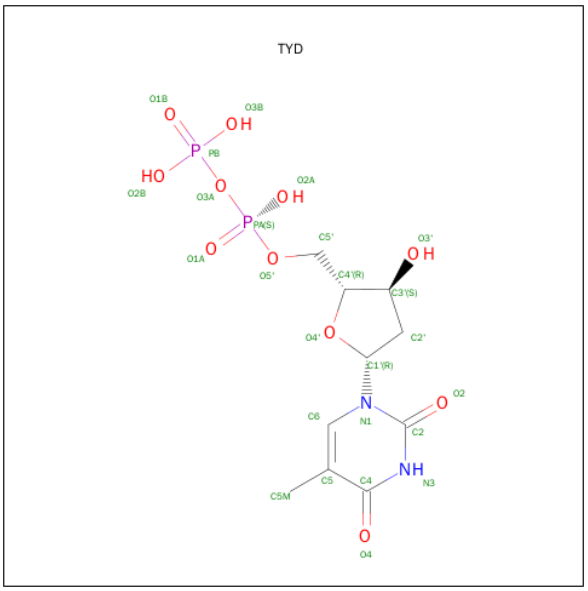
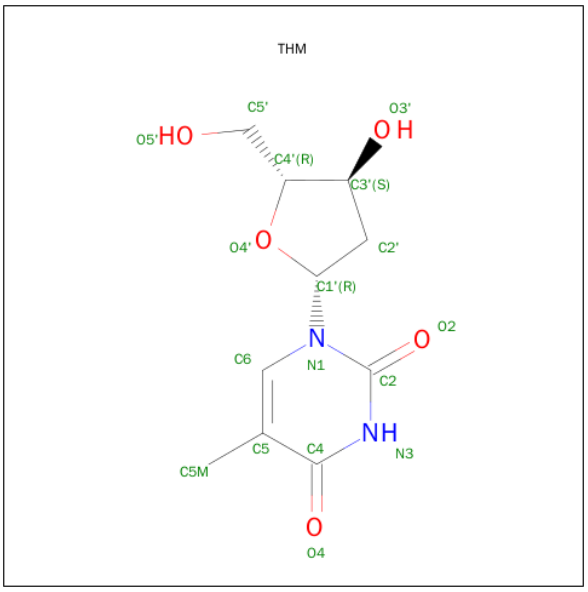
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



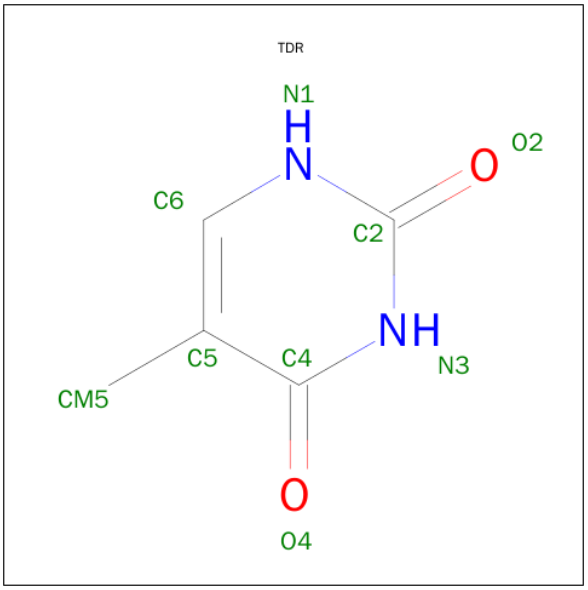
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 25 10 2 11 2	0	0
3	B	1	Total C N O P 25 10 2 11 2	0	0
3	C	1	Total C N O P 25 10 2 11 2	0	0
3	C	1	Total C N O P 25 10 2 11 2	0	0

- Molecule 4 is THYMIDINE (three-letter code: THM) (formula: $C_{10}H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	10	2	5		
4	B	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 5 is THYMINE (three-letter code: TDR) (formula: $C_5H_6N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			9	5	2	2		
5	D	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 6 is water.

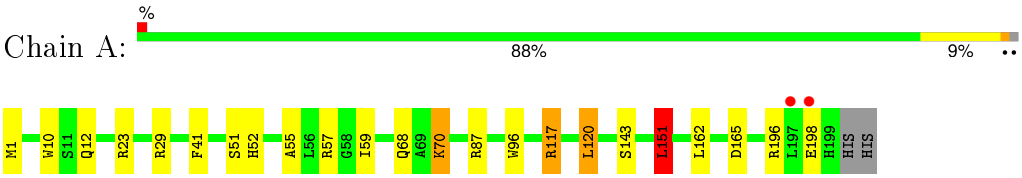
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	143	Total O 143 143	0	0
6	B	112	Total O 112 112	0	0
6	C	77	Total O 77 77	0	0
6	D	87	Total O 87 87	0	0

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.

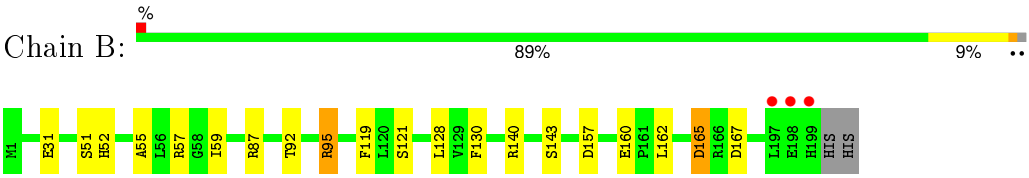
- Molecule 1: Putative 3-epimerase in D-allose pathway

Chain A:



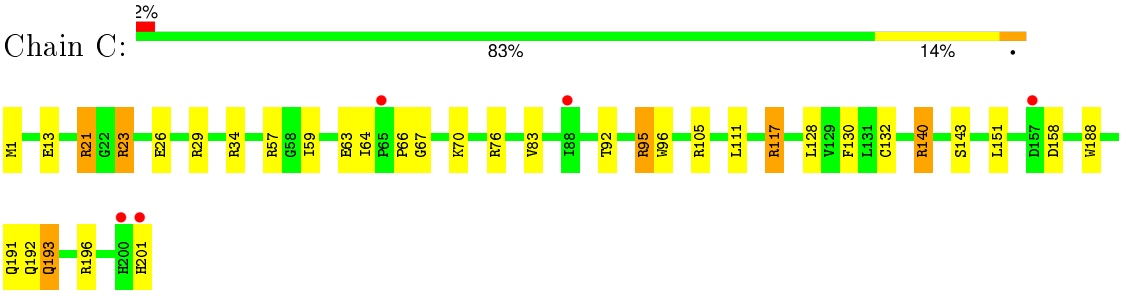
- Molecule 1: Putative 3-epimerase in D-allose pathway

Chain B:



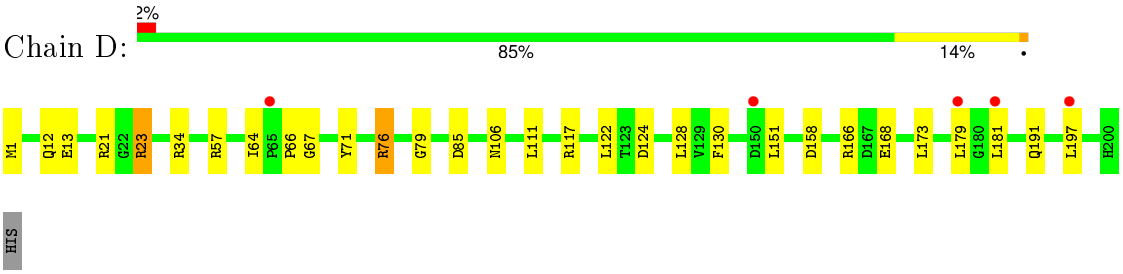
- Molecule 1: Putative 3-epimerase in D-allose pathway

Chain C:



- Molecule 1: Putative 3-epimerase in D-allose pathway

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	141.02Å 141.02Å 116.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 28.86 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-1.60) 96.1 (28.86-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.254 0.212 , 0.253	Depositor DCC
R_{free} test set	7511 reflections (5.50%)	DCC
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 30.0	EDS
Estimated twinning fraction	0.479 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 143836 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6909	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, 0.375 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: TYD, TDR, THM, EDO

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	0.54	0/1623	1.21	7/2215 (0.3%)
1	B	0.53	0/1634	1.19	7/2229 (0.3%)
1	C	0.47	0/1636	1.18	9/2233 (0.4%)
1	D	0.47	0/1612	1.17	14/2201 (0.6%)
All	All	0.50	0/6505	1.18	37/8878 (0.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	21	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	C	23	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	D	23	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	C	21	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	151	LEU	CB-CG-CD2	8.64	125.70	111.00
1	D	34	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	C	23	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	D	1	MET	CG-SD-CE	-6.97	89.04	100.20
1	D	23	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	120	LEU	CB-CG-CD2	6.79	122.55	111.00
1	B	87	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	165	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	87	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	1	MET	CG-SD-CE	-6.64	89.58	100.20
1	D	130	PHE	CB-CA-C	-6.55	97.31	110.40
1	B	57	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	167	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	87	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	173	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	D	197	LEU	CA-CB-CG	6.16	129.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	128	LEU	CA-CB-CG	-5.95	101.63	115.30
1	B	130	PHE	CB-CA-C	-5.83	98.73	110.40
1	A	70	LYS	CD-CE-NZ	-5.83	98.29	111.70
1	C	130	PHE	CB-CA-C	-5.82	98.77	110.40
1	A	87	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	76	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	21	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	41	PHE	CB-CG-CD2	5.56	124.69	120.80
1	D	111	LEU	CB-CG-CD2	5.51	120.36	111.00
1	C	111	LEU	CB-CG-CD2	5.46	120.29	111.00
1	D	34	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	128	LEU	CA-CB-CG	-5.38	102.93	115.30
1	B	128	LEU	CA-CB-CG	-5.19	103.36	115.30
1	D	124	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	85	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	34	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1568	0	1507	16	0
1	B	1576	0	1520	12	0
1	C	1585	0	1512	21	0
1	D	1565	0	1495	17	0
2	A	16	0	24	3	0
2	B	12	0	18	2	0
2	C	8	0	12	0	0
2	D	8	0	12	2	0
3	A	25	0	13	3	0
3	B	25	0	13	1	0
3	C	50	0	26	3	0
4	A	17	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	17	0	14	0	0
5	C	9	0	6	0	0
5	D	9	0	6	0	0
6	A	143	0	0	4	0
6	B	112	0	0	4	0
6	C	77	0	0	1	0
6	D	87	0	0	1	0
All	All	6909	0	6192	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (69) 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:C:105:ARG:HD3	6:C:477:HOH:O	1.52	1.06
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.23	1.00
3:C:303:TYD:O1B	1:D:57:ARG:NH1	2.10	0.84
1:A:117:ARG:HH11	1:A:117:ARG:CG	1.90	0.84
1:C:26[A]:GLU:OE1	1:C:29:ARG:NE	2.10	0.84
1:C:57:ARG:NH1	3:C:304:TYD:O2B	2.13	0.79
1:D:66:PRO:HA	1:D:191:GLN:HE22	1.48	0.78
1:A:10:TRP:CZ3	2:A:304:EDO:H22	2.18	0.78
1:C:70:LYS:NZ	1:C:132:CYS:SG	2.62	0.73
1:A:52:HIS:HD2	6:A:471:HOH:O	1.73	0.71
1:C:193:GLN:NE2	1:C:196:ARG:HH21	1.87	0.71
1:A:117:ARG:NH1	1:A:117:ARG:HG3	2.00	0.69
1:D:66:PRO:HA	1:D:191:GLN:NE2	2.08	0.69
1:C:26[A]:GLU:OE1	1:C:29:ARG:CD	2.43	0.67
1:D:71:TYR:OH	2:D:301:EDO:H21	1.94	0.67
1:B:52:HIS:ND1	6:B:508:HOH:O	2.28	0.66
1:C:66:PRO:HA	1:C:191:GLN:HE22	1.61	0.66
1:D:23:ARG:HH21	1:D:106:ASN:HD21	1.47	0.61
2:A:302:EDO:O1	3:B:304:TYD:H5'1	2.01	0.61
1:B:92:THR:HB	1:B:95:ARG:HG3	1.83	0.60
1:C:193:GLN:HE21	1:C:196:ARG:HH21	1.51	0.58
1:C:66:PRO:HA	1:C:191:GLN:NE2	2.18	0.58
3:A:305:TYD:O3'	6:A:487:HOH:O	2.06	0.57
1:C:21:ARG:NH1	3:C:303:TYD:O3B	2.27	0.57
1:D:23:ARG:HH21	1:D:106:ASN:ND2	2.03	0.57
3:A:305:TYD:H5'1	2:B:301:EDO:O1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLY:HA2	1:D:122:LEU:HG	1.90	0.53
1:D:168:GLU:OE1	6:D:464:HOH:O	2.18	0.53
1:A:117:ARG:NH1	1:A:117:ARG:CG	2.59	0.52
1:C:70:LYS:HD2	1:C:117:ARG:NH1	2.25	0.52
1:D:71:TYR:OH	2:D:301:EDO:C2	2.58	0.52
1:D:179:LEU:HD12	1:D:179:LEU:O	2.10	0.52
1:A:117:ARG:HD3	6:A:541:HOH:O	2.09	0.51
1:D:179:LEU:HD23	1:D:181:LEU:HD11	1.92	0.51
1:C:26[A]:GLU:OE1	1:C:29:ARG:CG	2.59	0.50
1:D:23:ARG:NH2	1:D:106:ASN:ND2	2.59	0.50
1:C:188:TRP:O	1:C:192:GLN:HG2	2.10	0.49
1:C:64:ILE:HG22	1:C:67:GLY:HA3	1.95	0.49
1:A:55:ALA:HA	1:A:162:LEU:HB2	1.94	0.49
1:A:96:TRP:HD1	1:A:151:LEU:HD22	1.78	0.48
1:A:196:ARG:NH1	6:A:500:HOH:O	2.45	0.48
1:A:68:GLN:OE1	1:A:70:LYS:HE3	2.14	0.48
1:B:59:ILE:O	1:B:143[B]:SER:HA	2.14	0.47
1:B:51:SER:HB2	1:B:121[B]:SER:OG	2.13	0.47
1:B:52:HIS:HA	6:B:508:HOH:O	2.14	0.47
1:B:160:GLU:OE2	1:B:160:GLU:HA	2.13	0.47
3:A:305:TYD:C5'	2:B:301:EDO:O1	2.63	0.47
1:C:76:ARG:HD2	1:D:76:ARG:HD2	1.98	0.45
1:C:158:ASP:N	1:C:158:ASP:OD1	2.47	0.45
1:B:59:ILE:O	1:B:143[A]:SER:HA	2.17	0.45
1:B:51:SER:HB3	1:B:55:ALA:HB3	1.97	0.45
1:A:1:MET:HG2	1:A:12:GLN:HE21	1.81	0.45
1:C:59:ILE:O	1:C:143:SER:HA	2.17	0.45
1:D:66:PRO:CA	1:D:191:GLN:HE22	2.26	0.44
1:A:59:ILE:O	1:A:143[A]:SER:HA	2.17	0.44
1:B:119:PHE:HE1	1:B:121[B]:SER:HG	1.66	0.44
1:D:179:LEU:HG	1:D:181:LEU:HG	2.00	0.43
1:C:63:GLU:HB2	1:C:140:ARG:HG3	2.00	0.43
1:C:83:VAL:O	1:C:96:TRP:HA	2.18	0.42
1:D:158:ASP:OD1	1:D:158:ASP:N	2.46	0.42
1:A:51:SER:HB3	1:A:55:ALA:HB3	2.02	0.41
1:B:119:PHE:HD1	6:B:463:HOH:O	2.03	0.41
1:B:55:ALA:HA	1:B:162:LEU:HB2	2.03	0.41
1:A:59:ILE:O	1:A:143[B]:SER:HA	2.21	0.41
1:C:66:PRO:CA	1:C:191:GLN:HE22	2.32	0.41
1:B:140:ARG:NH1	6:B:509:HOH:O	2.46	0.41
1:C:92:THR:HB	1:C:95:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:HG22	1:D:67:GLY:HA3	2.03	0.40
1:A:23:ARG:HA	2:A:302:EDO:H22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/201 (100%)	200 (100%)	1 (0%)	0	100	100
1	B	202/201 (100%)	201 (100%)	1 (0%)	0	100	100
1	C	201/201 (100%)	197 (98%)	4 (2%)	0	100	100
1	D	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
All	All	803/804 (100%)	794 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	167/165 (101%)	161 (96%)	6 (4%)	42	15
1	B	168/165 (102%)	164 (98%)	4 (2%)	57	27
1	C	167/165 (101%)	159 (95%)	8 (5%)	31	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	164/165 (99%)	159 (97%)	5 (3%)	48 19
All	All	666/660 (101%)	643 (96%)	23 (4%)	43 16

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	117	ARG
1	A	120	LEU
1	A	151	LEU
1	A	165	ASP
1	A	198	GLU
1	B	31	GLU
1	B	95	ARG
1	B	157	ASP
1	B	165	ASP
1	C	13	GLU
1	C	23	ARG
1	C	95	ARG
1	C	117	ARG
1	C	140	ARG
1	C	151	LEU
1	C	193	GLN
1	C	201	HIS
1	D	12	GLN
1	D	13	GLU
1	D	117	ARG
1	D	151	LEU
1	D	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	195	GLN
1	B	12	GLN
1	B	35	GLN
1	B	195	GLN
1	B	199	HIS
1	C	191	GLN
1	C	193	GLN

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Mol	Chain	Res	Type
1	D	12	GLN
1	D	106	ASN
1	D	191	GLN
1	D	193	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)

19 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	EDO	A	301	-	3,3,3	0.52	0	2,2,2	0.77	0
2	EDO	A	302	-	3,3,3	0.44	0	2,2,2	1.35	0
2	EDO	A	303	-	3,3,3	0.52	0	2,2,2	0.40	0
2	EDO	A	304	-	3,3,3	0.46	0	2,2,2	0.58	0
3	TYD	A	305	-	19,26,26	0.59	0	27,40,40	1.69	6 (22%)
4	THM	A	306	-	13,18,18	0.63	0	16,26,26	4.01	5 (31%)
2	EDO	B	301	-	3,3,3	0.45	0	2,2,2	0.18	0
2	EDO	B	302	-	3,3,3	0.54	0	2,2,2	0.29	0
2	EDO	B	303	-	3,3,3	0.49	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	TYD	B	304	-	19,26,26	0.61	0	27,40,40	1.91	5 (18%)
4	THM	B	305	-	13,18,18	0.62	0	16,26,26	3.58	4 (25%)
2	EDO	C	301	-	3,3,3	0.63	0	2,2,2	0.43	0
2	EDO	C	302	-	3,3,3	0.56	0	2,2,2	0.25	0
3	TYD	C	303	-	19,26,26	0.58	0	27,40,40	2.03	4 (14%)
3	TYD	C	304	-	19,26,26	0.60	0	27,40,40	2.01	6 (22%)
5	TDR	C	305	-	5,9,9	0.87	0	7,12,12	6.20	4 (57%)
2	EDO	D	301	-	3,3,3	0.44	0	2,2,2	0.78	0
2	EDO	D	302	-	3,3,3	0.63	0	2,2,2	0.46	0
5	TDR	D	303	-	5,9,9	1.06	1 (20%)	7,12,12	5.91	4 (57%)

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	EDO	A	301	-	-	0/1/1/1	0/0/0/0
2	EDO	A	302	-	-	0/1/1/1	0/0/0/0
2	EDO	A	303	-	-	0/1/1/1	0/0/0/0
2	EDO	A	304	-	-	0/1/1/1	0/0/0/0
3	TYD	A	305	-	-	0/12/28/28	0/2/2/2
4	THM	A	306	-	-	0/2/18/18	0/2/2/2
2	EDO	B	301	-	-	0/1/1/1	0/0/0/0
2	EDO	B	302	-	-	0/1/1/1	0/0/0/0
2	EDO	B	303	-	-	0/1/1/1	0/0/0/0
3	TYD	B	304	-	-	0/12/28/28	0/2/2/2
4	THM	B	305	-	-	0/2/18/18	0/2/2/2
2	EDO	C	301	-	-	0/1/1/1	0/0/0/0
2	EDO	C	302	-	-	0/1/1/1	0/0/0/0
3	TYD	C	303	-	-	0/12/28/28	0/2/2/2
3	TYD	C	304	-	-	0/12/28/28	0/2/2/2
5	TDR	C	305	-	-	0/0/0/0	0/1/1/1
2	EDO	D	301	-	-	0/1/1/1	0/0/0/0
2	EDO	D	302	-	-	0/1/1/1	0/0/0/0
5	TDR	D	303	-	-	0/0/0/0	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	303	TDR	C4-N3	2.06	1.36	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	305	TDR	N1-C2-N3	-11.22	121.18	128.33
5	D	303	TDR	N1-C2-N3	-10.98	121.33	128.33
4	A	306	THM	C5-C4-N3	-9.16	114.94	125.14
4	B	305	THM	C5-C4-N3	-7.52	116.76	125.14
5	C	305	TDR	C5-C4-N3	-7.16	117.17	125.14
5	D	303	TDR	C5-C4-N3	-6.90	117.45	125.14
3	C	304	TYD	C5-C4-N3	-5.30	119.24	125.14
3	C	303	TYD	C5-C4-N3	-4.64	119.97	125.14
3	B	304	TYD	C5-C4-N3	-3.64	121.09	125.14
3	A	305	TYD	C5-C4-N3	-3.59	121.14	125.14
3	A	305	TYD	O4'-C1'-N1	-3.24	102.11	107.72
5	D	303	TDR	C5-C6-N1	-3.19	122.39	125.23
5	C	305	TDR	C5-C6-N1	-2.77	122.75	125.23
3	C	304	TYD	O5'-PA-O1A	-2.62	99.44	109.62
3	A	305	TYD	O2B-PB-O1B	-2.51	102.50	110.58
4	B	305	THM	O3'-C3'-C2'	-2.33	103.03	110.74
4	A	306	THM	O3'-C3'-C2'	-2.31	103.11	110.74
4	A	306	THM	C2'-C1'-N1	-2.07	109.13	114.16
4	A	306	THM	C2'-C3'-C4'	2.05	107.03	102.77
3	C	304	TYD	C5M-C5-C4	2.21	122.90	120.05
3	C	304	TYD	O3B-PB-O3A	2.25	115.31	105.09
4	B	305	THM	O4'-C1'-N1	2.26	111.63	107.72
3	C	304	TYD	O3A-PA-O5'	2.37	109.24	102.94
3	B	304	TYD	O5'-C5'-C4'	2.60	118.70	109.12
3	A	305	TYD	O3B-PB-O2B	2.70	117.64	107.38
3	B	304	TYD	O2A-PA-O3A	3.04	118.86	105.09
3	A	305	TYD	C5M-C5-C4	3.44	124.49	120.05
3	C	303	TYD	C5M-C5-C4	3.46	124.51	120.05
3	A	305	TYD	C4-N3-C2	3.68	118.43	115.25
3	C	303	TYD	O3A-PA-O5'	4.08	113.75	102.94
3	B	304	TYD	C5M-C5-C4	4.67	126.08	120.05
3	B	304	TYD	C4-N3-C2	5.50	120.00	115.25
3	C	304	TYD	C4-N3-C2	6.43	120.80	115.25
3	C	303	TYD	C4-N3-C2	6.70	121.04	115.25
5	D	303	TDR	C4-N3-C2	7.97	122.14	115.25
5	C	305	TDR	C4-N3-C2	9.03	123.05	115.25
4	B	305	THM	C4-N3-C2	11.12	124.86	115.25
4	A	306	THM	C4-N3-C2	12.26	125.85	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	EDO	2	0
2	A	304	EDO	1	0
3	A	305	TYD	3	0
2	B	301	EDO	2	0
3	B	304	TYD	1	0
3	C	303	TYD	2	0
3	C	304	TYD	1	0
2	D	301	EDO	2	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, 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	199/201 (99%)	-0.11	2 (1%)	84	84	14, 24, 42, 65	0
1	B	199/201 (99%)	-0.08	3 (1%)	76	75	14, 24, 41, 67	0
1	C	201/201 (100%)	0.07	5 (2%)	61	58	17, 30, 48, 67	0
1	D	200/201 (99%)	0.09	5 (2%)	61	58	17, 30, 46, 56	0
All	All	799/804 (99%)	-0.01	15 (1%)	70	68	14, 26, 46, 67	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	GLU	4.2
1	C	200	HIS	3.9
1	C	201	HIS	3.7
1	D	179	LEU	3.4
1	B	197	LEU	3.1
1	D	65	PRO	2.8
1	A	197	LEU	2.7
1	B	199	HIS	2.7
1	C	88	ILE	2.4
1	C	157	ASP	2.2
1	A	198	GLU	2.1
1	D	150	ASP	2.0
1	C	65	PRO	2.0
1	D	181	LEU	2.0
1	D	197	LEU	2.0

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

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
2	EDO	A	304	4/4	0.91	0.12	4.55	34,44,44,48	0
2	EDO	A	302	4/4	0.88	0.12	3.14	25,27,34,50	0
2	EDO	B	303	4/4	0.91	0.15	3.02	32,32,33,37	0
2	EDO	A	301	4/4	0.96	0.12	1.60	30,32,33,35	0
3	TYD	C	303	25/25	0.93	0.13	1.29	37,41,66,69	0
2	EDO	D	301	4/4	0.87	0.11	0.97	35,37,37,39	0
3	TYD	A	305	25/25	0.90	0.12	0.62	31,40,53,59	0
3	TYD	B	304	25/25	0.89	0.12	0.51	28,40,54,61	0
3	TYD	C	304	25/25	0.92	0.11	0.43	35,42,63,68	0
2	EDO	D	302	4/4	0.94	0.09	0.31	21,21,23,30	0
2	EDO	C	301	4/4	0.95	0.09	-0.09	20,21,23,28	0
2	EDO	A	303	4/4	0.95	0.09	-0.39	25,28,30,38	0
2	EDO	C	302	4/4	0.94	0.07	-0.73	32,33,33,34	0
2	EDO	B	301	4/4	0.96	0.07	-1.31	25,25,34,45	0
2	EDO	B	302	4/4	0.97	0.07	-1.64	24,27,28,34	0
4	THM	B	305	17/17	0.87	0.17	-	27,42,55,61	0
5	TDR	C	305	9/9	0.86	0.24	-	30,35,40,48	0
5	TDR	D	303	9/9	0.87	0.17	-	30,35,41,42	0
4	THM	A	306	17/17	0.89	0.17	-	29,40,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.