Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 01:01 PM EDT

PDB ID	:	5U24
Title	:	X-ray structure of the WlaRG aminotransferase from campylobacter jejuni, K184A mutant in complex with TDP-Fuc3N
Authors	:	Holden, H.M.; Thoden, J.B.; Dow, G.T.; Gilbert, M.
Deposited on	:	2016-11-29
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

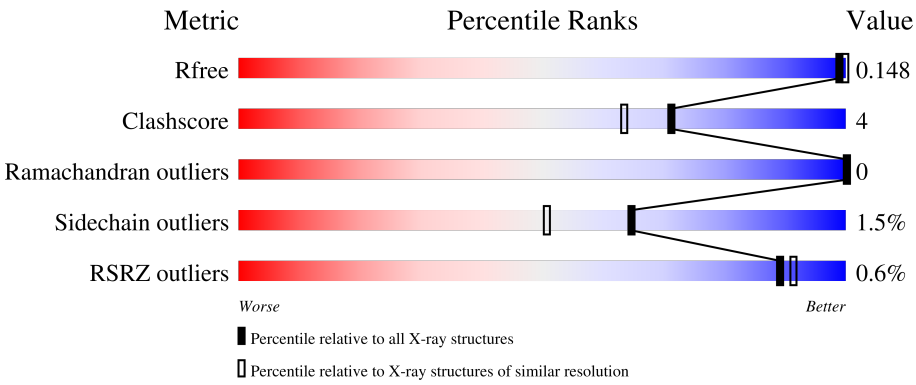
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

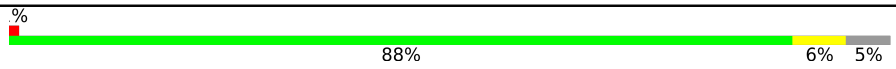
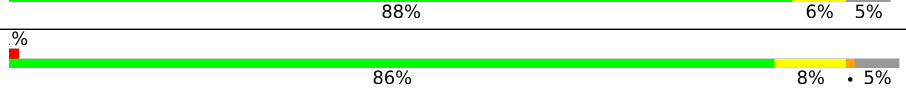
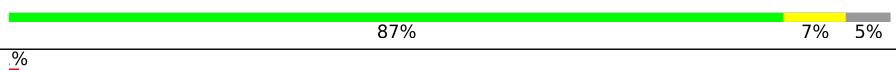
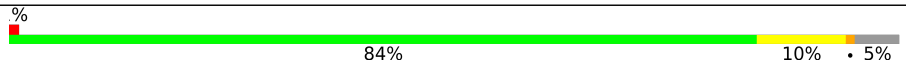
The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	382	
1	B	382	
1	C	382	
1	D	382	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13489 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 aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2938	1891	495	537	15	0	3	0
1	B	362	2938	1890	498	536	14	0	1	0
1	C	361	2945	1894	499	537	15	0	3	0
1	D	361	2939	1891	496	537	15	0	3	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q9ALS9
A	-20	GLY	-	expression tag	UNP Q9ALS9
A	-19	SER	-	expression tag	UNP Q9ALS9
A	-18	SER	-	expression tag	UNP Q9ALS9
A	-17	HIS	-	expression tag	UNP Q9ALS9
A	-16	HIS	-	expression tag	UNP Q9ALS9
A	-15	HIS	-	expression tag	UNP Q9ALS9
A	-14	HIS	-	expression tag	UNP Q9ALS9
A	-13	HIS	-	expression tag	UNP Q9ALS9
A	-12	HIS	-	expression tag	UNP Q9ALS9
A	-11	SER	-	expression tag	UNP Q9ALS9
A	-10	SER	-	expression tag	UNP Q9ALS9
A	-9	ARG	-	expression tag	UNP Q9ALS9
A	-8	ASN	-	expression tag	UNP Q9ALS9
A	-7	LEU	-	expression tag	UNP Q9ALS9
A	-6	TYR	-	expression tag	UNP Q9ALS9
A	-5	PHE	-	expression tag	UNP Q9ALS9
A	-4	GLN	-	expression tag	UNP Q9ALS9
A	-3	GLY	-	expression tag	UNP Q9ALS9
A	-2	GLY	-	expression tag	UNP Q9ALS9
A	-1	GLY	-	expression tag	UNP Q9ALS9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q9ALS9
A	184	ALA	LYS	engineered mutation	UNP Q9ALS9
B	-21	MET	-	initiating methionine	UNP Q9ALS9
B	-20	GLY	-	expression tag	UNP Q9ALS9
B	-19	SER	-	expression tag	UNP Q9ALS9
B	-18	SER	-	expression tag	UNP Q9ALS9
B	-17	HIS	-	expression tag	UNP Q9ALS9
B	-16	HIS	-	expression tag	UNP Q9ALS9
B	-15	HIS	-	expression tag	UNP Q9ALS9
B	-14	HIS	-	expression tag	UNP Q9ALS9
B	-13	HIS	-	expression tag	UNP Q9ALS9
B	-12	HIS	-	expression tag	UNP Q9ALS9
B	-11	SER	-	expression tag	UNP Q9ALS9
B	-10	SER	-	expression tag	UNP Q9ALS9
B	-9	ARG	-	expression tag	UNP Q9ALS9
B	-8	ASN	-	expression tag	UNP Q9ALS9
B	-7	LEU	-	expression tag	UNP Q9ALS9
B	-6	TYR	-	expression tag	UNP Q9ALS9
B	-5	PHE	-	expression tag	UNP Q9ALS9
B	-4	GLN	-	expression tag	UNP Q9ALS9
B	-3	GLY	-	expression tag	UNP Q9ALS9
B	-2	GLY	-	expression tag	UNP Q9ALS9
B	-1	GLY	-	expression tag	UNP Q9ALS9
B	0	HIS	-	expression tag	UNP Q9ALS9
B	184	ALA	LYS	engineered mutation	UNP Q9ALS9
C	-21	MET	-	initiating methionine	UNP Q9ALS9
C	-20	GLY	-	expression tag	UNP Q9ALS9
C	-19	SER	-	expression tag	UNP Q9ALS9
C	-18	SER	-	expression tag	UNP Q9ALS9
C	-17	HIS	-	expression tag	UNP Q9ALS9
C	-16	HIS	-	expression tag	UNP Q9ALS9
C	-15	HIS	-	expression tag	UNP Q9ALS9
C	-14	HIS	-	expression tag	UNP Q9ALS9
C	-13	HIS	-	expression tag	UNP Q9ALS9
C	-12	HIS	-	expression tag	UNP Q9ALS9
C	-11	SER	-	expression tag	UNP Q9ALS9
C	-10	SER	-	expression tag	UNP Q9ALS9
C	-9	ARG	-	expression tag	UNP Q9ALS9
C	-8	ASN	-	expression tag	UNP Q9ALS9
C	-7	LEU	-	expression tag	UNP Q9ALS9
C	-6	TYR	-	expression tag	UNP Q9ALS9
C	-5	PHE	-	expression tag	UNP Q9ALS9

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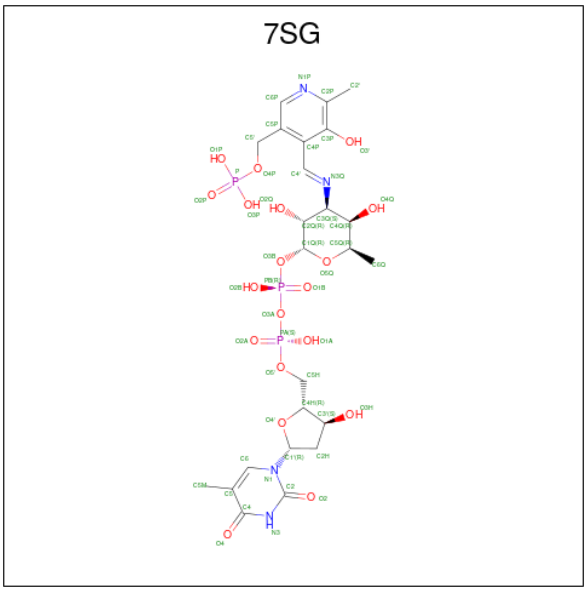
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLN	-	expression tag	UNP Q9ALS9
C	-3	GLY	-	expression tag	UNP Q9ALS9
C	-2	GLY	-	expression tag	UNP Q9ALS9
C	-1	GLY	-	expression tag	UNP Q9ALS9
C	0	HIS	-	expression tag	UNP Q9ALS9
C	184	ALA	LYS	engineered mutation	UNP Q9ALS9
D	-21	MET	-	initiating methionine	UNP Q9ALS9
D	-20	GLY	-	expression tag	UNP Q9ALS9
D	-19	SER	-	expression tag	UNP Q9ALS9
D	-18	SER	-	expression tag	UNP Q9ALS9
D	-17	HIS	-	expression tag	UNP Q9ALS9
D	-16	HIS	-	expression tag	UNP Q9ALS9
D	-15	HIS	-	expression tag	UNP Q9ALS9
D	-14	HIS	-	expression tag	UNP Q9ALS9
D	-13	HIS	-	expression tag	UNP Q9ALS9
D	-12	HIS	-	expression tag	UNP Q9ALS9
D	-11	SER	-	expression tag	UNP Q9ALS9
D	-10	SER	-	expression tag	UNP Q9ALS9
D	-9	ARG	-	expression tag	UNP Q9ALS9
D	-8	ASN	-	expression tag	UNP Q9ALS9
D	-7	LEU	-	expression tag	UNP Q9ALS9
D	-6	TYR	-	expression tag	UNP Q9ALS9
D	-5	PHE	-	expression tag	UNP Q9ALS9
D	-4	GLN	-	expression tag	UNP Q9ALS9
D	-3	GLY	-	expression tag	UNP Q9ALS9
D	-2	GLY	-	expression tag	UNP Q9ALS9
D	-1	GLY	-	expression tag	UNP Q9ALS9
D	0	HIS	-	expression tag	UNP Q9ALS9
D	184	ALA	LYS	engineered mutation	UNP Q9ALS9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

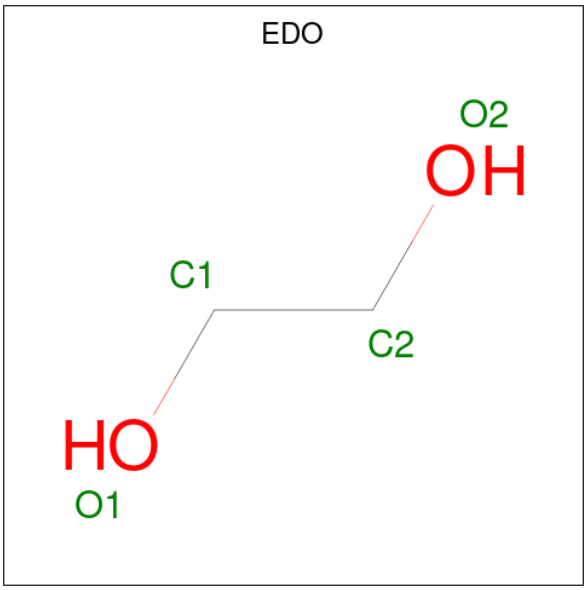
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
			Total	Na		
2	C	1	1	1	0	0

- Molecule 3 is (2R,3R,4S,5R,6R)-3,5-dihydroxy-4-[(E)-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)amino]-6-methyltetrahydro-2H-pyran-2-yl [(2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-2-yl]methyl dihydrogen diphosphate (non-preferred name) (three-letter code: 7SG) (formula: $C_{24}H_{35}N_4O_{19}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	50	24	4	19	3	0	0
3	B	1	50	24	4	19	3	0	0
3	C	1	50	24	4	19	3	0	0
3	D	1	50	24	4	19	3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0

- Molecule 6 is water.

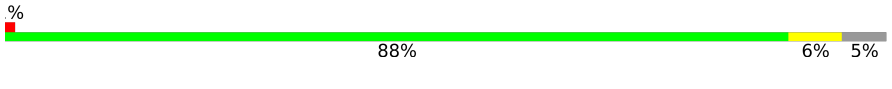
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	412	413	413	0	1
			Total	O		
6	B	368	368	368	0	0
			Total	O		
6	C	375	375	375	0	0
			Total	O		
6	D	338	338	338	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

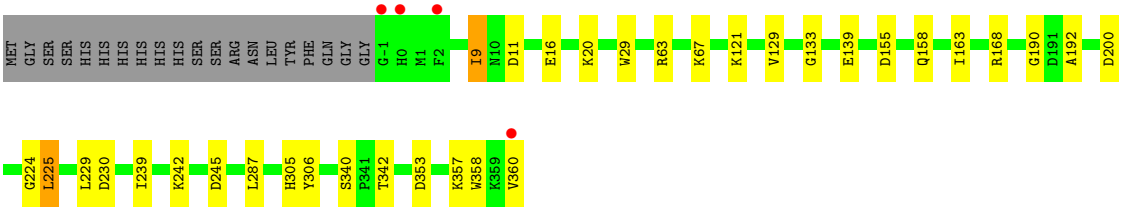
• Molecule 1: Putative aminotransferase

Chain A:



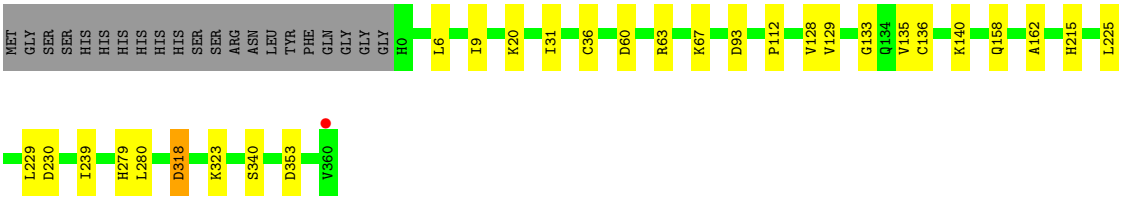
• Molecule 1: Putative aminotransferase

Chain B:



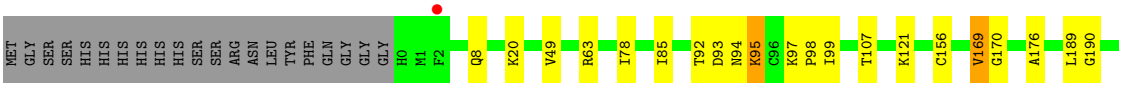
• Molecule 1: Putative aminotransferase

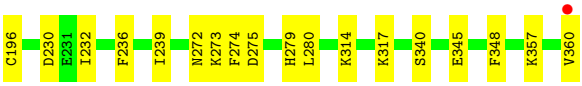
Chain C:



• Molecule 1: Putative aminotransferase

Chain D:




C196
D230
E231
I232
F236
I239
N272
K273
F274
D275
H279
L280
K314
K317
S340
E345
F348
K357
V360

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.06Å 56.80Å 124.31Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	28.53 – 1.70 28.53 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (28.53-1.70) 98.9 (28.53-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.105 , 0.146 0.108 , 0.148	Depositor DCC
R_{free} test set	8351 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
Reported twinning fraction	0.493 for H, K, L 0.507 for h,-k,-l	Depositor
Outliers	0 of 165117 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13489	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 7SG, EDO, NA

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	0.48	0/3009	0.83	0/4063
1	B	0.47	0/3004	0.85	6/4056 (0.1%)
1	C	0.48	0/3014	0.86	2/4070 (0.0%)
1	D	0.47	0/3007	0.83	2/4061 (0.0%)
All	All	0.47	0/12034	0.84	10/16250 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	230	ASP	CB-CG-OD1	7.48	125.03	118.30
1	C	230	ASP	CB-CG-OD1	7.15	124.73	118.30
1	B	200	ASP	CB-CG-OD1	6.85	124.47	118.30
1	B	200	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	B	245	ASP	CB-CG-OD1	6.14	123.83	118.30
1	C	353	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	275	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	11	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	230	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	230	ASP	CB-CG-OD1	5.03	122.82	118.30

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	2938	0	2967	19	0
1	B	2938	0	2964	22	0
1	C	2945	0	2971	17	0
1	D	2939	0	2967	25	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	50	0	0	1	0
3	B	50	0	0	0	0
3	C	50	0	0	1	0
3	D	50	0	0	0	0
4	A	12	0	18	1	0
4	B	8	0	12	0	0
4	C	4	0	6	0	0
4	D	8	0	12	1	0
5	A	1	0	0	0	0
6	A	413	0	0	5	0
6	B	368	0	0	4	0
6	C	375	0	0	2	0
6	D	338	0	0	4	0
All	All	13489	0	11917	84	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 4.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ARG:HD2	1:D:93:ASP:OD2	1.45	1.14
1:C:63:ARG:HD2	1:C:93:ASP:OD2	1.62	0.99
1:A:24:ILE:HD13	1:A:232:ILE:HD13	1.48	0.95
1:A:24:ILE:CD1	1:A:232:ILE:HD13	2.00	0.92
1:C:140:LYS:HE3	6:C:629:HOH:O	1.75	0.85
1:D:63:ARG:CD	1:D:93:ASP:OD2	2.27	0.82
1:D:8:GLN:OE1	6:D:501:HOH:O	1.98	0.81
1:B:9:ILE:HD12	1:B:342:THR:OG1	1.84	0.76
1:C:112:PRO:HB2	1:C:140:LYS:HD2	1.71	0.71
1:B:287:LEU:HD13	1:B:360:VAL:HG22	1.73	0.69
1:B:353:ASP:OD2	1:B:357:LYS:HE3	1.92	0.69
1:B:63:ARG:NH1	6:B:502:HOH:O	2.19	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ASN:O	1:D:95:LYS:HG2	1.98	0.64
1:C:63:ARG:CD	1:C:93:ASP:OD2	2.41	0.63
1:A:24:ILE:HD12	1:A:232:ILE:HD13	1.80	0.62
1:D:156:CYS:SG	1:D:169:VAL:HG13	2.40	0.61
1:B:29:TRP:HD1	6:B:681:HOH:O	1.84	0.59
1:D:272:ASN:ND2	6:D:508:HOH:O	2.35	0.58
1:D:121:LYS:HG2	6:D:746:HOH:O	2.03	0.57
1:C:67:LYS:HE2	6:C:829:HOH:O	2.04	0.57
1:A:141:ILE:HG13	6:A:504:HOH:O	2.04	0.57
1:C:318:ASP:OD1	1:C:318:ASP:N	2.39	0.56
1:D:232:ILE:HG22	1:D:236:PHE:CE2	2.41	0.56
1:B:287:LEU:HD13	1:B:360:VAL:CG2	2.36	0.56
1:D:345:GLU:HA	1:D:348:PHE:CE2	2.41	0.54
1:B:20:LYS:HG3	1:B:239:ILE:HD11	1.90	0.54
1:D:20:LYS:HG3	1:D:239:ILE:HD11	1.89	0.54
1:A:163:ILE:HG23	6:A:787:HOH:O	2.07	0.54
1:A:232:ILE:HG23	1:A:236:PHE:CZ	2.43	0.53
1:B:163:ILE:HG12	1:B:168:ARG:HD3	1.92	0.52
1:B:353:ASP:OD2	1:B:357:LYS:CE	2.58	0.51
1:A:81:ALA:HB2	1:A:100:LEU:HB3	1.92	0.51
1:B:358:TRP:CZ2	1:B:360:VAL:HG21	2.45	0.51
1:D:314:LYS:O	1:D:317:LYS:HE3	2.11	0.51
1:A:318:ASP:HB2	6:A:782:HOH:O	2.11	0.51
1:B:224:GLY:O	1:B:225:LEU:HD13	2.11	0.49
1:C:129:VAL:O	1:C:136[B]:CYS:SG	2.70	0.49
1:B:139:GLU:OE2	6:B:501:HOH:O	2.19	0.49
1:C:128:VAL:CG2	1:C:136[B]:CYS:SG	3.01	0.49
1:B:129:VAL:HG22	1:B:155:ASP:HB3	1.95	0.48
1:D:279:HIS:CD2	1:D:280:LEU:HG	2.48	0.48
1:C:135:VAL:CG1	1:C:162:ALA:HB1	2.42	0.48
1:D:189:LEU:HD22	1:D:236:PHE:CD2	2.49	0.48
1:D:97:LYS:HB2	6:D:744:HOH:O	2.13	0.48
1:A:163:ILE:CG2	6:A:787:HOH:O	2.60	0.48
1:D:232:ILE:CG2	1:D:236:PHE:CZ	2.96	0.48
1:D:273:LYS:HD3	1:D:274:PHE:CE2	2.49	0.48
1:C:279:HIS:CD2	1:C:280:LEU:HG	2.50	0.47
3:C:402:7SG:N3Q	3:C:402:7SG:O3'	2.48	0.46
1:A:242:LYS:HB3	1:A:242:LYS:HE2	1.63	0.46
1:A:345:GLU:HA	1:A:348:PHE:CE1	2.51	0.46
1:C:20:LYS:HG3	1:C:239:ILE:HD11	1.97	0.46
1:B:360:VAL:OXT	1:B:360:VAL:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:HIS:HA	1:B:306:TYR:CD1	2.52	0.45
1:C:60:ASP:OD1	1:C:63:ARG:NH2	2.50	0.45
1:C:6:LEU:HD23	1:C:9:ILE:HD12	1.99	0.45
1:A:31:ILE:HD11	1:B:190:GLY:HA2	1.98	0.45
1:C:36[A]:CYS:SG	1:C:229:LEU:O	2.75	0.45
1:D:78:ILE:HD13	1:D:99:ILE:HB	1.99	0.45
1:A:232:ILE:CG2	1:A:236:PHE:CE2	3.01	0.44
1:B:133:GLY:HA2	1:B:158:GLN:O	2.17	0.44
1:C:31:ILE:HD11	1:D:190:GLY:HA2	2.00	0.44
1:D:49:VAL:HG21	1:D:196:CYS:HB3	2.00	0.44
1:D:170:GLY:HA2	1:D:176:ALA:CB	2.47	0.44
1:A:305:HIS:HA	1:A:306:TYR:CD1	2.53	0.44
1:C:133:GLY:HA2	1:C:158:GLN:O	2.19	0.43
4:A:405:EDO:O1	6:A:501:HOH:O	2.19	0.43
1:B:16:GLU:HB3	1:B:239:ILE:HD13	2.00	0.43
1:D:232:ILE:CG2	1:D:236:PHE:CE2	3.01	0.43
1:A:21:PHE:HD1	1:A:232:ILE:HD12	1.83	0.43
1:D:107:THR:HA	4:D:403:EDO:H22	2.00	0.43
1:A:129:VAL:HG22	1:A:155:ASP:HB3	2.01	0.42
3:A:402:7SG:O3'	3:A:402:7SG:N3Q	2.51	0.42
1:D:357:LYS:O	1:D:360:VAL:HG12	2.19	0.42
1:A:311:HIS:O	1:A:320:ASN:HA	2.20	0.41
1:B:192:ALA:HB1	1:B:229:LEU:CD1	2.50	0.41
1:A:232:ILE:HG22	1:A:236:PHE:CE2	2.55	0.41
1:D:232:ILE:HG23	1:D:236:PHE:CZ	2.56	0.41
1:A:292:GLN:HG3	1:A:302:THR:OG1	2.20	0.41
1:B:287:LEU:CD1	1:B:360:VAL:CG2	2.99	0.40
1:C:6:LEU:HD23	1:C:6:LEU:HA	1.81	0.40
1:B:67:LYS:HE3	6:B:843:HOH:O	2.21	0.40
1:B:287:LEU:HD12	1:B:360:VAL:HG11	2.04	0.40
1:D:92:THR:HG22	1:D:98:PRO:HD3	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	362/382 (95%)	353 (98%)	9 (2%)	0	100	100
1	B	361/382 (94%)	350 (97%)	11 (3%)	0	100	100
1	C	362/382 (95%)	346 (96%)	16 (4%)	0	100	100
1	D	362/382 (95%)	351 (97%)	11 (3%)	0	100	100
All	All	1447/1528 (95%)	1400 (97%)	47 (3%)	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	323/338 (96%)	318 (98%)	5 (2%)	65	51
1	B	322/338 (95%)	317 (98%)	5 (2%)	62	48
1	C	324/338 (96%)	319 (98%)	5 (2%)	65	51
1	D	323/338 (96%)	319 (99%)	4 (1%)	71	59
All	All	1292/1352 (96%)	1273 (98%)	19 (2%)	65	51

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	97	LYS
1	A	242	LYS
1	A	340	SER
1	A	359	LYS
1	B	9	ILE
1	B	121	LYS
1	B	225	LEU
1	B	242	LYS
1	B	340	SER

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Mol	Chain	Res	Type
1	C	215	HIS
1	C	225	LEU
1	C	318	ASP
1	C	323	LYS
1	C	340	SER
1	D	85	ILE
1	D	95	LYS
1	D	169	VAL
1	D	340	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	B	41	ASN
1	B	260	GLN
1	C	201	ASN
1	C	256	ASN
1	C	260	GLN
1	C	297	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
4	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.34	0
3	7SG	B	401	-	50,53,53	1.73	6 (12%)	71,81,81	1.92	17 (23%)
4	EDO	B	403	-	3,3,3	0.64	0	2,2,2	0.63	0
4	EDO	C	403	-	3,3,3	0.57	0	2,2,2	0.34	0
3	7SG	A	402	-	50,53,53	1.68	6 (12%)	71,81,81	2.03	17 (23%)
4	EDO	D	403	-	3,3,3	0.50	0	2,2,2	0.41	0
4	EDO	D	402	-	3,3,3	0.50	0	2,2,2	0.10	0
4	EDO	B	402	-	3,3,3	0.63	0	2,2,2	0.17	0
4	EDO	A	405	-	3,3,3	0.41	0	2,2,2	0.39	0
3	7SG	C	402	-	50,53,53	1.81	8 (16%)	71,81,81	1.99	18 (25%)
4	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.18	0
3	7SG	D	401	-	50,53,53	1.61	6 (12%)	71,81,81	2.02	16 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	404	-	-	0/1/1/1	-
3	7SG	B	401	-	-	2/32/64/64	0/4/4/4
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
3	7SG	A	402	-	-	3/32/64/64	0/4/4/4
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	D	402	-	-	0/1/1/1	-
4	EDO	B	402	-	-	1/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
3	7SG	C	402	-	-	4/32/64/64	0/4/4/4
4	EDO	A	403	-	-	0/1/1/1	-
3	7SG	D	401	-	-	6/32/64/64	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	7SG	C3P-C2P	7.48	1.48	1.40
3	A	402	7SG	C3P-C2P	7.38	1.48	1.40
3	C	402	7SG	C3P-C2P	7.29	1.48	1.40
3	C	402	7SG	C4P-C5P	5.86	1.49	1.42
3	D	401	7SG	C4P-C3P	5.65	1.49	1.40
3	D	401	7SG	C4P-C5P	5.33	1.48	1.42
3	C	402	7SG	C4P-C3P	5.12	1.48	1.40
3	D	401	7SG	C3P-C2P	5.01	1.45	1.40
3	B	401	7SG	C4P-C3P	4.78	1.48	1.40
3	A	402	7SG	C4P-C5P	4.45	1.47	1.42
3	B	401	7SG	C4P-C5P	4.44	1.47	1.42
3	A	402	7SG	C4P-C3P	4.37	1.47	1.40
3	A	402	7SG	C6-C5	3.24	1.39	1.34
3	C	402	7SG	C6-C5	3.05	1.39	1.34
3	B	401	7SG	C6-C5	3.01	1.39	1.34
3	D	401	7SG	C6-C5	2.80	1.39	1.34
3	B	401	7SG	C4-N3	-2.45	1.34	1.38
3	A	402	7SG	C2-N3	-2.20	1.34	1.38
3	C	402	7SG	C4-C5	2.19	1.48	1.44
3	A	402	7SG	O2-C2	2.17	1.27	1.23
3	B	401	7SG	C4-C5	2.16	1.48	1.44
3	C	402	7SG	C2-N3	-2.14	1.34	1.38
3	C	402	7SG	C2-N1	2.14	1.41	1.38
3	C	402	7SG	O2-C2	2.04	1.26	1.23
3	D	401	7SG	C4-N3	-2.03	1.35	1.38
3	D	401	7SG	C4-C5	2.03	1.48	1.44

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	7SG	C3Q-N3Q-C4'	7.83	131.88	117.99
3	C	402	7SG	O4-C4-C5	-7.22	116.53	124.90
3	B	401	7SG	C3Q-N3Q-C4'	6.91	130.25	117.99
3	C	402	7SG	C3Q-N3Q-C4'	6.12	128.85	117.99
3	A	402	7SG	C3P-C4P-C5P	-6.11	113.57	118.26
3	A	402	7SG	O4-C4-C5	-5.65	118.35	124.90
3	D	401	7SG	O4-C4-C5	-5.38	118.67	124.90
3	A	402	7SG	O3A-PB-O3B	-5.06	92.28	102.48
3	B	401	7SG	O4-C4-C5	-5.00	119.11	124.90
3	D	401	7SG	C3P-C4P-C5P	-4.97	114.45	118.26
3	C	402	7SG	C5-C4-N3	4.95	119.53	115.31
3	D	401	7SG	C5-C4-N3	4.77	119.38	115.31
3	A	402	7SG	C5-C4-N3	4.68	119.30	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	7SG	C4-N3-C2	-4.53	121.48	127.35
3	B	401	7SG	O3A-PB-O3B	-4.48	93.45	102.48
3	A	402	7SG	C3Q-N3Q-C4'	4.38	125.76	117.99
3	B	401	7SG	C5-C4-N3	4.23	118.92	115.31
3	D	401	7SG	N3-C2-N1	4.07	120.29	114.89
3	A	402	7SG	C6Q-C5Q-C4Q	4.07	120.59	113.07
3	A	402	7SG	C2'-C2P-C3P	-3.79	116.20	120.89
3	B	401	7SG	N3-C2-N1	3.65	119.73	114.89
3	C	402	7SG	C5M-C5-C4	3.57	122.69	118.77
3	C	402	7SG	O3A-PB-O3B	-3.50	95.44	102.48
3	A	402	7SG	C4-N3-C2	-3.41	122.93	127.35
3	C	402	7SG	C4-N3-C2	-3.39	122.96	127.35
3	B	401	7SG	C4-N3-C2	-3.38	122.97	127.35
3	A	402	7SG	C4P-C4'-N3Q	-3.31	115.66	123.01
3	C	402	7SG	C6Q-C5Q-C4Q	3.25	119.09	113.07
3	B	401	7SG	C4P-C4'-N3Q	-3.16	115.99	123.01
3	A	402	7SG	O4P-C5'-C5P	3.15	115.35	109.35
3	C	402	7SG	C3P-C4P-C5P	-3.13	115.86	118.26
3	D	401	7SG	O5Q-C1Q-O3B	3.10	115.41	111.36
3	A	402	7SG	C2'-C2P-N1P	3.09	123.71	117.67
3	D	401	7SG	C4P-C4'-N3Q	-3.09	116.14	123.01
3	A	402	7SG	N3-C2-N1	3.04	118.92	114.89
3	C	402	7SG	O2-C2-N1	-2.96	118.85	122.79
3	B	401	7SG	C6P-N1P-C2P	2.95	124.63	119.17
3	B	401	7SG	C2H-C1'-N1	-2.94	107.00	113.77
3	A	402	7SG	O4Q-C4Q-C3Q	2.93	115.84	109.14
3	D	401	7SG	O4Q-C4Q-C3Q	2.84	115.64	109.14
3	C	402	7SG	N3-C2-N1	2.82	118.64	114.89
3	C	402	7SG	C6-C5-C4	-2.71	115.76	118.03
3	B	401	7SG	C1'-N1-C2	2.61	122.79	117.64
3	A	402	7SG	C5M-C5-C4	2.60	121.63	118.77
3	A	402	7SG	O5Q-C1Q-O3B	-2.54	108.05	111.36
3	C	402	7SG	O4Q-C4Q-C3Q	2.52	114.91	109.14
3	C	402	7SG	C4P-C4'-N3Q	-2.52	117.41	123.01
3	B	401	7SG	C6Q-C5Q-C4Q	2.50	117.69	113.07
3	C	402	7SG	C4P-C3P-C2P	-2.48	118.66	120.19
3	B	401	7SG	O4Q-C4Q-C3Q	2.45	114.75	109.14
3	B	401	7SG	O4'-C1'-N1	2.44	112.23	107.86
3	B	401	7SG	C3P-C2P-N1P	-2.43	117.63	120.77
3	D	401	7SG	O3A-PB-O3B	-2.32	97.80	102.48
3	A	402	7SG	C5-C6-N1	-2.25	121.02	123.34
3	C	402	7SG	C6P-N1P-C2P	2.23	123.29	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	7SG	O3'-C3P-C2P	2.21	122.30	117.49
3	D	401	7SG	C1'-N1-C2	2.20	121.97	117.64
3	D	401	7SG	O2Q-C2Q-C3Q	2.17	114.11	109.14
3	D	401	7SG	O2B-PB-O1B	2.15	122.85	112.24
3	B	401	7SG	C2'-C2P-N1P	2.13	121.84	117.67
3	C	402	7SG	O2B-PB-O1B	2.12	122.74	112.24
3	B	401	7SG	C5M-C5-C4	2.11	121.09	118.77
3	B	401	7SG	C1'-N1-C6	-2.09	117.17	120.77
3	A	402	7SG	C5P-C4P-C4'	2.09	124.99	121.56
3	D	401	7SG	C5-C6-N1	-2.06	121.22	123.34
3	D	401	7SG	C1Q-O5Q-C5Q	-2.02	110.20	113.67
3	D	401	7SG	C2H-C3'-C4H	2.01	106.95	102.76
3	C	402	7SG	C5P-C4P-C4'	2.01	124.86	121.56

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	7SG	C4Q-C3Q-N3Q-C4'
3	B	401	7SG	C4Q-C3Q-N3Q-C4'
3	C	402	7SG	C4Q-C3Q-N3Q-C4'
3	D	401	7SG	C4Q-C3Q-N3Q-C4'
3	D	401	7SG	C2Q-C1Q-O3B-PB
3	A	402	7SG	C1Q-O3B-PB-O3A
3	B	401	7SG	C1Q-O3B-PB-O3A
3	C	402	7SG	C2Q-C1Q-O3B-PB
3	D	401	7SG	C5'-O4P-P-O2P
4	B	402	EDO	O1-C1-C2-O2
3	D	401	7SG	PB-O3A-PA-O2A
3	C	402	7SG	C1Q-O3B-PB-O3A
3	A	402	7SG	PB-O3A-PA-O2A
3	D	401	7SG	PB-O3A-PA-O1A
3	C	402	7SG	C5'-O4P-P-O3P
3	D	401	7SG	C1Q-O3B-PB-O3A
4	B	403	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2

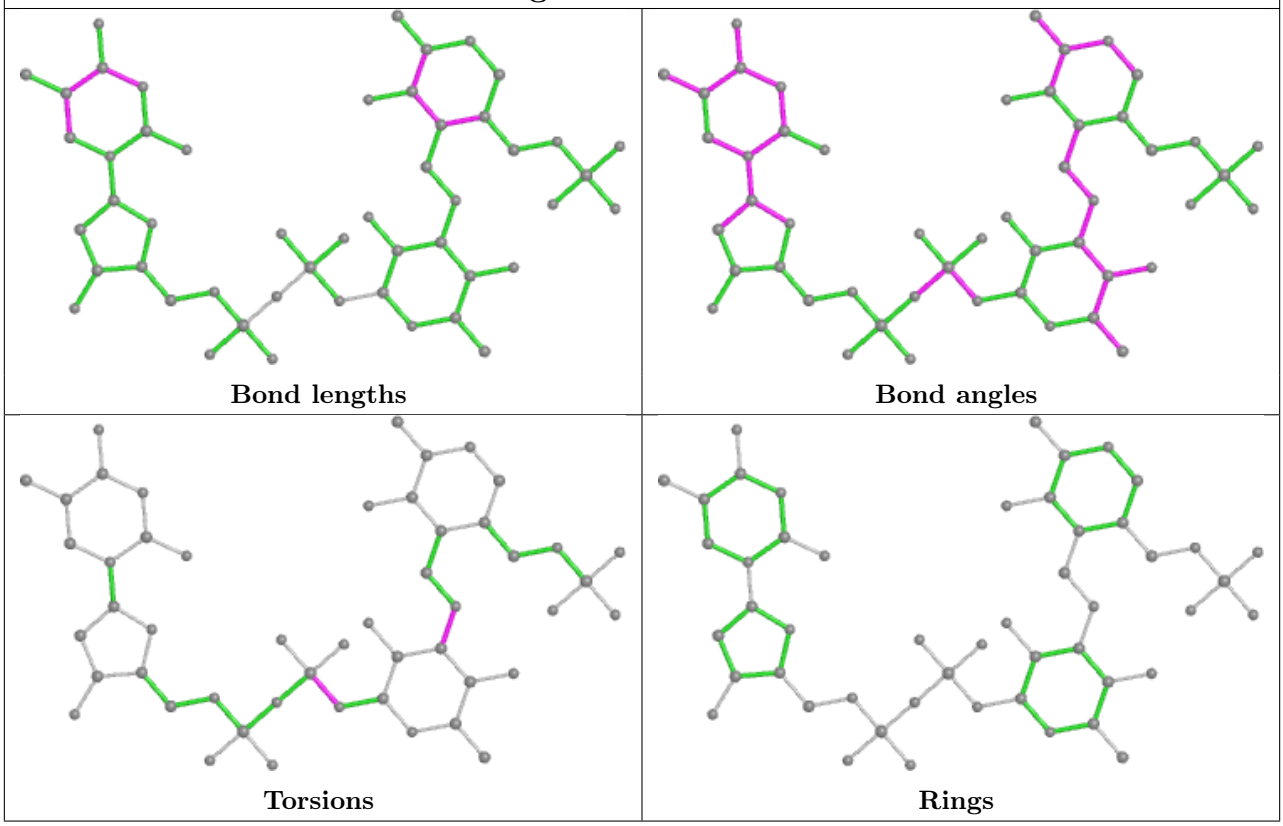
There are no ring outliers.

4 monomers are involved in 4 short contacts:

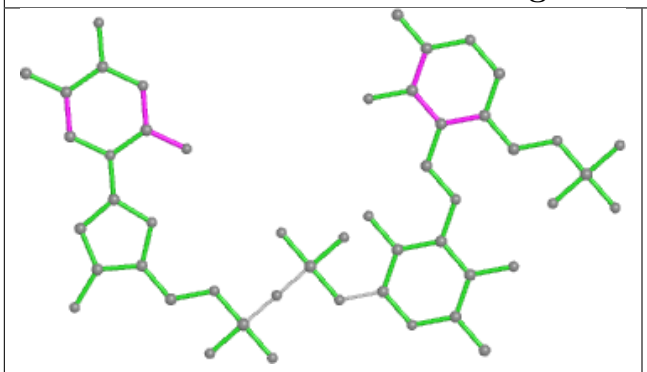
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	7SG	1	0
4	D	403	EDO	1	0
4	A	405	EDO	1	0
3	C	402	7SG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

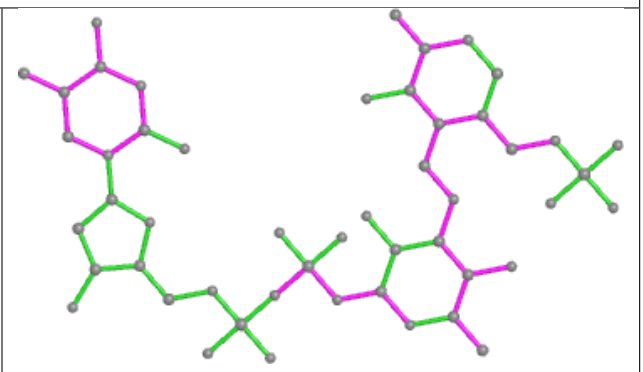
Ligand 7SG B 401



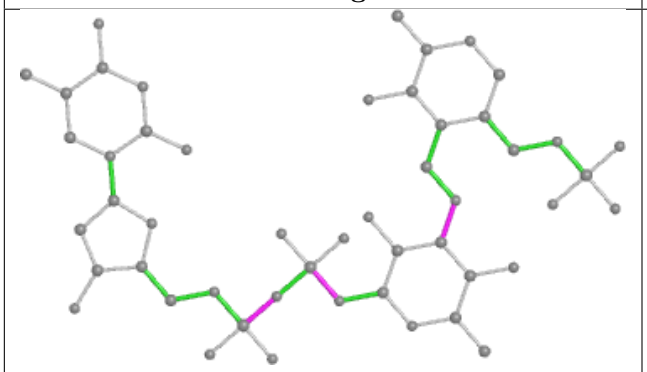
Ligand 7SG A 402



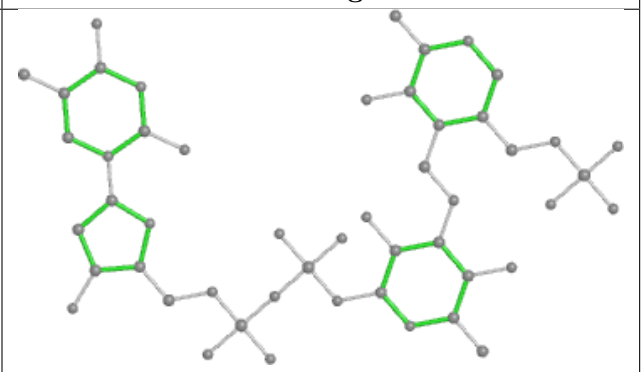
Bond lengths



Bond angles

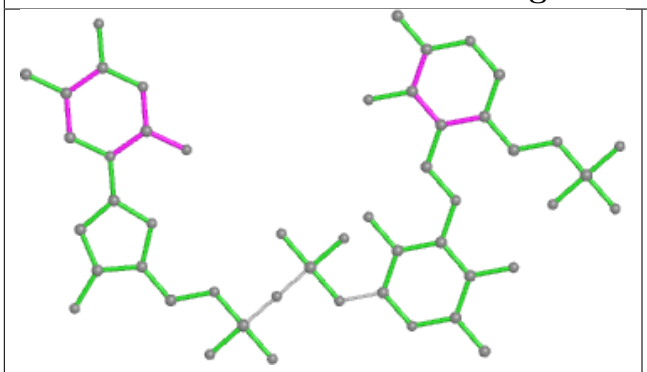


Torsions

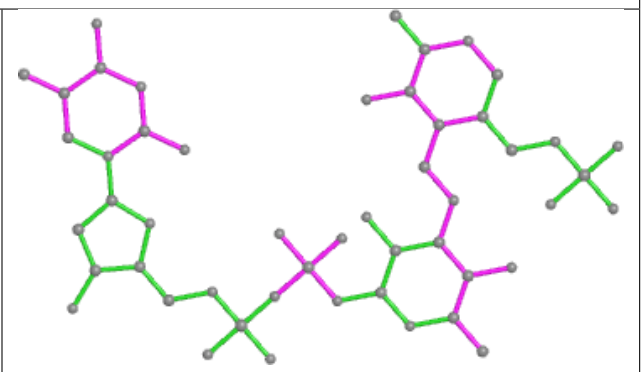


Rings

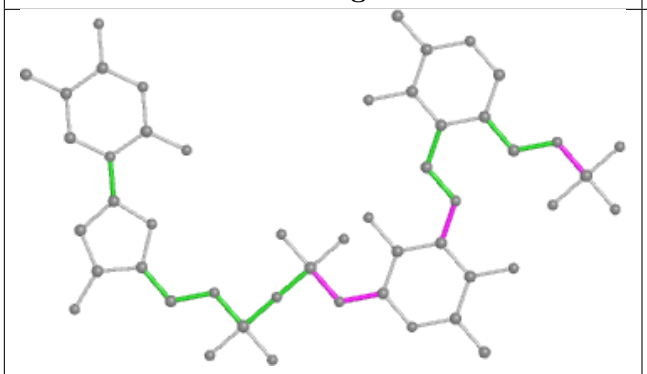
Ligand 7SG C 402



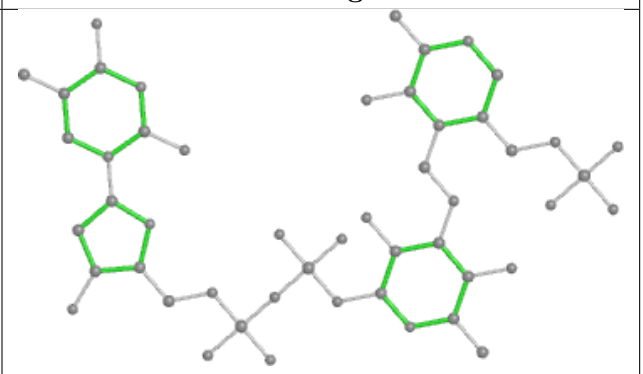
Bond lengths



Bond angles

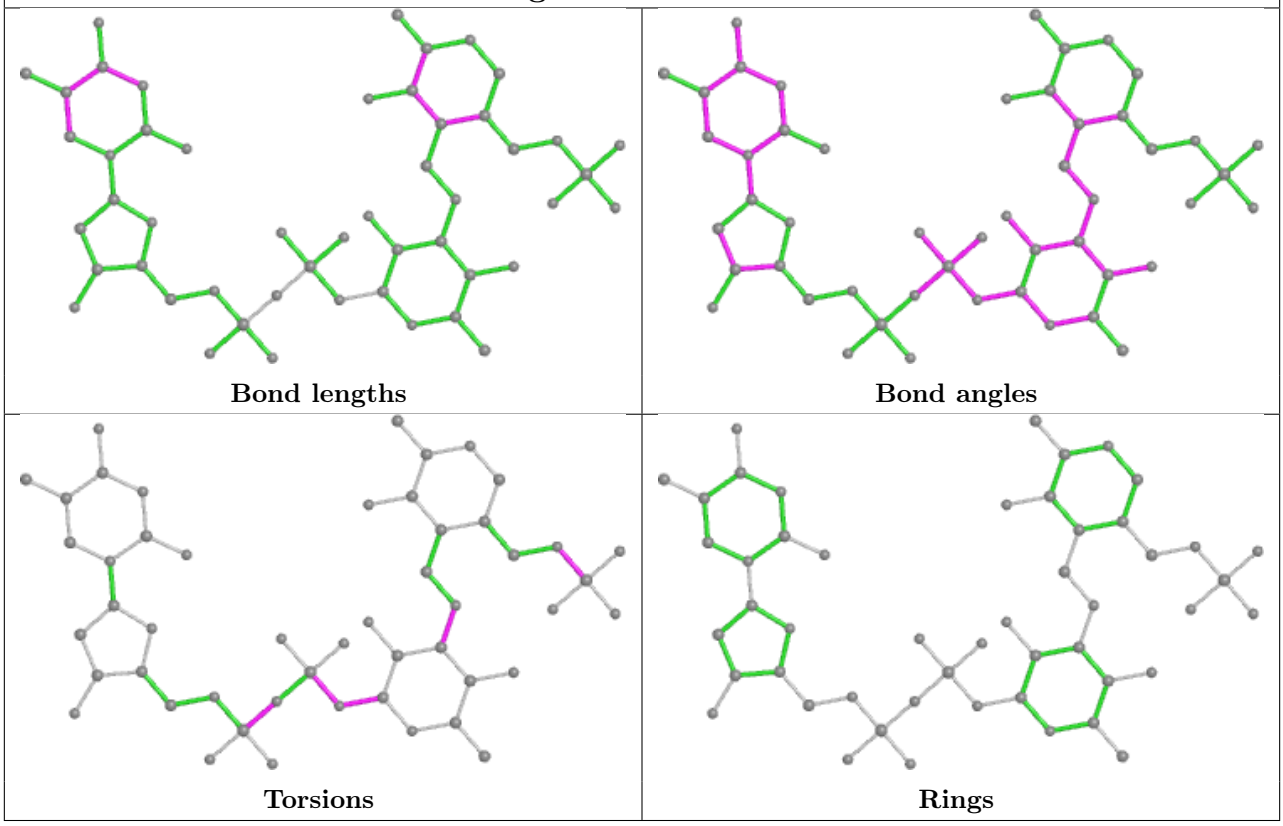


Torsions



Rings

Ligand 7SG D 401



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	361/382 (94%)	-0.45	2 (0%)	89	91	10, 17, 29, 68	0
1	B	362/382 (94%)	-0.39	4 (1%)	80	83	11, 18, 34, 66	0
1	C	361/382 (94%)	-0.42	1 (0%)	94	94	10, 17, 31, 43	0
1	D	361/382 (94%)	-0.40	2 (0%)	89	91	10, 17, 32, 44	0
All	All	1445/1528 (94%)	-0.41	9 (0%)	89	91	10, 17, 32, 68	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	VAL	5.1
1	D	360	VAL	3.7
1	B	-1	GLY	3.2
1	C	360	VAL	2.6
1	B	2	PHE	2.5
1	A	360	VAL	2.4
1	B	0	HIS	2.4
1	A	318	ASP	2.1
1	D	2	PHE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

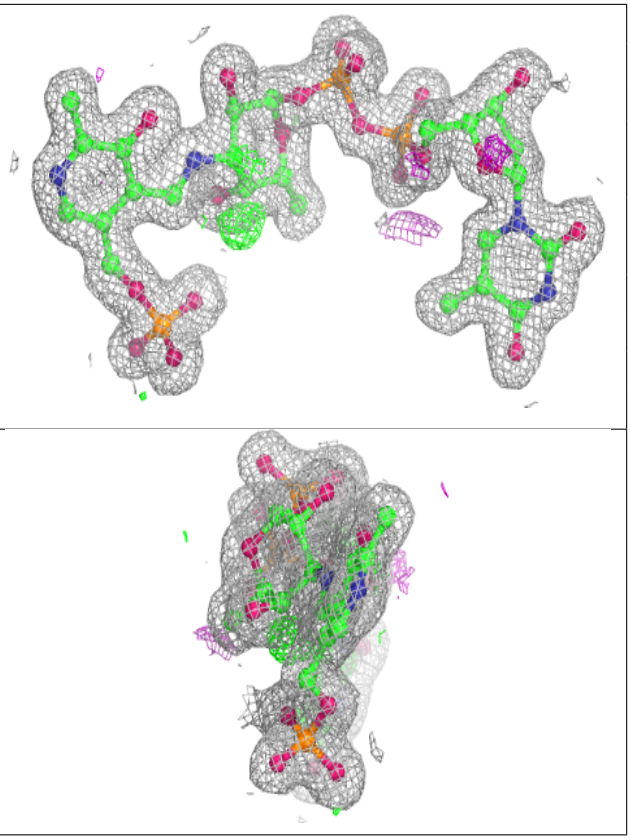
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	402	4/4	0.90	0.09	31,33,34,35	0
4	EDO	B	403	4/4	0.94	0.12	19,23,25,28	0
4	EDO	A	405	4/4	0.96	0.08	25,29,31,37	0
4	EDO	D	403	4/4	0.96	0.10	17,17,18,20	0
3	7SG	C	402	50/50	0.97	0.08	11,15,19,27	0
3	7SG	D	401	50/50	0.97	0.07	10,17,22,28	0
4	EDO	C	403	4/4	0.97	0.08	21,23,26,37	0
4	EDO	D	402	4/4	0.97	0.08	17,21,26,28	0
3	7SG	B	401	50/50	0.97	0.07	12,17,22,30	0
3	7SG	A	402	50/50	0.98	0.07	10,14,19,23	0
4	EDO	A	403	4/4	0.98	0.06	19,20,21,21	0
2	NA	A	401	1/1	0.99	0.08	14,14,14,14	0
4	EDO	A	404	4/4	0.99	0.05	15,17,18,19	0
2	NA	C	401	1/1	1.00	0.07	11,11,11,11	0
5	CL	A	406	1/1	1.00	0.03	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

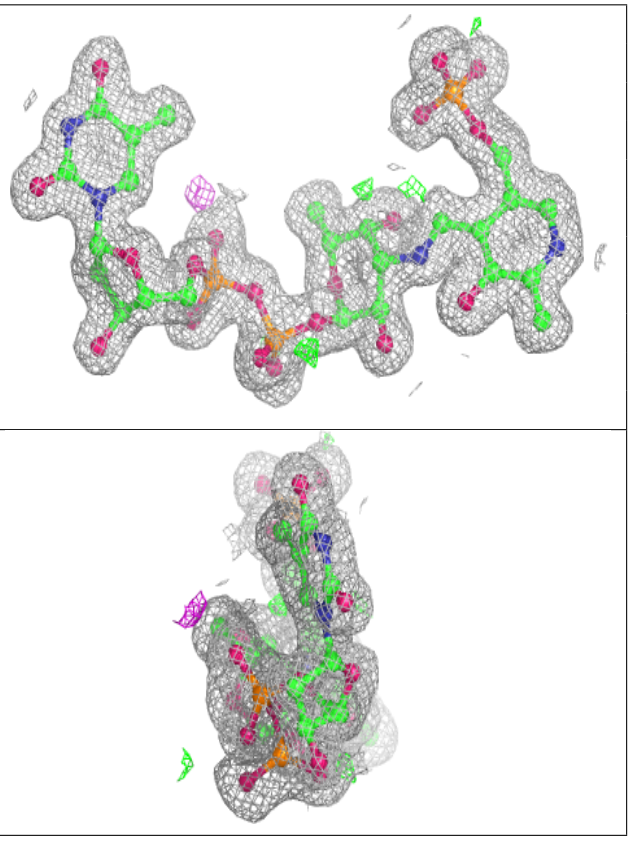
Electron density around 7SG C 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



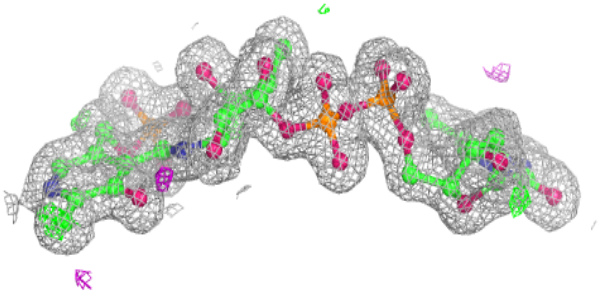
Electron density around 7SG D 401:

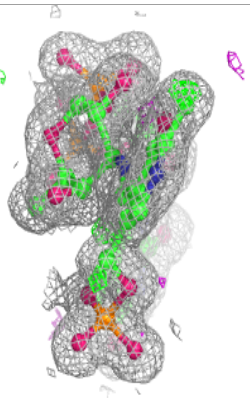
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7SG B 401:

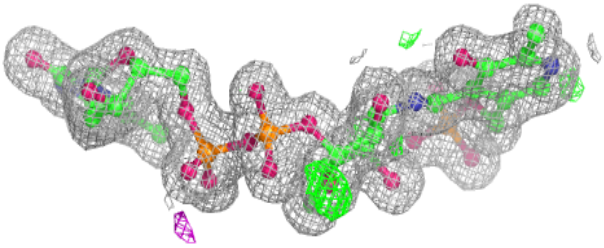
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

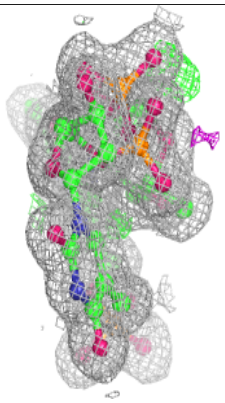




Electron density around 7SG A 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.