Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 09:11 PM EDT

PDB ID	:	5NFV
Title	:	Crystal structure of catalytically inactive FnCas12 mutant bound to an R-loop structure containing a pre-crRNA mimic and full-length DNA target
Authors	:	Swarts, D.C.; van der Oost, J.; Jinek, M.
Deposited on	:	2017-03-16
Resolution	:	2.50 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:

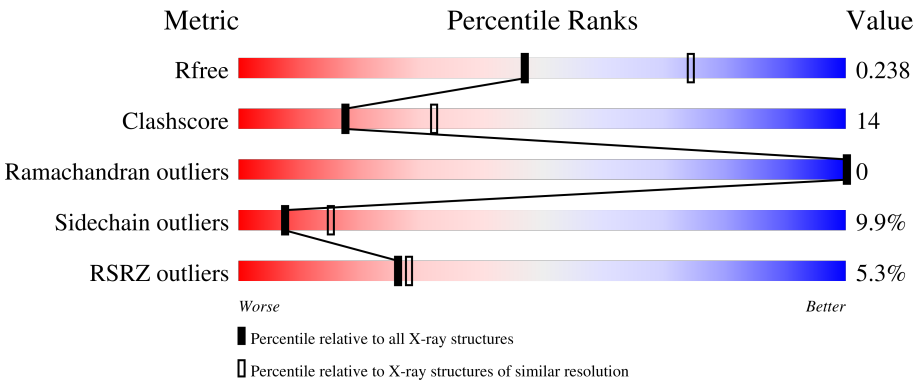
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	1302	5%, 65%, 27%, • •
2	B	46	52%, 39%, 9%
3	C	38	24%, 76%
4	D	38	8%, 32%, 32%, •, 34%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12573 atoms, of which 26 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 CRISPR-associated endonuclease Cpf1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1258	10387	6675	1712	1979	21	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0Q7Q2
A	0	ASN	-	expression tag	UNP A0Q7Q2
A	1	ALA	-	expression tag	UNP A0Q7Q2
A	1006	GLN	GLU	engineered mutation	UNP A0Q7Q2
A	1218	ALA	ARG	engineered mutation	UNP A0Q7Q2

- Molecule 2 is DNA/RNA hybrid called pre-crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	42	850	380	143	286	41	0	0	1

- Molecule 3 is a DNA chain called DNA target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	38	759	365	133	224	37	0	0	0

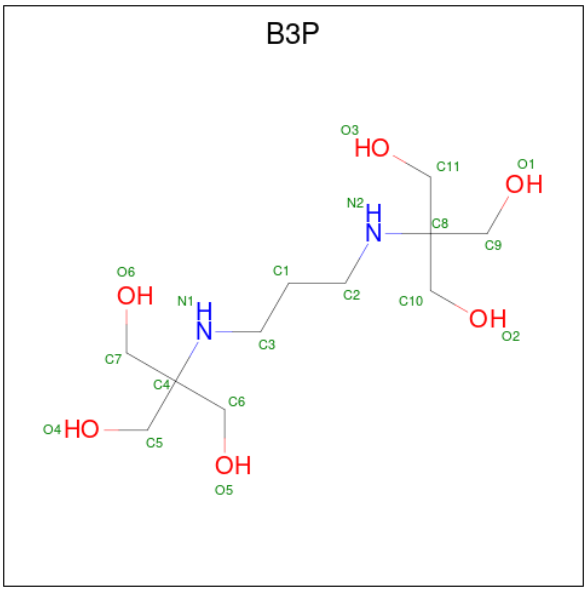
- Molecule 4 is a DNA chain called DNA non-target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	25	487	235	86	143	23	0	0	1

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	2	2	2	0	0
			Total	Mg		
5	B	1	1	1	0	0

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
6	A	1	45	11	26	2	6	0	0

- Molecule 7 is water.

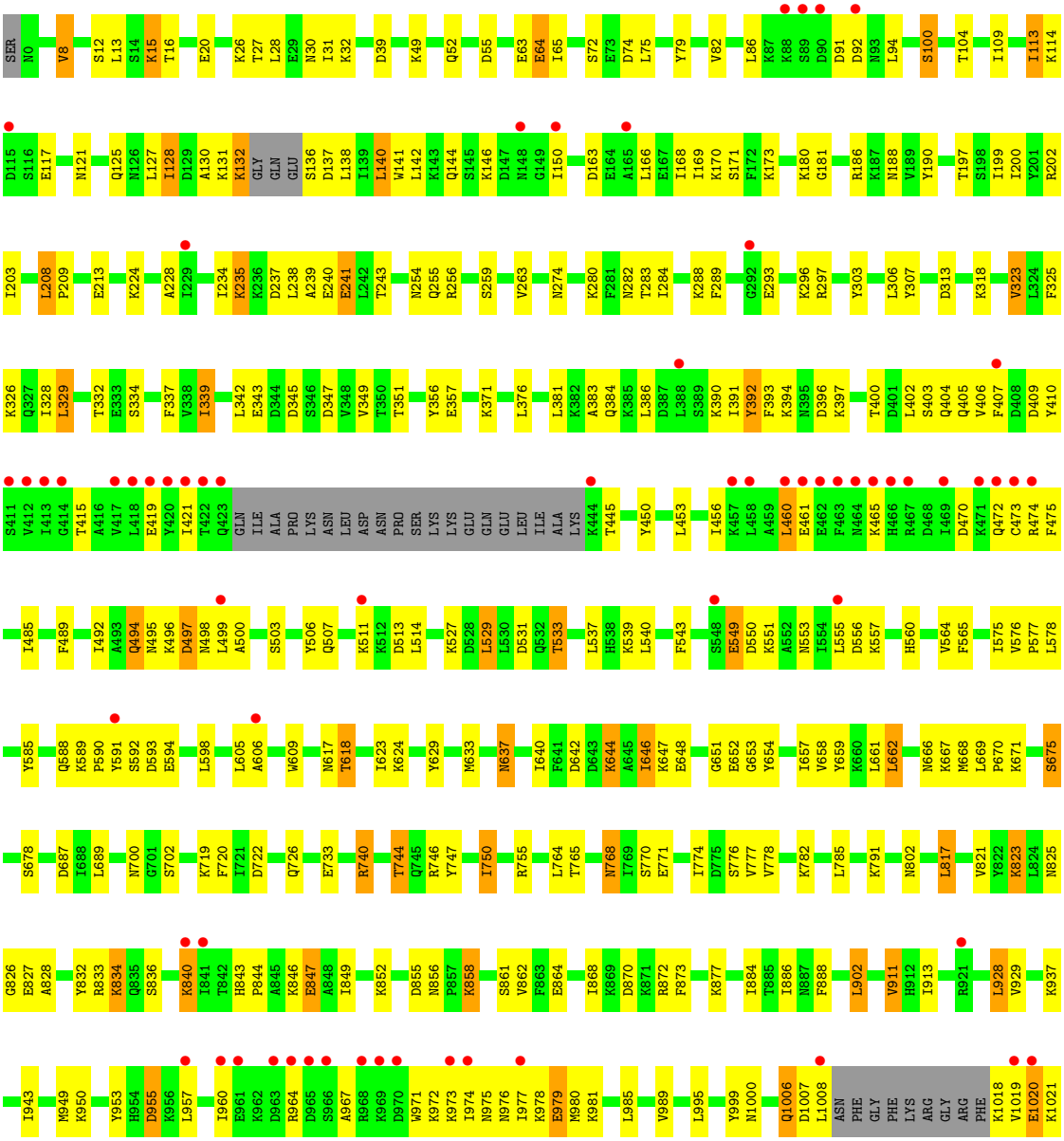
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	17	17	17	0	0
			Total	O		
7	B	19	19	19	0	0
			Total	O		
7	C	3	3	3	0	0
			Total	O		
7	D	3	3	3	0	0

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.

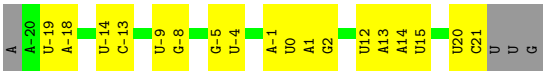
- Molecule 1: CRISPR-associated endonuclease Cpf1

Chain A:



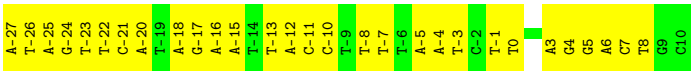
- Molecule 2: pre-crRNA

Chain B:



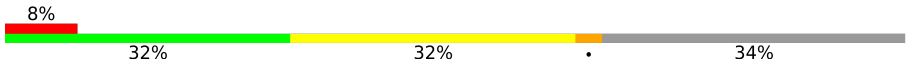
- Molecule 3: DNA target strand

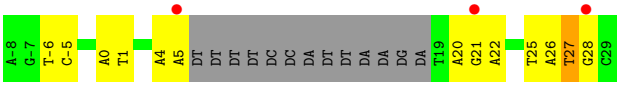
Chain C:



- Molecule 4: DNA non-target strand

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.42Å 143.70Å 84.63Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	46.57 – 2.50 46.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.57-2.50) 98.9 (46.57-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.205 , 0.238 0.206 , 0.238	Depositor DCC
R_{free} test set	3357 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12573	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: MG, B3P

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	0.27	0/10590	0.43	0/14215
2	B	1.63	14/949 (1.5%)	1.01	6/1476 (0.4%)
3	C	0.65	0/850	0.99	0/1311
4	D	0.67	0/544	0.99	1/836 (0.1%)
All	All	0.55	14/12933 (0.1%)	0.59	7/17838 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	-19	DU	C3'-C2'	-25.69	1.21	1.52
2	B	-19	DU	C4'-O4'	-17.15	1.27	1.45
2	B	-19	DU	C5-C6	16.86	1.49	1.34
2	B	-19	DU	C2-N3	15.26	1.48	1.37
2	B	-19	DU	N1-C2	12.90	1.50	1.38
2	B	-19	DU	C4-O4	-12.43	1.13	1.23
2	B	-19	DU	C4'-C3'	12.10	1.65	1.53
2	B	-19	DU	N1-C6	10.55	1.47	1.38
2	B	-19	DU	C1'-N1	-9.06	1.34	1.47
2	B	-19	DU	N3-C4	8.99	1.46	1.38
2	B	-19	DU	C4-C5	8.03	1.50	1.43
2	B	-19	DU	C3'-O3'	6.75	1.52	1.44
2	B	-19	DU	C2'-C1'	6.01	1.58	1.52
2	B	-19	DU	O4'-C1'	5.33	1.48	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	-19	DU	C2-N3-C4	-11.26	120.24	127.00
2	B	-19	DU	N1-C2-N3	9.64	120.68	114.90
2	B	-19	DU	C5-C4-O4	-9.23	120.36	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	-19	DU	N3-C4-C5	8.09	119.45	114.60
2	B	-19	DU	OP1-P-OP2	-6.13	110.40	119.60
2	B	-19	DU	C5-C6-N1	-5.83	119.78	122.70
4	D	27	DT	N3-C4-O4	5.45	123.17	119.90

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	10387	0	10361	277	1
2	B	850	0	420	22	0
3	C	759	0	422	32	0
4	D	487	0	275	24	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	19	26	26	1	0
7	A	17	0	0	3	0
7	B	19	0	0	1	0
7	C	3	0	0	0	0
7	D	3	0	0	2	0
All	All	12547	26	11504	329	1

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 14.

All (329) 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:1006:GLN:HG3	1:A:1079:ALA:HB2	1.15	1.13
1:A:576:VAL:HG22	1:A:577:PRO:HD3	1.46	0.97
1:A:403:SER:OG	1:A:409:ASP:O	1.83	0.95
1:A:960:ILE:HG23	1:A:977:ILE:HG12	1.51	0.93
1:A:913:ILE:HD12	1:A:1267:LEU:HD22	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:-5:DC:N4	7:D:101:HOH:O	2.06	0.89
1:A:400:THR:HG23	1:A:410:TYR:HB2	1.59	0.84
3:C:-25:DA:H2	4:D:25:DT:H3	1.25	0.83
1:A:964:ARG:HG2	1:A:977:ILE:HD13	1.61	0.82
1:A:170:LYS:O	1:A:173:LYS:HG3	1.79	0.81
1:A:1019:VAL:O	1:A:1022:GLN:HG2	1.80	0.81
1:A:1006:GLN:CG	1:A:1079:ALA:HB2	2.06	0.80
1:A:27:THR:HG21	1:A:785:LEU:H	1.46	0.79
1:A:960:ILE:HG21	1:A:977:ILE:HG23	1.65	0.77
1:A:823:LYS:HD3	1:A:888:PHE:CE1	2.19	0.77
4:D:20:DA:H1'	4:D:21:DG:O5'	1.86	0.76
1:A:1088:VAL:HG23	1:A:1089:THR:HG23	1.67	0.76
1:A:15:LYS:HG2	2:B:1:A:H5"	1.68	0.76
1:A:964:ARG:HG2	1:A:977:ILE:CD1	2.16	0.75
1:A:976:ASN:O	1:A:980:MET:HG3	1.86	0.75
3:C:-27:DA:N3	3:C:-27:DA:H5"	2.01	0.75
1:A:827:GLU:HG3	3:C:-1:DT:H4'	1.67	0.75
1:A:640:ILE:HG21	1:A:777:VAL:HG21	1.69	0.74
1:A:511:LYS:HE2	1:A:513:ASP:HB2	1.68	0.73
1:A:392:TYR:OH	1:A:556:ASP:O	2.06	0.72
1:A:394:LYS:HE3	1:A:396:ASP:OD2	1.90	0.72
1:A:140:LEU:O	1:A:144:GLN:HG2	1.91	0.71
3:C:-26:DT:H4'	3:C:-25:DA:OP1	1.90	0.71
4:D:4:DA:H1'	4:D:5:DA:N3	2.05	0.71
1:A:973:LYS:HD3	1:A:975:ASN:HD21	1.54	0.70
1:A:393:PHE:CZ	1:A:453:LEU:HD21	2.27	0.70
1:A:400:THR:HG21	3:C:-20:DA:H62	1.56	0.69
1:A:955:ASP:OD2	1:A:955:ASP:N	2.20	0.69
1:A:943:ILE:HD11	1:A:950:LYS:HD3	1.75	0.69
1:A:872:ARG:NH2	2:B:-13:C:OP2	2.24	0.69
1:A:1174:LEU:HG	1:A:1210:VAL:HG11	1.75	0.69
1:A:127:LEU:HB3	1:A:128:ILE:HD13	1.74	0.68
1:A:964:ARG:CG	1:A:977:ILE:HD13	2.24	0.68
1:A:421:ILE:HG21	1:A:445:THR:HG21	1.74	0.68
1:A:235:LYS:HE3	1:A:259:SER:HA	1.76	0.68
1:A:1191:ILE:HG22	1:A:1195:ILE:HG13	1.75	0.68
1:A:1183:ILE:HD12	1:A:1194:ALA:HB1	1.74	0.67
4:D:4:DA:OP2	4:D:4:DA:H2'	1.94	0.67
1:A:405:GLN:HE22	1:A:539:LYS:HE2	1.60	0.67
1:A:55:ASP:OD1	1:A:186:ARG:NH1	2.27	0.67
1:A:234:ILE:HD12	1:A:235:LYS:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:HD21	1:A:475:PHE:HD1	1.60	0.66
1:A:1283:ASN:OD1	1:A:1285:VAL:HG12	1.95	0.66
4:D:5:DA:H5"	4:D:5:DA:H8	1.61	0.66
4:D:4:DA:H1'	4:D:5:DA:C2	2.31	0.65
1:A:16:THR:HG23	2:B:1:A:N3	2.11	0.65
1:A:132:LYS:HZ2	1:A:136:SER:N	1.95	0.65
1:A:973:LYS:HD3	1:A:975:ASN:ND2	2.12	0.65
1:A:774:ILE:O	1:A:778:VAL:HG12	1.97	0.64
4:D:5:DA:H5"	4:D:5:DA:C8	2.32	0.64
1:A:974:ILE:CG2	1:A:977:ILE:HD12	2.27	0.64
1:A:168:ILE:O	1:A:171:SER:OG	2.13	0.64
1:A:1026:LYS:NZ	3:C:-7:DT:OP1	2.30	0.64
1:A:224:LYS:NZ	1:A:313:ASP:OD2	2.31	0.64
1:A:345:ASP:OD1	1:A:585:TYR:OH	2.14	0.64
1:A:1118:ASN:ND2	1:A:1121:LYS:H	1.95	0.64
1:A:296:LYS:HE3	3:C:-15:DA:H2"	1.80	0.63
4:D:26:DA:H8	4:D:28:DG:O6	1.81	0.63
1:A:456:ILE:O	1:A:460:LEU:HD23	1.99	0.63
1:A:606:ALA:HB3	1:A:828:ALA:O	1.98	0.63
1:A:624:LYS:HD2	1:A:654:TYR:CZ	2.34	0.63
1:A:1172:LYS:O	1:A:1176:LYS:HD3	1.98	0.63
2:B:-1:A:C2'	2:B:0:U:H5'	2.29	0.63
1:A:27:THR:CG2	1:A:785:LEU:H	2.11	0.62
1:A:1268:MET:HE3	1:A:1286:ILE:HD13	1.82	0.62
3:C:4:DG:H1'	3:C:5:DG:H5'	1.81	0.62
1:A:605:LEU:O	1:A:617:ASN:O	2.17	0.62
1:A:960:ILE:HD11	1:A:980:MET:CE	2.30	0.62
1:A:911:VAL:HG22	1:A:1270:LEU:HD11	1.81	0.62
1:A:128:ILE:HG22	1:A:169:ILE:HG23	1.83	0.61
1:A:1242:ASP:OD1	1:A:1244:ARG:NH1	2.26	0.61
1:A:844:PRO:HG2	1:A:847:GLU:HG3	1.84	0.60
1:A:618:THR:HG23	1:A:618:THR:O	2.01	0.60
1:A:576:VAL:CG2	1:A:577:PRO:HD3	2.28	0.60
1:A:637:ASN:N	1:A:637:ASN:OD1	2.35	0.60
1:A:678:SER:HB2	7:A:1506:HOH:O	2.00	0.60
1:A:960:ILE:CG2	1:A:977:ILE:HG12	2.29	0.59
4:D:28:DG:H8	4:D:28:DG:H3'	1.67	0.59
1:A:12:SER:OG	6:A:1403:B3P:H51	2.02	0.59
1:A:967:ALA:HB1	1:A:972:LYS:HD3	1.84	0.59
1:A:16:THR:HG21	2:B:2:G:H1'	1.84	0.59
1:A:960:ILE:CG2	1:A:977:ILE:HG23	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:DA:H2"	3:C:7:DC:O4'	2.02	0.59
1:A:1006:GLN:HG3	1:A:1079:ALA:CB	2.09	0.59
1:A:289:PHE:CE1	1:A:296:LYS:HB2	2.38	0.58
1:A:405:GLN:NE2	1:A:539:LYS:HE2	2.18	0.58
4:D:27:DT:H5'	4:D:28:DG:OP1	2.03	0.58
1:A:142:LEU:HD23	1:A:166:LEU:HD22	1.84	0.58
1:A:590:PRO:HG2	1:A:973:LYS:NZ	2.19	0.58
1:A:1260:TYR:OH	1:A:1298:ARG:NH2	2.37	0.58
4:D:20:DA:C1'	4:D:21:DG:O5'	2.50	0.58
1:A:356:TYR:HB3	1:A:496:LYS:HD2	1.87	0.57
1:A:383:ALA:O	1:A:384:GLN:HB2	2.05	0.57
3:C:6:DA:H2'	3:C:7:DC:C6	2.40	0.57
1:A:91:ASP:HB3	1:A:94:LEU:HG	1.87	0.57
3:C:-17:DG:H2'	3:C:-16:DA:C8	2.40	0.57
1:A:913:ILE:HB	1:A:929:VAL:HG22	1.88	0.56
1:A:1086:CYS:SG	1:A:1088:VAL:HG22	2.45	0.56
3:C:-27:DA:H2"	3:C:-26:DT:O5'	2.06	0.56
1:A:26:LYS:O	1:A:30:ASN:ND2	2.38	0.56
3:C:3:DA:H2"	3:C:4:DG:H5'	1.87	0.56
1:A:243:THR:O	1:A:280:LYS:NZ	2.35	0.56
1:A:823:LYS:NZ	1:A:825:ASN:OD1	2.35	0.55
1:A:28:LEU:HD11	1:A:32:LYS:HE3	1.88	0.55
3:C:-12:DA:H2'	3:C:-11:DC:C6	2.42	0.55
1:A:527:LYS:HD2	1:A:971:TRP:CD2	2.42	0.55
1:A:63:GLU:OE2	1:A:274:ASN:ND2	2.40	0.55
1:A:328:ILE:O	1:A:329:LEU:HB2	2.07	0.55
1:A:1138:ALA:O	1:A:1139:LYS:HG2	2.07	0.55
1:A:127:LEU:O	1:A:136:SER:OG	2.21	0.55
1:A:1269:LEU:HD13	1:A:1286:ILE:HD11	1.88	0.55
1:A:1048:THR:HA	1:A:1053:ARG:HB3	1.89	0.54
1:A:20:GLU:OE2	1:A:877:LYS:HG2	2.07	0.54
1:A:1119:LEU:HD21	1:A:1186:GLY:O	2.07	0.54
1:A:15:LYS:HG2	2:B:1:A:C5'	2.36	0.54
1:A:543:PHE:HB2	1:A:565:PHE:CZ	2.43	0.54
2:B:15:U:O4	7:B:201:HOH:O	2.17	0.54
1:A:642:ASP:O	1:A:646:ILE:HG23	2.07	0.54
1:A:687:ASP:OD2	1:A:719:LYS:NZ	2.28	0.54
4:D:28:DG:H3'	4:D:28:DG:C8	2.42	0.54
3:C:-1:DT:H5"	3:C:0:DT:H5"	1.90	0.54
1:A:15:LYS:CG	2:B:1:A:H5"	2.36	0.53
1:A:125:GLN:OE1	1:A:131:LYS:HE3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-17:DG:H2'	3:C:-16:DA:H8	1.72	0.53
1:A:460:LEU:HD11	1:A:475:PHE:N	2.24	0.53
1:A:722:ASP:OD2	1:A:744:THR:HG21	2.09	0.53
1:A:870:ASP:HB3	1:A:873:PHE:HD2	1.73	0.53
1:A:1260:TYR:O	1:A:1264:LEU:HD23	2.09	0.53
1:A:188:ASN:HB3	1:A:197:THR:OG1	2.08	0.53
1:A:884:ILE:HD11	1:A:886:ILE:HD11	1.91	0.53
1:A:334:SER:OG	3:C:-13:DT:OP1	2.18	0.53
1:A:1209:SER:O	1:A:1213:THR:HG22	2.09	0.53
1:A:141:TRP:CE3	1:A:142:LEU:HD12	2.43	0.53
1:A:202:ARG:NH1	1:A:326:LYS:O	2.42	0.52
1:A:928:LEU:HD11	1:A:999:TYR:CG	2.43	0.52
1:A:337:PHE:CE2	1:A:339:ILE:HD13	2.44	0.52
1:A:404:GLN:HE21	1:A:410:TYR:N	2.08	0.52
1:A:1018:LYS:O	1:A:1021:LYS:HG2	2.10	0.52
1:A:722:ASP:O	1:A:726:GLN:HG3	2.09	0.52
1:A:1264:LEU:HD12	1:A:1294:PHE:HE2	1.75	0.52
3:C:-18:DA:H2'	3:C:-17:DG:H8	1.74	0.52
1:A:827:GLU:HG3	3:C:-1:DT:C4'	2.36	0.52
1:A:492:ILE:HG23	1:A:529:LEU:HD21	1.92	0.52
4:D:1:DT:OP1	7:D:102:HOH:O	2.18	0.52
2:B:-1:A:O2'	2:B:0:U:H5'	2.10	0.52
1:A:407:PHE:CD1	1:A:473:CYS:HB3	2.45	0.51
1:A:644:LYS:O	1:A:648:GLU:HG2	2.09	0.51
1:A:840:LYS:O	1:A:868:ILE:HG23	2.09	0.51
1:A:985:LEU:O	1:A:989:VAL:HG13	2.09	0.51
1:A:394:LYS:HD3	1:A:450:TYR:CE1	2.45	0.51
1:A:1265:LYS:HA	1:A:1268:MET:HE3	1.92	0.51
1:A:402:LEU:O	1:A:406:VAL:HG12	2.11	0.51
1:A:976:ASN:ND2	1:A:979:GLU:OE1	2.44	0.51
1:A:618:THR:HA	1:A:633:MET:HE2	1.92	0.51
1:A:1118:ASN:HD22	1:A:1121:LYS:H	1.59	0.51
1:A:973:LYS:HD3	1:A:975:ASN:OD1	2.11	0.50
1:A:91:ASP:OD1	1:A:92:ASP:N	2.44	0.50
1:A:1265:LYS:HA	1:A:1268:MET:CE	2.41	0.50
1:A:576:VAL:HG22	1:A:577:PRO:CD	2.30	0.50
1:A:669:LEU:HB2	1:A:670:PRO:HD3	1.91	0.50
1:A:843:HIS:CE1	1:A:849:ILE:HG23	2.47	0.50
1:A:1155:ARG:NH2	3:C:-24:DG:O6	2.45	0.50
1:A:109:ILE:O	1:A:113:ILE:HG23	2.12	0.50
1:A:200:ILE:HD12	1:A:200:ILE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:CB	1:A:132:LYS:HD2	2.41	0.50
1:A:130:ALA:HB1	1:A:132:LYS:HD2	1.94	0.49
1:A:237:ASP:HB3	1:A:297:ARG:HB3	1.94	0.49
1:A:495:ASN:HA	1:A:498:ASN:ND2	2.26	0.49
1:A:964:ARG:CD	1:A:977:ILE:HD13	2.42	0.49
1:A:293:GLU:OE2	1:A:297:ARG:NH1	2.45	0.49
1:A:836:SER:OG	1:A:873:PHE:HB3	2.11	0.49
1:A:240:GLU:HB3	1:A:241:GLU:OE2	2.13	0.49
2:B:20:U:H5'	2:B:21:C:OP2	2.12	0.49
1:A:957:LEU:HD11	1:A:981:LYS:HG2	1.94	0.49
1:A:1146:SER:OG	1:A:1171:THR:HB	2.12	0.49
2:B:1:A:H1'	2:B:2:G:C8	2.48	0.48
1:A:646:ILE:HG12	1:A:647:LYS:N	2.28	0.48
1:A:15:LYS:CG	2:B:1:A:C5'	2.92	0.48
1:A:1038:LEU:HB3	1:A:1055:TYR:HB2	1.95	0.48
1:A:640:ILE:CG2	1:A:777:VAL:HG21	2.41	0.48
1:A:342:LEU:HD22	1:A:347:ASP:HB3	1.95	0.48
1:A:498:ASN:OD1	1:A:499:LEU:N	2.46	0.48
1:A:506:TYR:CE1	1:A:514:LEU:HD13	2.48	0.48
1:A:351:THR:HG22	1:A:578:LEU:HD13	1.96	0.48
1:A:744:THR:HA	1:A:747:TYR:CD1	2.49	0.48
4:D:21:DG:H2"	4:D:22:DA:OP2	2.13	0.48
1:A:82:VAL:O	1:A:86:LEU:HG	2.14	0.48
1:A:296:LYS:HE3	3:C:-15:DA:C2'	2.44	0.47
1:A:653:GLY:HA3	1:A:771:GLU:N	2.29	0.47
3:C:-16:DA:H2'	3:C:-15:DA:H5"	1.96	0.47
1:A:114:LYS:NZ	1:A:190:TYR:O	2.47	0.47
1:A:667:LYS:HD3	4:D:1:DT:O2	2.14	0.47
4:D:28:DG:C8	4:D:28:DG:C3'	2.95	0.47
1:A:592:SER:O	1:A:594:GLU:HG2	2.14	0.47
1:A:949:MET:O	1:A:950:LYS:HG3	2.13	0.47
1:A:202:ARG:NH1	1:A:325:PHE:HB3	2.29	0.47
1:A:1006:GLN:NE2	1:A:1008:LEU:HD21	2.29	0.47
1:A:113:ILE:HD11	1:A:190:TYR:HB3	1.97	0.47
1:A:858:LYS:NZ	1:A:861:SER:OG	2.47	0.47
1:A:957:LEU:CD1	1:A:981:LYS:HG2	2.45	0.47
1:A:8:VAL:HG11	1:A:1053:ARG:HG3	1.97	0.46
1:A:394:LYS:HG2	1:A:450:TYR:CE1	2.50	0.46
1:A:494:GLN:H	1:A:494:GLN:HG3	1.48	0.46
4:D:4:DA:H1'	4:D:5:DA:C4	2.50	0.46
1:A:404:GLN:HE21	1:A:410:TYR:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HE21	1:A:474:ARG:HE	1.63	0.46
1:A:750:ILE:HG22	7:A:1512:HOH:O	2.15	0.46
2:B:-9:U:H4'	2:B:-8:G:O5'	2.14	0.46
2:B:-5:G:H2'	2:B:-4:U:H5'	1.97	0.46
1:A:100:SER:O	1:A:104:THR:HG23	2.15	0.46
1:A:337:PHE:HE2	1:A:339:ILE:HD13	1.81	0.46
1:A:624:LYS:HD2	1:A:654:TYR:CE1	2.51	0.46
1:A:802:ASN:HB3	2:B:0:U:O4	2.16	0.46
1:A:817:LEU:HD12	1:A:817:LEU:HA	1.83	0.46
1:A:598:LEU:HD11	1:A:832:TYR:HB2	1.97	0.45
1:A:974:ILE:HG21	1:A:977:ILE:HD12	1.97	0.45
1:A:228:ALA:HA	1:A:307:TYR:CD1	2.51	0.45
1:A:667:LYS:HG2	4:D:1:DT:O4'	2.17	0.45
1:A:823:LYS:HD3	1:A:888:PHE:CD1	2.52	0.45
1:A:1121:LYS:HB3	1:A:1123:TYR:CE1	2.51	0.45
3:C:-5:DA:H2"	3:C:-4:DA:H8	1.81	0.45
1:A:64:GLU:HG3	1:A:65:ILE:N	2.31	0.45
1:A:497:ASP:O	1:A:500:ALA:HB3	2.17	0.45
1:A:856:ASN:ND2	2:B:-9:U:H5"	2.31	0.45
1:A:884:ILE:CD1	1:A:886:ILE:HD11	2.47	0.45
3:C:-8:DT:H2'	3:C:-7:DT:C6	2.51	0.45
1:A:72:SER:HB3	1:A:75:LEU:HG	1.99	0.45
1:A:390:LYS:O	1:A:557:LYS:HA	2.16	0.45
1:A:235:LYS:O	1:A:239:ALA:HB2	2.17	0.45
1:A:1151:LEU:HB2	1:A:1219:ASN:HB3	1.98	0.45
3:C:-25:DA:H2	4:D:25:DT:N3	2.03	0.45
3:C:-15:DA:H5"	3:C:-15:DA:H8	1.81	0.45
1:A:472:GLN:NE2	1:A:474:ARG:HE	2.14	0.44
1:A:527:LYS:HD2	1:A:971:TRP:CG	2.53	0.44
1:A:886:ILE:HG21	1:A:1037:TYR:CZ	2.52	0.44
1:A:234:ILE:HG23	1:A:303:TYR:HE2	1.81	0.44
1:A:259:SER:O	1:A:263:VAL:HG13	2.18	0.44
1:A:407:PHE:CE1	1:A:473:CYS:HB3	2.53	0.44
1:A:671:LYS:HB2	4:D:0:DA:O4'	2.17	0.44
1:A:1189:GLU:H	1:A:1189:GLU:CD	2.21	0.44
1:A:637:ASN:ND2	1:A:782:LYS:HG2	2.32	0.44
1:A:651:GLY:HA3	1:A:770:SER:OG	2.17	0.44
3:C:-22:DT:H2"	3:C:-21:DC:C6	2.52	0.44
4:D:26:DA:C8	4:D:28:DG:O6	2.67	0.44
1:A:128:ILE:HD13	1:A:128:ILE:N	2.33	0.44
1:A:282:ASN:ND2	1:A:323:VAL:HG13	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ASN:HA	1:A:498:ASN:HD21	1.83	0.44
1:A:973:LYS:HD3	1:A:975:ASN:CG	2.38	0.44
1:A:1150:ARG:O	1:A:1151:LEU:HD12	2.17	0.44
1:A:768:ASN:OD1	1:A:768:ASN:N	2.51	0.44
1:A:1021:LYS:HG3	1:A:1022:GLN:N	2.33	0.44
1:A:241:GLU:OE1	1:A:288:LYS:HD3	2.18	0.43
1:A:609:TRP:O	1:A:659:TYR:HB3	2.18	0.43
2:B:-5:G:C2'	2:B:-4:U:H5'	2.48	0.43
1:A:27:THR:O	1:A:31:ILE:HG12	2.18	0.43
1:A:833:ARG:NH2	2:B:-14:U:OP1	2.51	0.43
1:A:1126:PHE:HB2	1:A:1144:ILE:HG12	1.99	0.43
1:A:415:THR:O	1:A:419:GLU:HG2	2.18	0.43
1:A:1006:GLN:HB2	1:A:1262:ILE:HD12	2.01	0.43
1:A:1150:ARG:NH1	1:A:1214:ILE:O	2.51	0.43
1:A:27:THR:HG21	1:A:785:LEU:N	2.23	0.43
2:B:13:A:H2'	2:B:14:A:C8	2.53	0.43
1:A:560:HIS:O	1:A:564:VAL:HG22	2.18	0.43
1:A:662:LEU:C	1:A:662:LEU:HD12	2.39	0.43
1:A:937:LYS:HE2	1:A:999:TYR:OH	2.19	0.43
1:A:345:ASP:O	1:A:349:VAL:HG22	2.19	0.43
1:A:180:LYS:HG3	1:A:181:GLY:N	2.34	0.43
1:A:589:LYS:HB2	3:C:-10:DC:H5"	1.99	0.43
1:A:1049:GLY:N	1:A:1053:ARG:O	2.47	0.43
4:D:-6:DT:H2"	4:D:-5:DC:C6	2.54	0.42
1:A:953:TYR:O	1:A:957:LEU:HD23	2.19	0.42
1:A:1019:VAL:HG13	1:A:1020:GLU:N	2.35	0.42
2:B:-1:A:H2'	2:B:0:U:H5'	2.01	0.42
4:D:25:DT:H1'	4:D:26:DA:H5'	2.01	0.42
1:A:485:ILE:HG21	1:A:540:LEU:HD21	2.01	0.42
1:A:49:LYS:HA	1:A:52:GLN:HE21	1.84	0.42
1:A:27:THR:HG23	1:A:778:VAL:CG2	2.50	0.42
1:A:1063:THR:HG22	1:A:1066:LYS:H	1.85	0.42
3:C:-24:DG:H2'	3:C:-23:DT:H72	2.00	0.42
1:A:658:VAL:CG2	1:A:765:THR:OG1	2.68	0.42
1:A:967:ALA:CB	1:A:972:LYS:HD3	2.50	0.42
1:A:533:THR:HB	1:A:575:ILE:CD1	2.49	0.42
1:A:777:VAL:HG22	1:A:782:LYS:HB2	2.01	0.42
1:A:911:VAL:HA	1:A:1000:ASN:O	2.19	0.42
2:B:12:U:H2'	2:B:13:A:C8	2.54	0.42
1:A:150:ILE:HG23	1:A:150:ILE:O	2.19	0.41
1:A:662:LEU:HD13	1:A:668:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:DC:C6	3:C:8:DT:H72	2.53	0.41
1:A:238:LEU:HD13	1:A:284:ILE:HA	2.02	0.41
3:C:-4:DA:H3'	3:C:-3:DT:H71	2.02	0.41
1:A:506:TYR:CZ	1:A:514:LEU:HD13	2.56	0.41
1:A:1088:VAL:HG23	1:A:1089:THR:N	2.35	0.41
1:A:886:ILE:CG2	1:A:1037:TYR:CZ	3.04	0.41
1:A:1087:PRO:HG3	1:A:1257:ASN:OD1	2.20	0.41
1:A:623:ILE:HG13	1:A:657:ILE:HD11	2.02	0.41
1:A:902:LEU:HD23	1:A:902:LEU:HA	1.85	0.41
1:A:588:GLN:HA	3:C:-11:DC:O3'	2.20	0.41
1:A:593:ASP:OD1	1:A:834:LYS:NZ	2.45	0.41
1:A:658:VAL:HG22	1:A:765:THR:OG1	2.20	0.41
1:A:661:LEU:HD13	1:A:823:LYS:HE3	2.01	0.41
1:A:371:LYS:HE2	1:A:489:PHE:HB3	2.02	0.41
1:A:392:TYR:CD1	1:A:392:TYR:N	2.89	0.41
1:A:618:THR:OG1	1:A:633:MET:HB2	2.20	0.41
1:A:675:SER:HB3	7:A:1506:HOH:O	2.20	0.41
1:A:1082:THR:O	1:A:1258:GLY:HA2	2.20	0.41
1:A:1113:ASP:O	1:A:1114:LYS:HG2	2.21	0.41
1:A:1183:ILE:HG21	1:A:1191:ILE:HG23	2.03	0.41
1:A:146:LYS:NZ	1:A:163:ASP:OD2	2.51	0.41
1:A:624:LYS:HB3	1:A:629:TYR:CE2	2.55	0.41
1:A:1206:LYS:HD2	1:A:1206:LYS:HA	1.82	0.41
1:A:241:GLU:OE1	1:A:283:THR:HG21	2.20	0.41
1:A:852:LYS:NZ	2:B:-18:A:OP2	2.30	0.41
1:A:1006:GLN:HE22	1:A:1008:LEU:HD21	1.86	0.41
1:A:208:LEU:HB3	1:A:209:PRO:HD3	2.03	0.41
1:A:394:LYS:HG2	1:A:450:TYR:HE1	1.84	0.41
1:A:1165:THR:CG2	1:A:1222:THR:HB	2.51	0.41
1:A:79:TYR:CE2	1:A:208:LEU:HD13	2.56	0.40
1:A:199:ILE:O	1:A:203:ILE:HG13	2.21	0.40
1:A:527:LYS:HG2	1:A:531:ASP:OD1	2.20	0.40
1:A:549:GLU:OE1	1:A:549:GLU:HA	2.21	0.40
1:A:339:ILE:H	1:A:339:ILE:HG12	1.56	0.40
1:A:1085:ILE:HG23	1:A:1261:HIS:CE1	2.56	0.40
1:A:826:GLY:O	1:A:827:GLU:HB2	2.21	0.40
1:A:1113:ASP:C	1:A:1114:LYS:HG2	2.42	0.40

All (1) 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)
1:A:357:GLU:OE1	1:A:740:ARG:NH2[2_8511]	2.11	0.09

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	1246/1302 (96%)	1220 (98%)	26 (2%)	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	1146/1184 (97%)	1033 (90%)	113 (10%)	8 15

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	13	LEU
1	A	15	LYS
1	A	39	ASP
1	A	64	GLU
1	A	74	ASP
1	A	100	SER
1	A	113	ILE

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Mol	Chain	Res	Type
1	A	117	GLU
1	A	121	ASN
1	A	128	ILE
1	A	132	LYS
1	A	137	ASP
1	A	138	LEU
1	A	140	LEU
1	A	208	LEU
1	A	213	GLU
1	A	235	LYS
1	A	241	GLU
1	A	254	ASN
1	A	255	GLN
1	A	256	ARG
1	A	306	LEU
1	A	318	LYS
1	A	323	VAL
1	A	329	LEU
1	A	332	THR
1	A	339	ILE
1	A	343	GLU
1	A	376	LEU
1	A	381	LEU
1	A	386	LEU
1	A	391	ILE
1	A	392	TYR
1	A	397	LYS
1	A	460	LEU
1	A	461	GLU
1	A	465	LYS
1	A	470	ASP
1	A	494	GLN
1	A	497	ASP
1	A	503	SER
1	A	507	GLN
1	A	529	LEU
1	A	533	THR
1	A	537	LEU
1	A	549	GLU
1	A	550	ASP
1	A	551	LYS
1	A	553	ASN

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Mol	Chain	Res	Type
1	A	555	LEU
1	A	591	TYR
1	A	618	THR
1	A	637	ASN
1	A	644	LYS
1	A	646	ILE
1	A	652	GLU
1	A	662	LEU
1	A	666	ASN
1	A	675	SER
1	A	689	LEU
1	A	700	ASN
1	A	702	SER
1	A	720	PHE
1	A	733	GLU
1	A	740	ARG
1	A	744	THR
1	A	746	ARG
1	A	750	ILE
1	A	755	ARG
1	A	764	LEU
1	A	768	ASN
1	A	776	SER
1	A	791	LYS
1	A	817	LEU
1	A	821	VAL
1	A	823	LYS
1	A	834	LYS
1	A	840	LYS
1	A	846	LYS
1	A	847	GLU
1	A	855	ASP
1	A	858	LYS
1	A	862	VAL
1	A	864	GLU
1	A	902	LEU
1	A	911	VAL
1	A	928	LEU
1	A	955	ASP
1	A	978	LYS
1	A	979	GLU
1	A	995	LEU

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Mol	Chain	Res	Type
1	A	1006	GLN
1	A	1007	ASP
1	A	1020	GLU
1	A	1022	GLN
1	A	1034	LYS
1	A	1053	ARG
1	A	1063	THR
1	A	1069	LYS
1	A	1084	LYS
1	A	1092	VAL
1	A	1101	SER
1	A	1103	SER
1	A	1116	CYS
1	A	1118	ASN
1	A	1150	ARG
1	A	1153	ASN
1	A	1171	THR
1	A	1176	LYS
1	A	1267	LEU
1	A	1270	LEU
1	A	1295	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	121	ASN
1	A	188	ASN
1	A	404	GLN
1	A	405	GLN
1	A	472	GLN
1	A	713	ASN
1	A	843	HIS
1	A	976	ASN
1	A	990	HIS
1	A	1118	ASN
1	A	1153	ASN
1	A	1296	GLN
1	A	1297	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
6	B3P	A	1403	-	18,18,18	0.49	0	21,23,23	1.04	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
6	B3P	A	1403	-	-	11/28/28/28	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1403	B3P	C5-C4-N1-C3
6	A	1403	B3P	C6-C4-N1-C3
6	A	1403	B3P	C7-C4-N1-C3
6	A	1403	B3P	N1-C4-C5-O4
6	A	1403	B3P	C6-C4-C5-O4
6	A	1403	B3P	C7-C4-C5-O4
6	A	1403	B3P	C10-C8-C9-O1
6	A	1403	B3P	C3-C1-C2-N2
6	A	1403	B3P	N2-C8-C9-O1
6	A	1403	B3P	C2-C1-C3-N1
6	A	1403	B3P	C11-C8-C9-O1

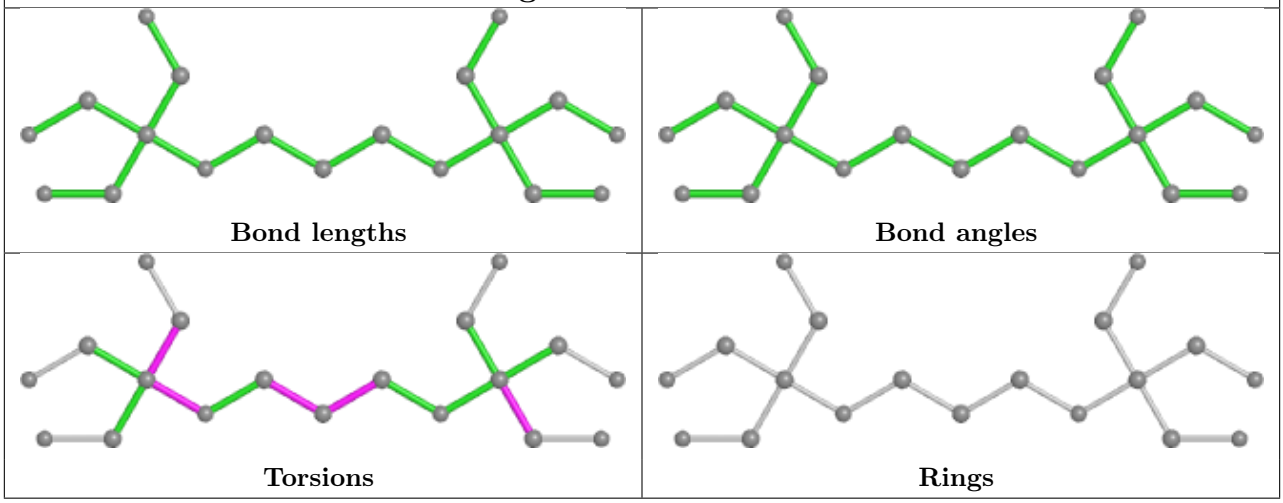
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1403	B3P	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 B3P A 1403



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	1258/1302 (96%)	0.28	69 (5%) 25 26	34, 67, 113, 146	0
2	B	41/46 (89%)	-0.23	0 100 100	40, 51, 74, 134	0
3	C	38/38 (100%)	-0.09	0 100 100	42, 59, 127, 137	0
4	D	25/38 (65%)	0.51	3 (12%) 4 4	46, 96, 160, 186	0
All	All	1362/1424 (95%)	0.26	72 (5%) 26 28	34, 66, 116, 186	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	974	ILE	6.7
1	A	965	ASP	6.0
1	A	960	ILE	5.4
1	A	460	LEU	5.3
1	A	421	ILE	5.2
1	A	473	CYS	5.2
1	A	474	ARG	5.1
1	A	1020	GLU	4.8
1	A	1019	VAL	4.5
1	A	499	LEU	4.1
1	A	418	LEU	4.0
1	A	966	SER	4.0
1	A	466	HIS	3.9
1	A	461	GLU	3.7
1	A	463	PHE	3.7
1	A	964	ARG	3.6
1	A	471	LYS	3.6
4	D	21	DG	3.5
1	A	465	LYS	3.5
1	A	467	ARG	3.5
1	A	963	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	458	LEU	3.2
1	A	969	LYS	3.2
1	A	970	ASP	3.1
1	A	422	THR	3.0
1	A	1221	LYS	3.0
1	A	1008	LEU	3.0
1	A	419	GLU	2.9
1	A	423	GLN	2.9
1	A	420	TYR	2.9
1	A	417	VAL	2.8
1	A	957	LEU	2.8
1	A	977	ILE	2.8
1	A	464	ASN	2.8
1	A	1278	GLU	2.7
1	A	841	ILE	2.6
1	A	89	SER	2.6
1	A	606	ALA	2.6
1	A	407	PHE	2.6
4	D	28	DG	2.6
1	A	411	SER	2.6
1	A	469	ILE	2.6
1	A	88	LYS	2.6
1	A	444	LYS	2.6
1	A	414	GLY	2.5
1	A	511	LYS	2.5
1	A	840	LYS	2.5
1	A	548	SER	2.5
1	A	413	ILE	2.5
1	A	1098	LYS	2.4
1	A	973	LYS	2.4
1	A	457	LYS	2.4
1	A	150	ILE	2.4
1	A	412	VAL	2.3
1	A	148	ASN	2.3
1	A	92	ASP	2.3
1	A	591	TYR	2.3
4	D	5	DA	2.3
1	A	90	ASP	2.3
1	A	921	ARG	2.3
1	A	555	LEU	2.2
1	A	462	GLU	2.2
1	A	115	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1104	LYS	2.2
1	A	968	ARG	2.1
1	A	1281	LYS	2.1
1	A	229	ILE	2.1
1	A	388	LEU	2.1
1	A	292	GLY	2.1
1	A	961	GLU	2.0
1	A	165	ALA	2.0
1	A	472	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

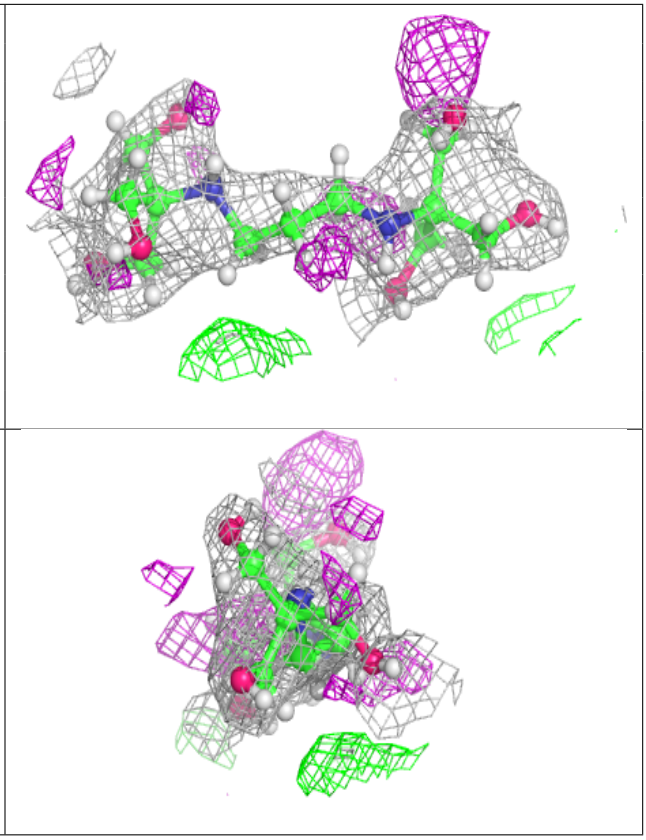
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1402	1/1	0.73	0.13	60,60,60,60	0
6	B3P	A	1403	19/19	0.89	0.26	50,68,104,108	0
5	MG	B	101	1/1	0.98	0.07	48,48,48,48	0
5	MG	A	1401	1/1	0.98	0.20	38,38,38,38	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 B3P A 1403:

$2mF_o$-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.