Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:58 am BST

PDB ID	:	5GWW
Title	:	Structure of MoeN5-Sso7d fusion protein in complex with a permethylated substrate analogue
Authors	:	Ko, T.-P.; Guo, R.-T.; Chen, C.-C.
Deposited on	:	2016-09-14
Resolution	:	2.30 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 ⓘ symbol.

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

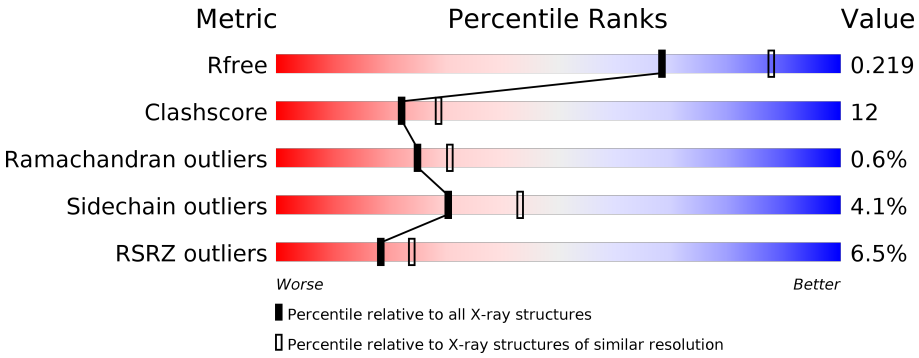
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	343	3% 62% 13% • 23%
1	B	343	6% 80% 15% • •
1	C	343	% 62% 13% • 24%
1	D	343	12% 75% 20% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10096 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2013	1243	374	385	11			
1	B	332	Total	C	N	O	S	0	0	0
			2533	1571	463	485	14			
1	C	262	Total	C	N	O	S	0	0	0
			1998	1234	372	381	11			
1	D	333	Total	C	N	O	S	0	0	0
			2544	1579	466	485	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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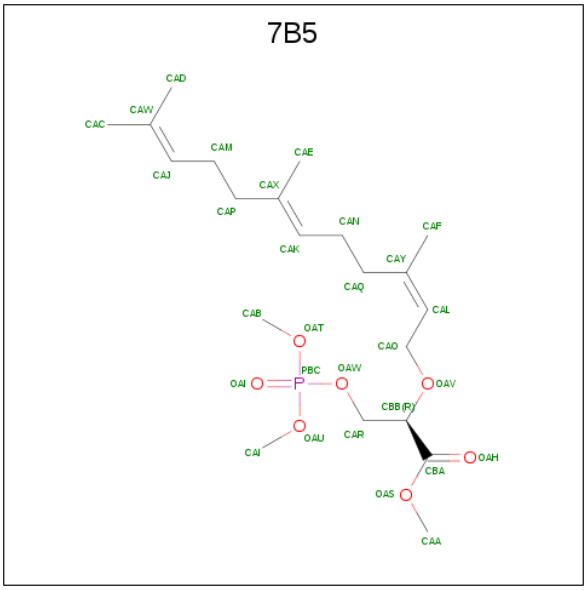
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

- Molecule 2 is methyl (2R)-3-dimethoxyphosphoryloxy-2-[(2Z,6E)-3,7,11-trimethyldodeca-2,6,10-trienoxy]propanoate (three-letter code: 7B5) (formula: $C_{21}H_{37}O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C 15 15	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	232	Total O 232 232	0	0

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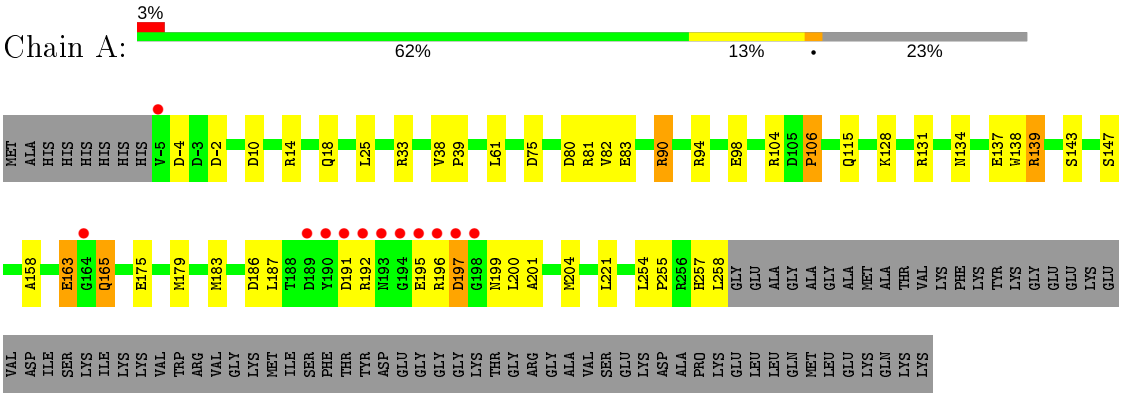
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	275	Total O 275 275	0	0
3	C	199	Total O 199 199	0	0
3	D	287	Total O 287 287	0	0

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 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.

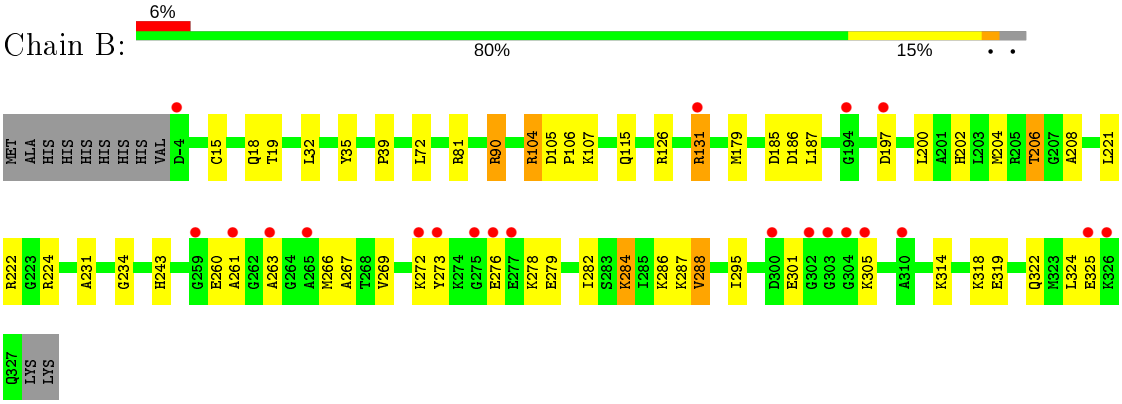
- Molecule 1: MoeN5,DNA-binding protein 7d

Chain A:



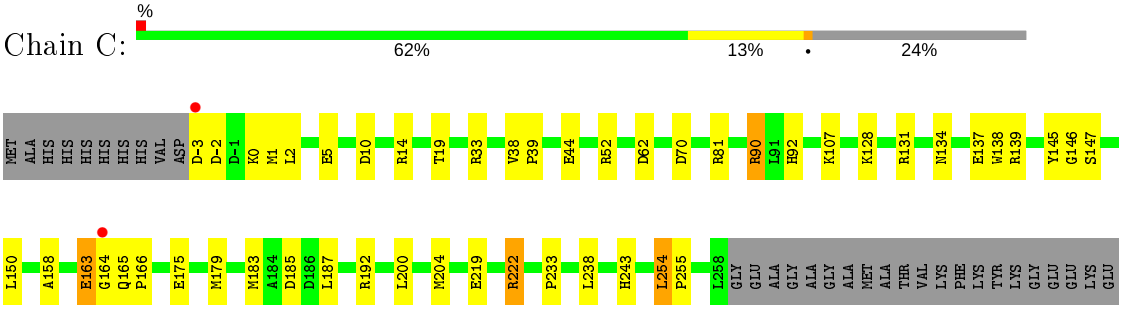
- Molecule 1: MoeN5,DNA-binding protein 7d

Chain B:



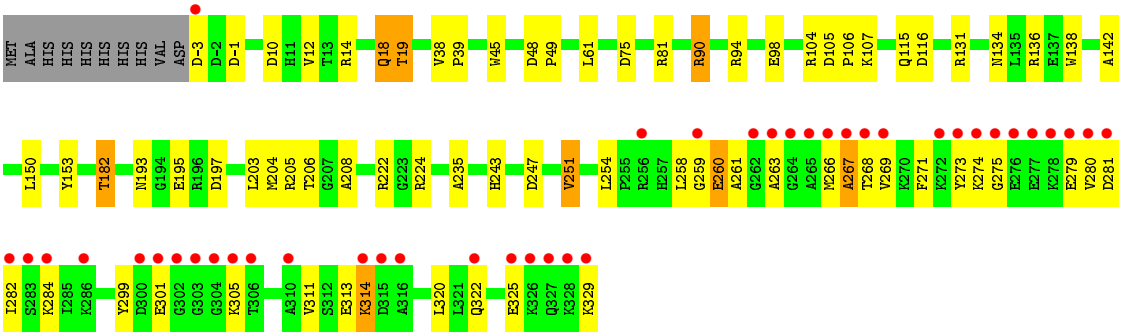
- Molecule 1: MoeN5,DNA-binding protein 7d

Chain C:



- Molecule 1: MoeN5,DNA-binding protein 7d

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	137.86Å 217.33Å 104.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (25.00-2.30) 94.8 (25.01-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 2.31Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.174 , 0.221 0.171 , 0.219	Depositor DCC
R_{free} test set	3342 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10096	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7B5

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	0.61	0/2045	0.74	0/2780
1	B	0.62	1/2572 (0.0%)	0.75	0/3478
1	C	0.64	0/2030	0.76	1/2759 (0.0%)
1	D	0.58	0/2583	0.71	0/3489
All	All	0.61	1/9230 (0.0%)	0.74	1/12506 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	CYS	CB-SG	-5.80	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	222	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	153	TYR	Sidechain

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	2013	0	1996	54	0
1	B	2533	0	2532	52	0
1	C	1998	0	1983	42	0
1	D	2544	0	2554	70	0
2	D	15	0	0	0	0
3	A	232	0	0	10	0
3	B	275	0	0	8	0
3	C	199	0	0	5	0
3	D	287	0	0	3	0
All	All	10096	0	9065	213	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 12.

All (213) 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:325:GLU:HB2	1:D:329:LYS:HD2	1.51	0.92
1:D:10:ASP:HB2	3:D:708:HOH:O	1.76	0.86
1:A:192:ARG:HB2	3:A:401:HOH:O	1.78	0.83
1:A:192:ARG:N	3:A:401:HOH:O	2.12	0.82
1:B:284:LYS:HE3	1:B:284:LYS:HA	1.61	0.82
1:D:94:ARG:HD2	1:D:98:GLU:OE2	1.82	0.80
1:C:219:GLU:OE1	1:C:222:ARG:NE	2.13	0.80
1:D:267:ALA:HB1	1:D:282:ILE:HB	1.63	0.80
1:D:325:GLU:HA	1:D:329:LYS:HB3	1.65	0.79
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.46	0.79
1:A:38:VAL:HG12	1:A:39:PRO:HD3	1.65	0.78
1:C:1:MET:HE2	3:C:539:HOH:O	1.83	0.77
1:B:263:ALA:HB2	3:B:523:HOH:O	1.87	0.74
1:A:115:GLN:HG3	3:A:547:HOH:O	1.88	0.73
1:D:222:ARG:HH11	1:D:243:HIS:HD2	1.36	0.73
1:A:61:LEU:HD13	1:A:94:ARG:HG3	1.72	0.71
1:A:94:ARG:HD2	1:A:98:GLU:OE2	1.90	0.71
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ALA:HB1	1:D:282:ILE:CG1	2.21	0.70
1:D:254:LEU:HG	1:D:258:LEU:HD22	1.73	0.69
1:D:267:ALA:HB1	1:D:282:ILE:CB	2.23	0.69
1:C:187:LEU:HD21	1:C:204:MET:HE3	1.75	0.69
1:C:187:LEU:HD21	1:C:204:MET:CE	2.24	0.67
1:D:38:VAL:HG12	1:D:39:PRO:HD3	1.76	0.67
1:A:158:ALA:CB	1:A:165:GLN:HG2	2.25	0.66
1:B:222:ARG:HH11	1:B:243:HIS:HD2	1.43	0.65
1:C:219:GLU:CD	1:C:222:ARG:HE	1.99	0.65
1:D:61:LEU:HD13	1:D:94:ARG:HG3	1.79	0.64
1:A:163:GLU:HA	3:A:453:HOH:O	1.98	0.63
1:B:179:MET:HE3	1:B:221:LEU:HD11	1.80	0.63
1:D:142:ALA:HB1	1:D:182:THR:HG21	1.81	0.63
1:D:10:ASP:O	1:D:14:ARG:HG3	1.99	0.63
1:D:329:LYS:OXT	1:D:329:LYS:HD3	1.99	0.62
1:D:206:THR:HG23	1:D:208:ALA:H	1.65	0.61
1:A:158:ALA:HB1	1:A:165:GLN:HG2	1.82	0.61
1:D:263:ALA:HB3	1:D:266:MET:O	1.99	0.61
1:D:75:ASP:HB2	1:D:81:ARG:NH1	2.16	0.61
1:A:158:ALA:HA	1:A:165:GLN:HG2	1.83	0.61
1:D:131:ARG:NH1	1:D:131:ARG:HG2	2.16	0.60
1:A:179:MET:HG2	1:A:221:LEU:HD11	1.82	0.60
1:B:301:GLU:CD	1:B:305:LYS:HE3	2.22	0.59
1:C:187:LEU:CD2	1:C:204:MET:HE3	2.31	0.59
1:C:107:LYS:O	1:C:107:LYS:HD3	2.03	0.58
1:C:81:ARG:NH2	3:C:403:HOH:O	2.37	0.58
1:A:139:ARG:HD3	1:A:179:MET:HE1	1.86	0.58
1:C:222:ARG:HH11	1:C:243:HIS:HD2	1.51	0.58
1:D:10:ASP:O	1:D:14:ARG:CG	2.52	0.57
1:D:325:GLU:CB	1:D:329:LYS:HD2	2.29	0.57
1:D:203:LEU:O	1:D:206:THR:HG22	2.03	0.57
1:D:138:TRP:CH2	1:D:182:THR:HG22	2.40	0.57
1:B:325:GLU:O	3:B:401:HOH:O	2.18	0.57
1:A:131:ARG:HG3	1:A:197:ASP:HB3	1.87	0.57
1:D:267:ALA:CB	1:D:282:ILE:HB	2.33	0.57
1:C:5:GLU:OE2	1:C:33:ARG:HG2	2.04	0.56
1:A:199:ASN:OD1	1:A:201:ALA:HB3	2.05	0.56
1:A:158:ALA:CA	1:A:165:GLN:HG2	2.36	0.56
1:C:145:TYR:CD1	1:C:146:GLY:N	2.74	0.56
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.70	0.56
1:A:38:VAL:CG1	1:A:39:PRO:HD3	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LEU:HG	1:C:204:MET:HE2	1.89	0.55
1:D:105:ASP:OD2	1:D:106:PRO:HD2	2.07	0.55
1:D:254:LEU:O	1:D:258:LEU:HB2	2.06	0.55
1:B:224:ARG:HD2	3:B:496:HOH:O	2.06	0.55
1:C:222:ARG:NH1	1:C:243:HIS:HD2	2.04	0.55
1:B:106:PRO:HA	3:B:488:HOH:O	2.07	0.55
1:C:19:THR:O	1:C:19:THR:HG22	2.07	0.55
1:D:269:VAL:O	1:D:279:GLU:HA	2.06	0.55
1:C:-3:ASP:HB3	1:C:2:LEU:HD11	1.89	0.54
1:A:139:ARG:HD3	1:A:179:MET:CE	2.37	0.54
1:C:38:VAL:CG1	1:C:39:PRO:HD3	2.37	0.54
1:D:271:PHE:CE2	1:D:273:TYR:HB2	2.43	0.54
1:A:104:ARG:NH1	1:A:158:ALA:O	2.41	0.54
1:C:131:ARG:HH11	1:C:131:ARG:CG	2.20	0.54
1:D:224:ARG:HG2	1:D:224:ARG:HH21	1.73	0.54
1:A:106:PRO:HB2	1:B:106:PRO:HB2	1.89	0.54
1:B:179:MET:CE	1:B:221:LEU:HD21	2.38	0.54
1:B:126:ARG:NH2	3:B:405:HOH:O	2.29	0.54
1:D:138:TRP:HH2	1:D:182:THR:HG22	1.73	0.54
1:D:38:VAL:CG1	1:D:39:PRO:HD3	2.37	0.54
1:C:38:VAL:HG12	1:C:39:PRO:HD3	1.90	0.54
1:B:269:VAL:O	1:B:279:GLU:HA	2.08	0.53
1:C:44:GLU:HG2	1:C:238:LEU:HG	1.90	0.53
1:D:268:THR:HB	1:D:279:GLU:CG	2.39	0.53
1:B:295:ILE:HD12	1:B:324:LEU:HD11	1.91	0.53
1:D:281:ASP:HB3	1:D:284:LYS:HG2	1.91	0.53
1:C:-2:ASP:OD2	1:C:0:LYS:HB3	2.09	0.53
1:A:187:LEU:HD21	1:A:204:MET:HE1	1.91	0.53
1:B:104:ARG:HB3	1:B:104:ARG:NH1	2.24	0.53
1:B:319:GLU:CD	1:B:319:GLU:H	2.12	0.53
1:D:193:ASN:HB2	1:D:195:GLU:HG3	1.91	0.53
1:D:12:VAL:HG22	1:D:61:LEU:HD23	1.91	0.52
1:D:266:MET:O	1:D:267:ALA:HB2	2.09	0.52
1:C:166:PRO:HD3	1:C:233:PRO:HD2	1.90	0.52
1:A:186:ASP:OD1	1:A:200:LEU:N	2.43	0.52
1:A:138:TRP:CH2	1:A:183:MET:HG2	2.44	0.52
1:B:243:HIS:HE1	3:B:551:HOH:O	1.92	0.52
1:B:301:GLU:HB2	1:B:305:LYS:HG2	1.91	0.51
1:D:271:PHE:HB3	1:D:311:VAL:CG1	2.41	0.51
1:A:187:LEU:HD22	1:A:204:MET:HE3	1.92	0.51
1:A:196:ARG:O	1:A:199:ASN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HD3	1:A:90:ARG:C	2.31	0.51
3:A:529:HOH:O	1:B:107:LYS:HG2	2.11	0.51
1:A:134:ASN:OD1	1:A:137:GLU:HG3	2.11	0.50
1:B:179:MET:HE3	1:B:221:LEU:HD21	1.93	0.50
1:A:14:ARG:HD2	3:A:514:HOH:O	2.11	0.50
3:C:501:HOH:O	1:D:107:LYS:HD3	2.12	0.50
1:A:81:ARG:NH2	1:B:72:LEU:O	2.43	0.50
1:B:105:ASP:CG	1:B:106:PRO:HD2	2.31	0.50
1:B:206:THR:HG22	1:B:208:ALA:H	1.77	0.49
1:A:90:ARG:NH1	1:A:94:ARG:HB2	2.27	0.49
1:B:115:GLN:NE2	3:B:412:HOH:O	2.45	0.49
1:A:200:LEU:HG	1:A:204:MET:CE	2.43	0.49
1:B:202:HIS:O	1:B:206:THR:HB	2.13	0.48
1:A:33:ARG:NH1	1:A:33:ARG:HG2	2.27	0.48
1:B:267:ALA:O	1:B:282:ILE:HG12	2.13	0.48
1:B:131:ARG:HG3	1:B:197:ASP:HB3	1.95	0.48
1:B:273:TYR:HB3	1:B:278:LYS:CD	2.44	0.48
1:B:287:LYS:HG2	1:B:288:VAL:N	2.27	0.48
1:D:222:ARG:NH1	1:D:243:HIS:HD2	2.08	0.48
1:A:25:LEU:HD22	1:A:83:GLU:HB3	1.95	0.48
1:D:280:VAL:HG21	1:D:299:TYR:CE2	2.49	0.47
1:D:313:GLU:HG2	1:D:314:LYS:N	2.29	0.47
1:D:105:ASP:OD2	1:D:106:PRO:CD	2.61	0.47
1:B:104:ARG:HG3	1:B:105:ASP:N	2.30	0.47
1:B:314:LYS:CB	1:B:314:LYS:NZ	2.77	0.47
1:C:134:ASN:OD1	1:C:137:GLU:HG3	2.14	0.47
1:D:247:ASP:O	1:D:251:VAL:HG13	2.15	0.47
1:D:267:ALA:HB1	1:D:282:ILE:HG12	1.96	0.47
1:A:192:ARG:CB	3:A:401:HOH:O	2.49	0.47
1:C:147:SER:O	1:C:175:GLU:HG2	2.15	0.47
1:D:203:LEU:C	1:D:206:THR:HG22	2.35	0.46
1:D:19:THR:CG2	1:D:90:ARG:HG3	2.46	0.46
1:A:200:LEU:HG	1:A:204:MET:HE2	1.97	0.46
1:C:10:ASP:CG	1:C:14:ARG:HH12	2.19	0.46
1:B:200:LEU:HG	1:B:204:MET:CE	2.46	0.46
1:D:90:ARG:HD3	1:D:90:ARG:C	2.36	0.46
1:C:62:ASP:OD1	1:C:92:HIS:ND1	2.50	0.45
1:D:134:ASN:HD21	1:D:136:ARG:NH1	2.15	0.45
1:C:81:ARG:HD3	1:D:81:ARG:NH2	2.31	0.45
1:A:61:LEU:CD1	1:A:94:ARG:HG3	2.43	0.45
1:A:254:LEU:HB2	1:A:255:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:OD1	1:B:81:ARG:NH2	2.49	0.45
1:C:254:LEU:N	1:C:255:PRO:CD	2.80	0.45
1:B:266:MET:HE3	1:B:267:ALA:H	1.81	0.45
1:A:80:ASP:OD1	1:A:82:VAL:HB	2.17	0.44
1:B:231:ALA:O	1:B:234:GLY:N	2.51	0.44
1:C:158:ALA:HA	1:C:165:GLN:NE2	2.32	0.44
1:C:187:LEU:HD21	1:C:204:MET:HE1	1.99	0.44
1:B:187:LEU:HD21	1:B:204:MET:CE	2.47	0.44
1:D:267:ALA:O	1:D:281:ASP:HA	2.18	0.44
1:B:272:LYS:HA	1:B:276:GLU:O	2.17	0.44
1:D:75:ASP:O	1:D:75:ASP:CG	2.56	0.44
1:B:35:TYR:O	1:B:39:PRO:HD3	2.18	0.44
1:D:116:ASP:HA	3:D:686:HOH:O	2.18	0.44
1:A:195:GLU:O	1:A:196:ARG:HD2	2.17	0.44
1:C:1:MET:C	1:C:1:MET:SD	2.96	0.44
1:D:273:TYR:O	1:D:275:GLY:N	2.51	0.44
1:B:266:MET:HE2	1:B:267:ALA:O	2.18	0.44
1:B:273:TYR:HB3	1:B:278:LYS:HD3	2.00	0.44
1:D:224:ARG:NH2	1:D:224:ARG:HG2	2.33	0.44
1:C:131:ARG:NH1	3:C:409:HOH:O	2.51	0.44
1:C:222:ARG:HH11	1:C:243:HIS:CD2	2.34	0.43
1:A:-4:ASP:HB2	3:A:499:HOH:O	2.18	0.43
1:B:187:LEU:HD21	1:B:204:MET:HE3	2.00	0.43
1:D:205:ARG:NH1	1:D:260:GLU:HG3	2.32	0.43
1:A:187:LEU:CD2	1:A:204:MET:CE	2.96	0.43
1:A:179:MET:HG2	1:A:221:LEU:CD1	2.49	0.43
1:A:187:LEU:HD21	1:A:204:MET:CE	2.48	0.43
1:B:261:ALA:C	1:B:263:ALA:H	2.21	0.43
1:D:104:ARG:HD2	3:D:690:HOH:O	2.19	0.43
1:B:272:LYS:HG3	1:B:276:GLU:O	2.19	0.43
1:C:150:LEU:HD12	1:C:150:LEU:HA	1.91	0.42
1:D:75:ASP:HB2	1:D:81:ARG:HH12	1.84	0.42
1:A:179:MET:HG3	1:A:179:MET:O	2.19	0.42
1:D:18:GLN:HG2	1:D:18:GLN:O	2.18	0.42
1:D:45:TRP:CE2	1:D:235:ALA:HB2	2.54	0.42
1:C:70:ASP:OD2	1:C:128:LYS:HE3	2.20	0.42
1:D:301:GLU:HG2	1:D:305:LYS:O	2.18	0.42
1:B:106:PRO:CA	3:B:488:HOH:O	2.66	0.42
1:B:90:ARG:C	1:B:90:ARG:HD3	2.40	0.42
1:A:183:MET:O	1:A:187:LEU:HG	2.19	0.42
1:A:257:HIS:O	1:A:258:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HB3	1:B:35:TYR:CD2	2.54	0.42
1:B:314:LYS:HB3	1:B:314:LYS:HZ3	1.85	0.42
1:B:104:ARG:HB3	1:B:104:ARG:HH11	1.85	0.42
1:C:90:ARG:HD3	1:C:90:ARG:C	2.40	0.42
1:A:10:ASP:OD2	1:C:192:ARG:HD2	2.20	0.42
1:A:139:ARG:HG2	3:A:478:HOH:O	2.20	0.42
1:D:206:THR:CG2	1:D:208:ALA:H	2.31	0.41
1:C:131:ARG:NH1	1:C:131:ARG:CG	2.80	0.41
1:C:163:GLU:HG2	1:C:163:GLU:O	2.20	0.41
1:C:138:TRP:CH2	1:C:183:MET:HG2	2.54	0.41
1:A:131:ARG:HA	1:A:131:ARG:HD2	1.80	0.41
1:B:301:GLU:HB2	1:B:305:LYS:CG	2.49	0.41
1:D:269:VAL:HG21	1:D:320:LEU:HD22	2.02	0.41
1:D:19:THR:HG23	1:D:90:ARG:HG3	2.02	0.41
1:B:222:ARG:NH1	1:B:243:HIS:HD2	2.14	0.41
1:B:266:MET:HE3	1:B:267:ALA:N	2.36	0.41
1:D:134:ASN:ND2	1:D:136:ARG:HH12	2.19	0.41
1:A:147:SER:O	1:A:175:GLU:HG2	2.21	0.41
1:B:314:LYS:HB3	1:B:314:LYS:NZ	2.35	0.41
1:D:94:ARG:HD3	1:D:98:GLU:HG3	2.02	0.41
1:B:318:LYS:O	1:B:322:GLN:HG3	2.21	0.41
1:C:14:ARG:HG2	3:C:488:HOH:O	2.20	0.41
1:D:150:LEU:HD12	1:D:150:LEU:HA	1.91	0.41
1:D:204:MET:HE3	1:D:258:LEU:HD13	2.02	0.41
1:A:179:MET:O	1:A:183:MET:HG3	2.21	0.41
1:C:139:ARG:HG3	1:C:179:MET:CE	2.51	0.41
1:A:163:GLU:H	1:A:163:GLU:HG2	1.74	0.40
1:A:192:ARG:CA	3:A:401:HOH:O	2.63	0.40
1:D:273:TYR:C	1:D:275:GLY:H	2.24	0.40
1:D:48:ASP:OD1	1:D:49:PRO:HD2	2.22	0.40
1:D:48:ASP:HA	1:D:49:PRO:HD3	1.82	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	262/343 (76%)	255 (97%)	7 (3%)	0	100	100
1	B	330/343 (96%)	314 (95%)	15 (4%)	1 (0%)	41	50
1	C	260/343 (76%)	253 (97%)	5 (2%)	2 (1%)	19	23
1	D	331/343 (96%)	313 (95%)	14 (4%)	4 (1%)	13	14
All	All	1183/1372 (86%)	1135 (96%)	41 (4%)	7 (1%)	25	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	261	ALA
1	B	260	GLU
1	D	274	LYS
1	D	267	ALA
1	C	163	GLU
1	C	164	GLY
1	D	259	GLY

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	208/270 (77%)	197 (95%)	11 (5%)	22	31
1	B	260/270 (96%)	249 (96%)	11 (4%)	30	42
1	C	206/270 (76%)	202 (98%)	4 (2%)	57	73
1	D	261/270 (97%)	249 (95%)	12 (5%)	27	38
All	All	935/1080 (87%)	897 (96%)	38 (4%)	30	43

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	ASP

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Mol	Chain	Res	Type
1	A	18	GLN
1	A	90	ARG
1	A	106	PRO
1	A	128	LYS
1	A	139	ARG
1	A	143	SER
1	A	163	GLU
1	A	165	GLN
1	A	191	ASP
1	A	197	ASP
1	B	18	GLN
1	B	19	THR
1	B	90	ARG
1	B	104	ARG
1	B	131	ARG
1	B	185	ASP
1	B	186	ASP
1	B	206	THR
1	B	284	LYS
1	B	286	LYS
1	B	288	VAL
1	C	52	ARG
1	C	90	ARG
1	C	185	ASP
1	C	254	LEU
1	D	-3	ASP
1	D	-1	ASP
1	D	18	GLN
1	D	19	THR
1	D	90	ARG
1	D	115	GLN
1	D	182	THR
1	D	197	ASP
1	D	251	VAL
1	D	260	GLU
1	D	314	LYS
1	D	322	GLN

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

Mol	Chain	Res	Type
1	B	243	HIS

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Mol	Chain	Res	Type
1	C	115	GLN
1	C	124	GLN
1	C	165	GLN
1	C	243	HIS
1	D	165	GLN
1	D	243	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	7B5	D	501	-	14,14,28	3.55	3 (21%)	16,16,35	2.43	7 (43%)

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	7B5	D	501	-	-	6/14/14/36	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	7B5	CAK-CAX	8.59	1.53	1.33
2	D	501	7B5	CAJ-CAW	7.32	1.53	1.32
2	D	501	7B5	CAL-CAY	6.21	1.53	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	7B5	CAO-CAL-CAY	-4.99	115.11	126.57
2	D	501	7B5	CAN-CAK-CAX	-4.48	116.86	127.66
2	D	501	7B5	CAM-CAJ-CAW	-3.32	116.41	127.75
2	D	501	7B5	CAF-CAY-CAQ	3.22	120.69	115.27
2	D	501	7B5	CAE-CAX-CAP	3.18	120.62	115.27
2	D	501	7B5	CAD-CAW-CAC	2.48	120.07	114.60
2	D	501	7B5	CAF-CAY-CAL	-2.09	119.67	123.81

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	7B5	CAK-CAN-CAQ-CAY
2	D	501	7B5	CAM-CAP-CAX-CAE
2	D	501	7B5	CAN-CAQ-CAY-CAF
2	D	501	7B5	CAM-CAP-CAX-CAK
2	D	501	7B5	CAN-CAQ-CAY-CAL
2	D	501	7B5	CAJ-CAM-CAP-CAX

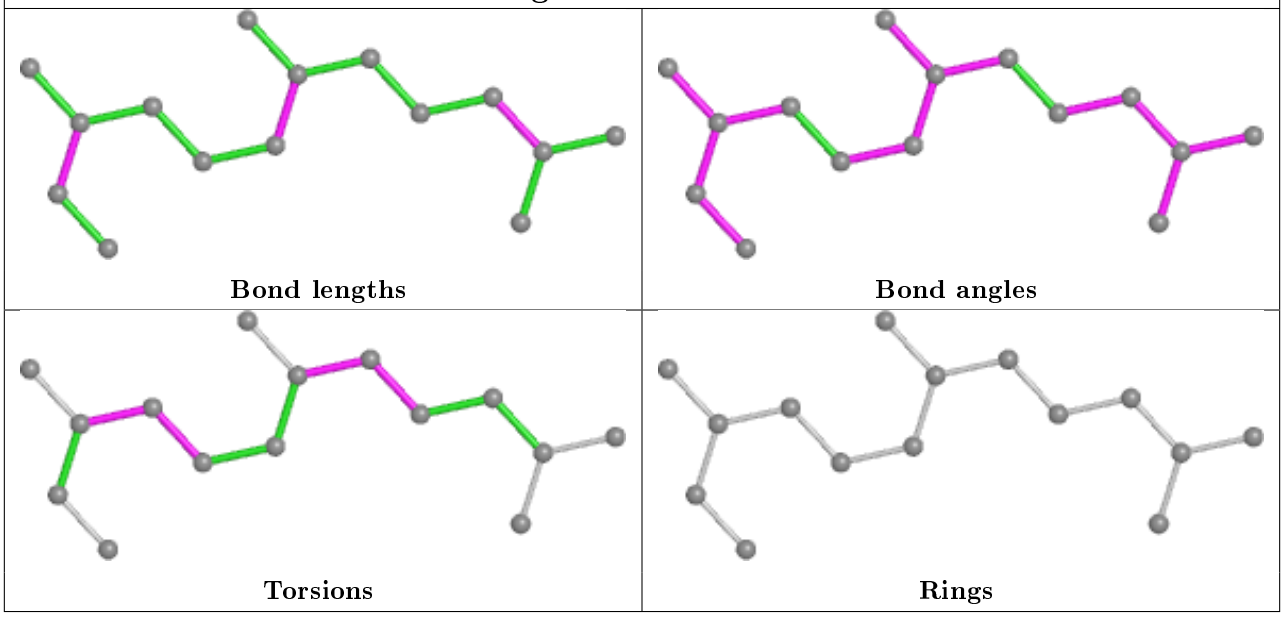
There are no ring outliers.

No monomer is involved in short contacts.

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 7B5 D 501



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	264/343 (76%)	-0.18	12 (4%) 33 40	25, 35, 70, 110	0
1	B	332/343 (96%)	-0.03	21 (6%) 20 25	25, 39, 82, 100	0
1	C	262/343 (76%)	-0.39	2 (0%) 86 89	21, 37, 55, 85	0
1	D	333/343 (97%)	0.29	42 (12%) 3 5	22, 38, 126, 140	0
All	All	1191/1372 (86%)	-0.05	77 (6%) 18 24	21, 37, 95, 140	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	ALA	10.4
1	D	266	MET	9.1
1	D	268	THR	8.0
1	D	267	ALA	7.8
1	D	263	ALA	7.7
1	A	164	GLY	7.6
1	D	275	GLY	7.5
1	D	276	GLU	7.2
1	D	264	GLY	6.9
1	D	303	GLY	6.9
1	B	304	GLY	6.6
1	A	194	GLY	6.0
1	D	328	LYS	6.0
1	D	283	SER	5.8
1	A	-5	VAL	5.7
1	B	194	GLY	5.3
1	D	329	LYS	5.2
1	D	262	GLY	5.2
1	D	273	TYR	5.0
1	D	327	GLN	4.9
1	D	325	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	274	LYS	4.8
1	D	277	GLU	4.7
1	A	195	GLU	4.7
1	A	196	ARG	4.5
1	A	190	TYR	4.4
1	B	263	ALA	4.4
1	D	304	GLY	4.3
1	D	305	LYS	4.3
1	B	277	GLU	4.3
1	D	301	GLU	4.2
1	B	276	GLU	4.2
1	B	326	LYS	4.2
1	B	303	GLY	4.1
1	D	302	GLY	4.1
1	D	314	LYS	3.9
1	D	326	LYS	3.9
1	B	305	LYS	3.7
1	A	197	ASP	3.7
1	A	193	ASN	3.6
1	D	281	ASP	3.5
1	C	-3	ASP	3.4
1	B	261	ALA	3.2
1	D	284	LYS	3.1
1	B	-4	ASP	3.1
1	D	269	VAL	3.1
1	D	286	LYS	3.0
1	D	300	ASP	3.0
1	A	198	GLY	3.0
1	D	272	LYS	3.0
1	B	325	GLU	2.9
1	B	197	ASP	2.8
1	D	306	THR	2.7
1	B	265	ALA	2.7
1	D	280	VAL	2.7
1	D	259	GLY	2.7
1	B	273	TYR	2.6
1	D	278	LYS	2.6
1	D	310	ALA	2.5
1	B	131	ARG	2.4
1	D	322	GLN	2.4
1	A	191	ASP	2.4
1	B	310	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	279	GLU	2.4
1	D	256	ARG	2.3
1	B	275	GLY	2.3
1	C	164	GLY	2.3
1	D	-3	ASP	2.2
1	B	302	GLY	2.2
1	D	315	ASP	2.2
1	B	300	ASP	2.2
1	D	282	ILE	2.2
1	B	259	GLY	2.1
1	A	189	ASP	2.1
1	B	272	LYS	2.1
1	A	192	ARG	2.0
1	D	316	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

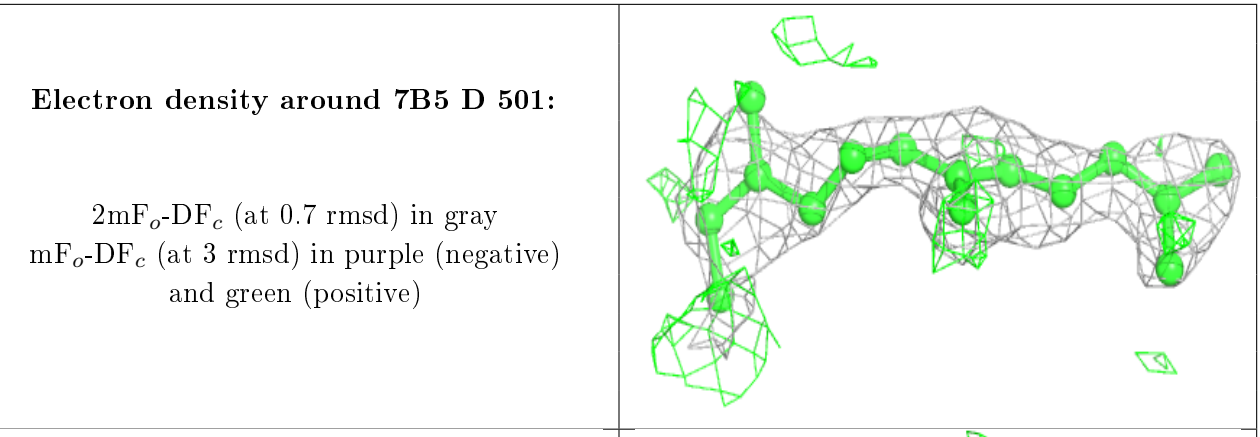
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

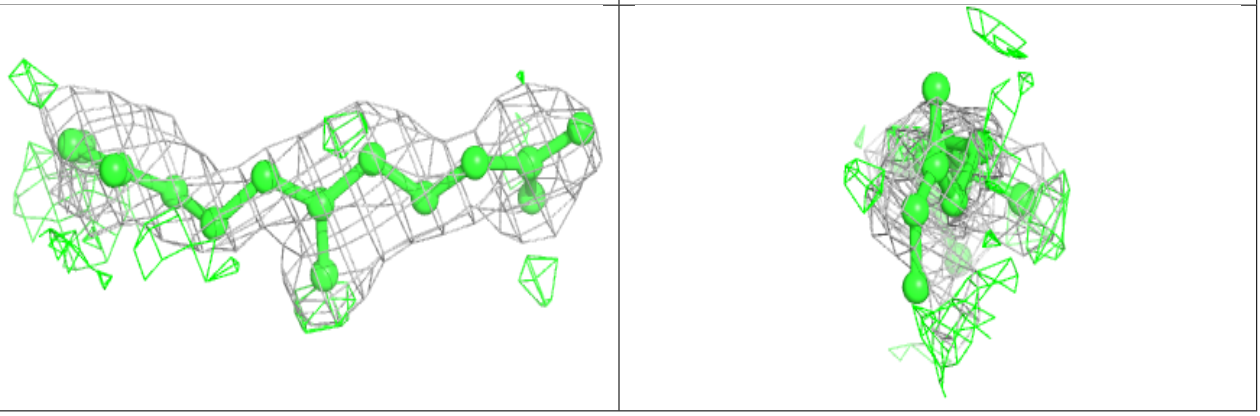
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7B5	D	501	15/29	0.77	0.31	62,66,73,74	0

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 7B5 D 501:

$2mF_o$-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.