



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:27 PM EDT

PDB ID : 3M2P
Title : The crystal structure of UDP-N-acetylglucosamine 4-epimerase from *Bacillus cereus*
Authors : Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-03-08
Resolution : 2.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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

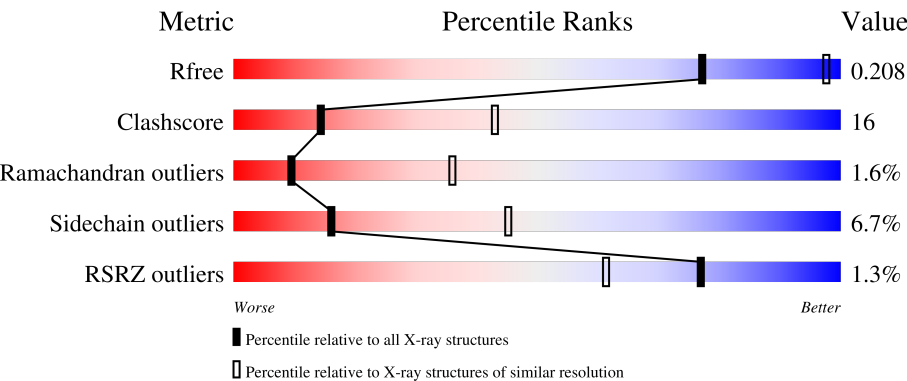
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 $\leq 5\%$. 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	311	<div><div></div><div>63%24%5%8%</div></div>
1	B	311	<div><div>2%</div><div>57%22%18%</div></div>
1	C	311	<div><div>2%</div><div>64%23%10%</div></div>
1	D	311	<div><div>%</div><div>66%24%7%</div></div>

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Mol	Chain	Length	Quality of chain
1	E	311	<div><div>%</div><div><div></div><div>58%</div><div>24%</div><div>•</div><div>16%</div></div></div>
1	F	311	<div><div>%</div><div><div></div><div>59%</div><div>24%</div><div>•</div><div>14%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13067 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 UDP-N-acetylglucosamine 4-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	Se	0	0	0
			2261	1428	382	444	3	4			
1	B	255	Total	C	N	O	S	Se	0	0	0
			2010	1273	334	396	3	4			
1	C	280	Total	C	N	O	S	Se	0	0	0
			2212	1399	372	434	3	4			
1	D	289	Total	C	N	O	S	Se	0	0	0
			2289	1451	382	449	3	4			
1	E	262	Total	C	N	O	S	Se	0	0	0
			2076	1317	348	404	3	4			
1	F	267	Total	C	N	O	S	Se	0	0	0
			2080	1315	346	413	3	3			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q814Z6
A	0	SER	-	expression tag	UNP Q814Z6
A	1	LEU	-	expression tag	UNP Q814Z6
A	302	GLU	-	expression tag	UNP Q814Z6
A	303	GLY	-	expression tag	UNP Q814Z6
A	304	HIS	-	expression tag	UNP Q814Z6
A	305	HIS	-	expression tag	UNP Q814Z6
A	306	HIS	-	expression tag	UNP Q814Z6
A	307	HIS	-	expression tag	UNP Q814Z6
A	308	HIS	-	expression tag	UNP Q814Z6
A	309	HIS	-	expression tag	UNP Q814Z6
B	-1	MSE	-	expression tag	UNP Q814Z6
B	0	SER	-	expression tag	UNP Q814Z6
B	1	LEU	-	expression tag	UNP Q814Z6
B	302	GLU	-	expression tag	UNP Q814Z6
B	303	GLY	-	expression tag	UNP Q814Z6
B	304	HIS	-	expression tag	UNP Q814Z6

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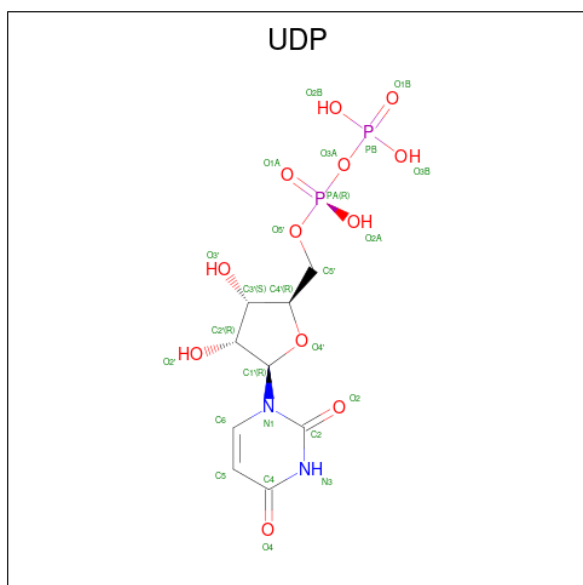
Chain	Residue	Modelled	Actual	Comment	Reference
B	305	HIS	-	expression tag	UNP Q814Z6
B	306	HIS	-	expression tag	UNP Q814Z6
B	307	HIS	-	expression tag	UNP Q814Z6
B	308	HIS	-	expression tag	UNP Q814Z6
B	309	HIS	-	expression tag	UNP Q814Z6
C	-1	MSE	-	expression tag	UNP Q814Z6
C	0	SER	-	expression tag	UNP Q814Z6
C	1	LEU	-	expression tag	UNP Q814Z6
C	302	GLU	-	expression tag	UNP Q814Z6
C	303	GLY	-	expression tag	UNP Q814Z6
C	304	HIS	-	expression tag	UNP Q814Z6
C	305	HIS	-	expression tag	UNP Q814Z6
C	306	HIS	-	expression tag	UNP Q814Z6
C	307	HIS	-	expression tag	UNP Q814Z6
C	308	HIS	-	expression tag	UNP Q814Z6
C	309	HIS	-	expression tag	UNP Q814Z6
D	-1	MSE	-	expression tag	UNP Q814Z6
D	0	SER	-	expression tag	UNP Q814Z6
D	1	LEU	-	expression tag	UNP Q814Z6
D	304	GLU	-	expression tag	UNP Q814Z6
D	305	GLY	-	expression tag	UNP Q814Z6
D	306	HIS	-	expression tag	UNP Q814Z6
D	307	HIS	-	expression tag	UNP Q814Z6
D	308	HIS	-	expression tag	UNP Q814Z6
D	309	HIS	-	expression tag	UNP Q814Z6
D	310	HIS	-	expression tag	UNP Q814Z6
D	311	HIS	-	expression tag	UNP Q814Z6
E	-1	MSE	-	expression tag	UNP Q814Z6
E	0	SER	-	expression tag	UNP Q814Z6
E	1	LEU	-	expression tag	UNP Q814Z6
E	302	GLU	-	expression tag	UNP Q814Z6
E	303	GLY	-	expression tag	UNP Q814Z6
E	304	HIS	-	expression tag	UNP Q814Z6
E	305	HIS	-	expression tag	UNP Q814Z6
E	306	HIS	-	expression tag	UNP Q814Z6
E	307	HIS	-	expression tag	UNP Q814Z6
E	308	HIS	-	expression tag	UNP Q814Z6
E	309	HIS	-	expression tag	UNP Q814Z6
F	-1	MSE	-	expression tag	UNP Q814Z6
F	0	SER	-	expression tag	UNP Q814Z6
F	1	LEU	-	expression tag	UNP Q814Z6
F	302	GLU	-	expression tag	UNP Q814Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	303	GLY	-	expression tag	UNP Q814Z6
F	304	HIS	-	expression tag	UNP Q814Z6
F	305	HIS	-	expression tag	UNP Q814Z6
F	306	HIS	-	expression tag	UNP Q814Z6
F	307	HIS	-	expression tag	UNP Q814Z6
F	308	HIS	-	expression tag	UNP Q814Z6
F	309	HIS	-	expression tag	UNP Q814Z6

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	
			25	9	2	12	2	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	12	Total	O	0	0
			12	12		
3	C	23	Total	O	0	0
			23	23		
3	D	22	Total	O	0	0
			22	22		
3	E	12	Total	O	0	0
			12	12		

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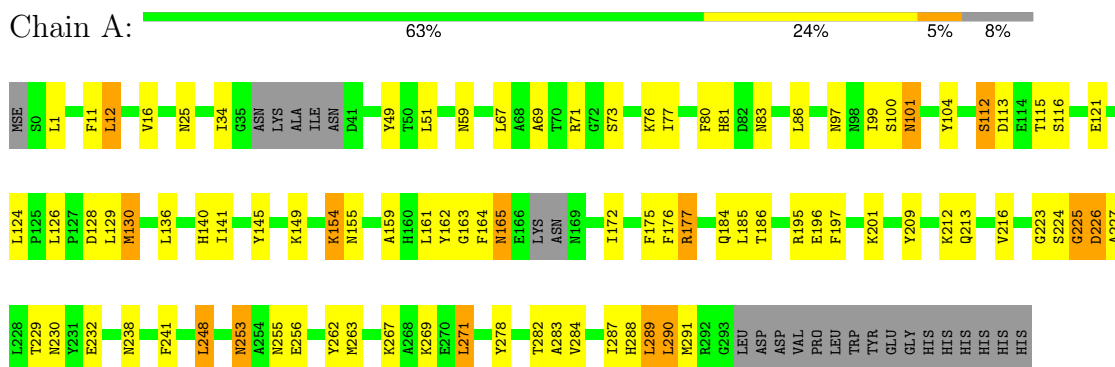
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	18	Total	O	0	0
			18	18		

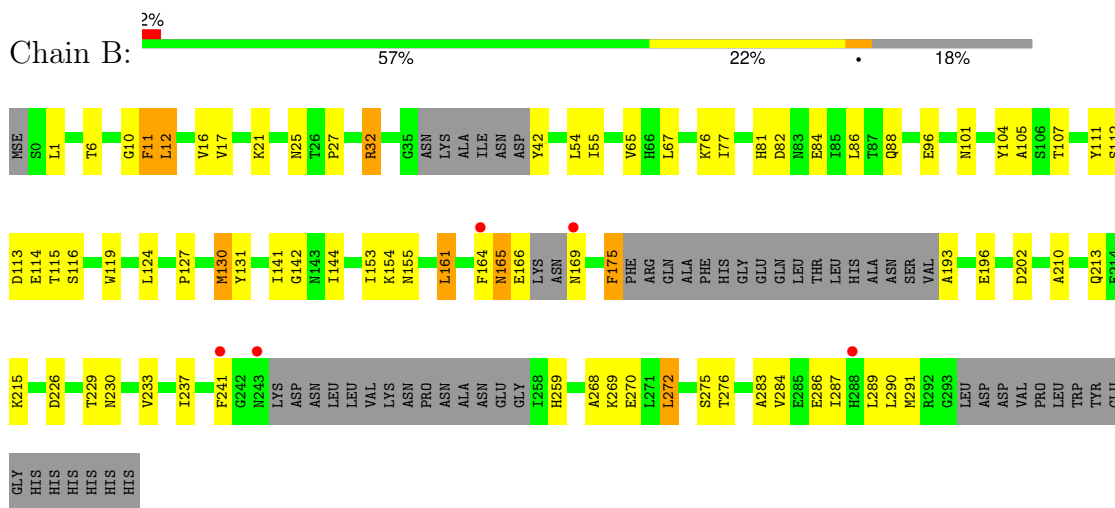
3 Residue-property plots

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.

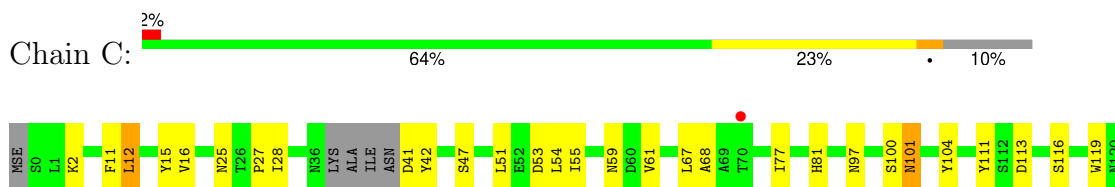
• Molecule 1: UDP-N-acetylglucosamine 4-epimerase

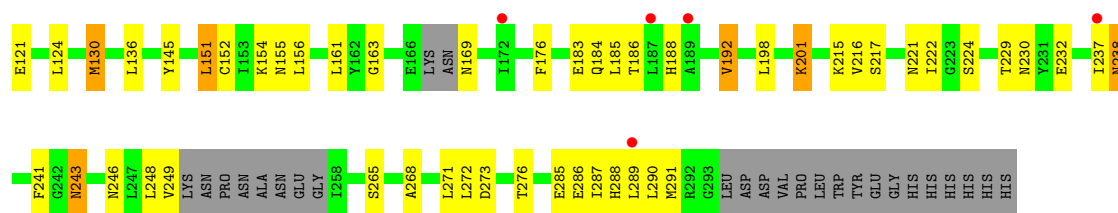


• Molecule 1: UDP-N-acetylglucosamine 4-epimerase

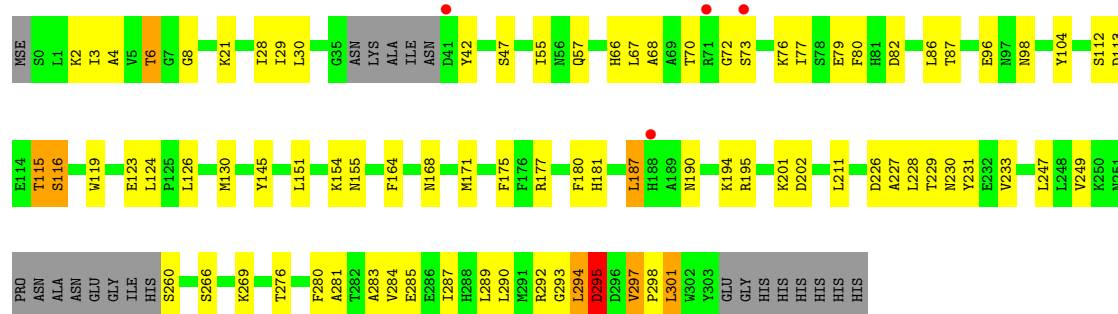


• Molecule 1: UDP-N-acetylglucosamine 4-epimerase

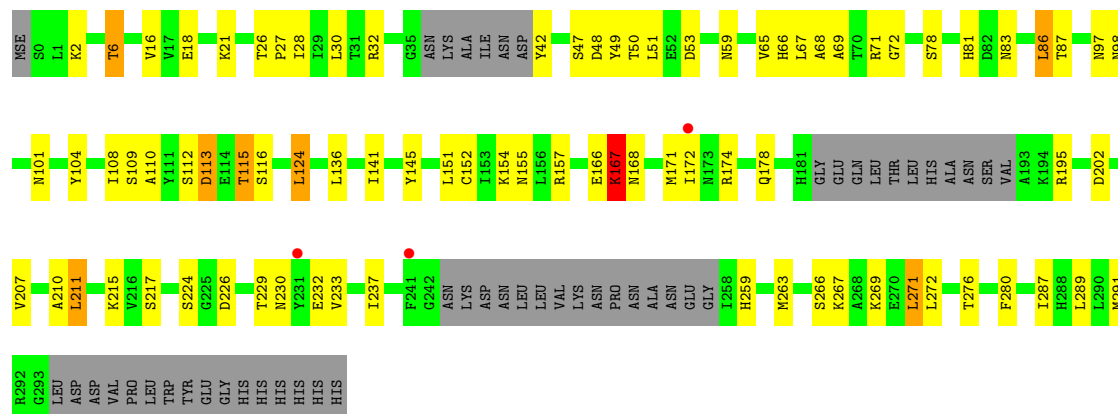




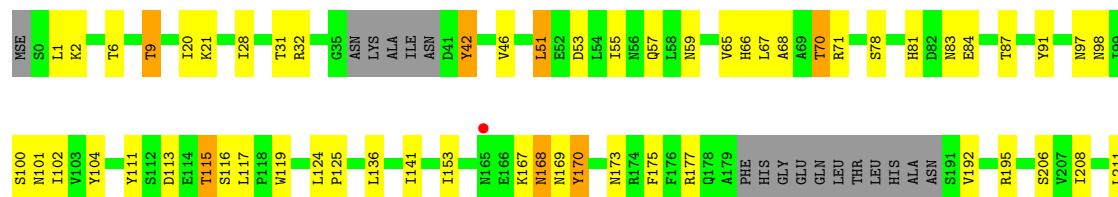
• Molecule 1: UDP-N-acetylglucosamine 4-epimerase

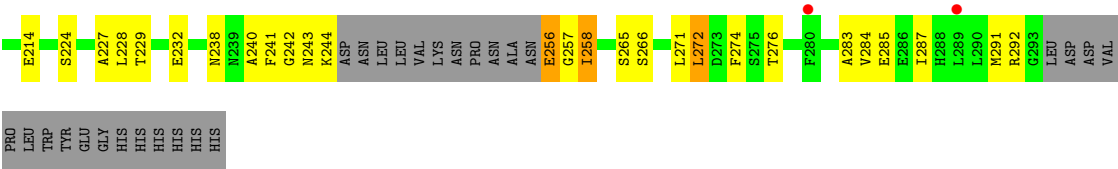


• Molecule 1: UDP-N-acetylglucosamine 4-epimerase



• Molecule 1: UDP-N-acetylglucosamine 4-epimerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.12Å 149.72Å 166.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.70 – 2.95 111.28 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.70-2.95) 100.0 (111.28-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.212 , 0.276 0.214 , 0.208	Depositor DCC
R_{free} test set	2816 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13067	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: UDP

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	0.39	0/2298	0.56	0/3101
1	B	0.37	0/2040	0.53	0/2748
1	C	0.38	0/2247	0.53	0/3030
1	D	0.42	0/2328	0.55	0/3144
1	E	0.39	0/2110	0.54	0/2842
1	F	0.39	0/2111	0.57	0/2845
All	All	0.39	0/13134	0.55	0/17710

There are no bond length outliers.

There are no bond angle outliers.

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	2261	0	2194	96	0
1	B	2010	0	1956	62	0
1	C	2212	0	2150	62	0
1	D	2289	0	2221	74	0
1	E	2076	0	2021	57	0
1	F	2080	0	2007	74	0
2	B	25	0	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	0	1	0
3	B	12	0	0	0	0
3	C	23	0	0	0	0
3	D	22	0	0	1	0
3	E	12	0	0	0	0
3	F	18	0	0	1	0
All	All	13067	0	12559	396	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 16.

All (396) 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:6:THR:HG21	1:D:66:HIS:HD2	1.10	1.14
1:E:6:THR:HG21	1:E:66:HIS:HD2	1.02	1.13
1:E:6:THR:HG21	1:E:66:HIS:CD2	1.88	1.06
1:C:130:MSE:HE1	1:F:141:ILE:HG12	1.38	1.05
1:D:6:THR:HG21	1:D:66:HIS:CD2	1.92	1.05
1:A:177:ARG:HH11	1:A:177:ARG:HG2	1.19	1.03
1:D:77:ILE:HB	1:D:130:MSE:CE	1.89	1.02
1:A:225:GLY:HA3	1:A:226:ASP:HB2	1.42	1.01
1:F:6:THR:HG21	1:F:66:HIS:HD2	1.25	1.01
1:D:77:ILE:HB	1:D:130:MSE:HE3	1.40	1.00
1:D:292:ARG:O	1:D:294:LEU:HD12	1.61	0.98
1:D:130:MSE:HE1	1:E:141:ILE:HG12	1.45	0.98
1:D:293:GLY:HA2	1:D:294:LEU:CB	1.98	0.93
1:D:293:GLY:HA2	1:D:294:LEU:HB2	1.48	0.92
1:B:32:ARG:HG3	1:B:32:ARG:HH21	1.34	0.91
1:E:2:LYS:HD2	1:E:28:ILE:HD11	1.53	0.90
1:F:6:THR:HG21	1:F:66:HIS:CD2	2.07	0.90
1:F:6:THR:HG22	1:F:68:ALA:H	1.35	0.90
1:E:6:THR:CG2	1:E:66:HIS:HD2	1.86	0.87
1:A:225:GLY:CA	1:A:226:ASP:HB2	2.06	0.85
1:E:195:ARG:HH21	1:E:230:ASN:HD21	1.22	0.85
1:C:201:LYS:HE3	1:C:286:GLU:OE2	1.76	0.84
1:A:69:ALA:HA	1:A:83:ASN:HD21	1.42	0.84
1:A:287:ILE:HG22	1:A:291:MSE:HE2	1.60	0.83
1:E:229:THR:OG1	1:E:232:GLU:HG3	1.79	0.81
1:C:77:ILE:HB	1:C:130:MSE:HE2	1.61	0.81
1:D:6:THR:HG22	1:D:68:ALA:H	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:GLY:CA	1:D:294:LEU:HB2	2.09	0.81
1:C:243:ASN:HD21	1:C:246:ASN:HD22	1.29	0.81
1:D:8:GLY:HA3	1:D:29:ILE:HG23	1.62	0.80
1:A:177:ARG:HG2	1:A:177:ARG:NH1	1.93	0.79
1:C:130:MSE:CE	1:F:141:ILE:HG12	2.12	0.78
1:E:113:ASP:OD1	1:E:115:THR:HB	1.83	0.78
1:D:21:LYS:HD3	1:D:42:TYR:HE1	1.47	0.77
1:A:186:THR:HG22	1:A:248:LEU:HB3	1.66	0.77
1:E:66:HIS:HE1	1:E:87:THR:OG1	1.68	0.77
1:B:77:ILE:HB	1:B:130:MSE:HE3	1.67	0.77
1:C:124:LEU:HD12	1:F:124:LEU:HD23	1.66	0.76
1:D:177:ARG:HD2	1:D:298:PRO:O	1.84	0.76
1:B:32:ARG:HH21	1:B:32:ARG:CG	1.98	0.76
1:A:241:PHE:CZ	1:A:291:MSE:HE1	2.22	0.75
1:B:10:GLY:HA3	2:B:7517:UDP:H5'1	1.67	0.74
1:D:124:LEU:HD23	1:E:124:LEU:HD23	1.68	0.74
1:D:104:TYR:HB3	1:D:155:ASN:HD22	1.52	0.74
1:A:289:LEU:HD13	1:A:289:LEU:O	1.89	0.73
1:A:76:LYS:HA	1:B:88:GLN:HE22	1.56	0.71
1:A:77:ILE:HB	1:A:130:MSE:HE3	1.73	0.71
1:D:124:LEU:HD23	1:E:124:LEU:CD2	2.20	0.70
1:B:161:LEU:H	1:B:161:LEU:HD12	1.57	0.70
1:A:278:TYR:HD2	1:A:282:THR:HG22	1.57	0.69
1:F:229:THR:OG1	1:F:232:GLU:HG3	1.93	0.68
1:A:77:ILE:HB	1:A:130:MSE:CE	2.24	0.68
1:A:81:HIS:HE1	1:B:84:GLU:OE1	1.77	0.68
1:B:164:PHE:O	1:B:165:ASN:HB2	1.94	0.68
1:B:283:ALA:O	1:B:287:ILE:HG13	1.94	0.67
1:B:104:TYR:HB3	1:B:155:ASN:HD22	1.58	0.67
1:D:77:ILE:HB	1:D:130:MSE:HE2	1.76	0.67
1:B:12:LEU:HD22	1:B:16:VAL:HG23	1.76	0.67
1:C:12:LEU:HD22	1:C:16:VAL:HG23	1.75	0.67
1:C:145:TYR:HB3	1:C:151:LEU:HD22	1.75	0.67
1:E:145:TYR:HB3	1:E:151:LEU:HD22	1.77	0.66
1:E:6:THR:CG2	1:E:68:ALA:H	2.08	0.66
1:A:241:PHE:HZ	1:A:291:MSE:HE1	1.59	0.66
1:D:187:LEU:HB3	1:D:190:ASN:HB2	1.78	0.66
1:D:294:LEU:O	1:D:295:ASP:HB2	1.94	0.66
1:D:293:GLY:CA	1:D:294:LEU:CB	2.73	0.65
1:D:6:THR:CG2	1:D:68:ALA:H	2.08	0.65
1:D:181:HIS:HE1	1:D:297:VAL:O	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ARG:HD2	1:E:178:GLN:NE2	2.12	0.65
1:A:126:LEU:HD23	1:A:126:LEU:O	1.97	0.65
1:A:288:HIS:HA	1:A:291:MSE:HE3	1.77	0.65
1:E:6:THR:HG22	1:E:67:LEU:H	1.61	0.65
1:E:287:ILE:O	1:E:291:MSE:HG3	1.97	0.65
1:D:6:THR:CG2	1:D:66:HIS:HD2	1.98	0.65
1:B:113:ASP:OD1	1:B:115:THR:HB	1.97	0.65
1:A:278:TYR:CD2	1:A:282:THR:HG22	2.32	0.64
1:D:171:MSE:HE1	1:D:230:ASN:HB3	1.78	0.64
1:F:6:THR:HG23	1:F:68:ALA:HB2	1.80	0.64
1:A:161:LEU:N	1:A:161:LEU:HD12	2.12	0.64
1:A:104:TYR:HB3	1:A:155:ASN:HD22	1.62	0.64
1:D:293:GLY:HA2	1:D:294:LEU:CD1	2.27	0.63
1:A:101:ASN:ND2	1:A:154:LYS:HZ1	1.95	0.63
1:A:101:ASN:ND2	1:A:154:LYS:NZ	2.47	0.62
1:B:161:LEU:HD12	1:B:161:LEU:N	2.13	0.62
1:A:177:ARG:HH11	1:A:177:ARG:CG	2.04	0.62
1:E:78:SER:HA	1:E:81:HIS:CD2	2.34	0.62
1:A:225:GLY:CA	1:A:226:ASP:CB	2.76	0.62
1:B:241:PHE:HE1	1:B:284:VAL:HG13	1.64	0.62
1:E:6:THR:HG23	1:E:68:ALA:CB	2.29	0.62
1:A:130:MSE:HE1	1:B:141:ILE:HG12	1.82	0.62
1:D:66:HIS:HE1	1:D:87:THR:OG1	1.81	0.62
1:F:6:THR:HG22	1:F:68:ALA:N	2.13	0.62
1:C:183:GLU:HG2	1:C:184:GLN:N	2.15	0.61
1:F:240:ALA:HB1	1:F:285:GLU:HG3	1.82	0.61
1:A:121:GLU:HG3	1:A:267:LYS:HE3	1.81	0.61
1:F:66:HIS:HE1	1:F:87:THR:OG1	1.84	0.61
1:E:195:ARG:NH2	1:E:230:ASN:HD21	1.98	0.61
1:D:70:THR:HG22	1:D:72:GLY:H	1.66	0.60
1:B:32:ARG:HH22	2:B:7517:UDP:H2'	1.65	0.60
1:E:167:LYS:HE3	1:E:167:LYS:HA	1.83	0.60
1:D:2:LYS:HD3	1:D:28:ILE:HD11	1.83	0.60
1:A:229:THR:OG1	1:A:232:GLU:HG3	2.02	0.60
1:B:287:ILE:O	1:B:291:MSE:HG3	2.02	0.60
1:D:3:ILE:HD13	1:D:211:LEU:HD13	1.84	0.60
1:E:48:ASP:OD1	1:E:50:THR:HG23	2.02	0.60
1:C:224:SER:HA	1:C:276:THR:HG21	1.83	0.59
1:E:233:VAL:O	1:E:237:ILE:HG13	2.03	0.59
1:B:67:LEU:HD23	1:B:105:ALA:HB2	1.85	0.58
1:F:175:PHE:HB3	1:F:291:MSE:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:THR:HG22	1:E:68:ALA:H	1.68	0.58
1:C:25:ASN:O	1:C:27:PRO:HD3	2.03	0.58
1:E:6:THR:HG23	1:E:68:ALA:HB2	1.84	0.58
1:C:77:ILE:HG13	1:C:77:ILE:O	2.04	0.58
1:D:289:LEU:O	1:D:292:ARG:HB2	2.03	0.57
1:D:187:LEU:HD21	1:D:231:TYR:HA	1.85	0.57
1:D:145:TYR:HB3	1:D:151:LEU:HD22	1.86	0.57
1:F:287:ILE:HG22	1:F:291:MSE:HE2	1.87	0.57
1:B:32:ARG:HG3	1:B:32:ARG:NH2	2.09	0.57
1:F:66:HIS:HD1	1:F:104:TYR:HD1	1.53	0.57
1:A:141:ILE:HG12	1:B:130:MSE:HE1	1.86	0.57
1:B:230:ASN:N	1:B:230:ASN:HD22	2.01	0.56
1:F:113:ASP:OD1	1:F:115:THR:HB	2.05	0.56
1:D:70:THR:O	1:D:80:PHE:HE2	1.88	0.56
1:B:1:LEU:HB2	1:B:25:ASN:OD1	2.05	0.56
1:B:269:LYS:HG3	1:B:269:LYS:O	2.04	0.56
1:D:171:MSE:HE2	1:D:175:PHE:CZ	2.40	0.56
1:F:65:VAL:HG12	1:F:67:LEU:HD21	1.86	0.56
1:F:283:ALA:O	1:F:287:ILE:HG13	2.06	0.56
1:A:101:ASN:HD21	1:A:154:LYS:NZ	2.04	0.56
1:D:195:ARG:HH21	1:D:230:ASN:HD21	1.53	0.56
1:A:140:HIS:ND1	1:B:127:PRO:HD2	2.20	0.56
1:A:11:PHE:HZ	1:A:163:GLY:HA3	1.71	0.56
1:B:107:THR:HG21	1:B:131:TYR:CE2	2.41	0.56
1:E:154:LYS:HE3	1:E:210:ALA:O	2.06	0.56
1:F:111:TYR:HB2	1:F:119:TRP:CE3	2.41	0.55
1:C:101:ASN:ND2	1:C:154:LYS:NZ	2.54	0.55
1:F:241:PHE:CZ	1:F:291:MSE:HE3	2.42	0.55
1:D:281:ALA:O	1:D:285:GLU:HG3	2.07	0.55
1:B:101:ASN:HD21	1:B:154:LYS:NZ	2.05	0.55
1:D:6:THR:HG23	1:D:68:ALA:CB	2.37	0.55
1:D:21:LYS:HD3	1:D:42:TYR:CE1	2.36	0.55
1:F:71:ARG:O	1:F:71:ARG:HG3	2.05	0.55
1:F:6:THR:CG2	1:F:66:HIS:HD2	2.10	0.54
1:C:130:MSE:HE1	1:F:141:ILE:CG1	2.27	0.54
1:F:224:SER:HA	1:F:276:THR:HG21	1.89	0.54
1:A:159:ALA:O	1:A:161:LEU:HD12	2.08	0.54
1:D:113:ASP:OD1	1:D:115:THR:HB	2.08	0.54
1:E:59:ASN:HA	1:E:97:ASN:OD1	2.08	0.54
1:C:111:TYR:HB2	1:C:119:TRP:CE3	2.43	0.53
1:A:130:MSE:CE	1:B:141:ILE:HG12	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:SER:CB	1:A:126:LEU:HD23	2.38	0.53
1:B:55:ILE:HD13	1:B:96:GLU:HG3	1.90	0.53
1:C:183:GLU:HG2	1:C:184:GLN:H	1.73	0.53
1:C:104:TYR:HB3	1:C:155:ASN:HD22	1.74	0.53
1:C:59:ASN:HA	1:C:97:ASN:OD1	2.09	0.53
1:F:70:THR:H	1:F:83:ASN:HD21	1.56	0.53
1:F:51:LEU:O	1:F:55:ILE:HG13	2.09	0.53
1:E:266:SER:O	1:E:269:LYS:HB3	2.09	0.53
1:A:162:TYR:CD1	1:A:197:PHE:HB3	2.44	0.52
1:A:71:ARG:HG3	3:A:321:HOH:O	2.09	0.52
1:D:233:VAL:HG13	1:D:280:PHE:CZ	2.44	0.52
1:F:32:ARG:O	1:F:46:VAL:HG13	2.09	0.52
1:A:195:ARG:HH21	1:A:230:ASN:HD21	1.58	0.52
1:C:101:ASN:ND2	1:C:154:LYS:HZ1	2.08	0.52
1:A:175:PHE:CD1	1:A:185:LEU:HG	2.44	0.52
1:E:202:ASP:OD2	1:E:276:THR:HB	2.10	0.52
1:F:87:THR:HG23	1:F:91:TYR:CE2	2.45	0.52
1:F:241:PHE:HE1	1:F:284:VAL:HG13	1.75	0.52
1:A:177:ARG:NH1	1:A:177:ARG:CG	2.67	0.52
1:D:47:SER:HB2	1:D:57:GLN:HG3	1.92	0.52
1:E:2:LYS:HD2	1:E:28:ILE:CD1	2.34	0.52
1:C:229:THR:OG1	1:C:232:GLU:HG3	2.11	0.51
1:E:6:THR:HG22	1:E:67:LEU:N	2.25	0.51
1:A:186:THR:HA	1:A:248:LEU:O	2.11	0.51
1:A:12:LEU:HD13	1:A:67:LEU:HD22	1.92	0.51
1:C:154:LYS:HE2	1:C:216:VAL:O	2.11	0.51
1:D:283:ALA:O	1:D:287:ILE:HG13	2.10	0.51
1:E:207:VAL:O	1:E:211:LEU:HB2	2.10	0.51
1:B:21:LYS:HD3	1:B:42:TYR:HE1	1.75	0.51
1:C:81:HIS:HE1	1:F:84:GLU:OE1	1.93	0.51
1:C:285:GLU:O	1:C:288:HIS:HB3	2.10	0.51
1:B:202:ASP:OD2	1:B:276:THR:HB	2.11	0.51
1:C:248:LEU:HD22	1:C:249:VAL:H	1.76	0.51
1:D:77:ILE:CB	1:D:130:MSE:HE3	2.27	0.51
1:A:101:ASN:HD21	1:A:154:LYS:HZ2	1.58	0.51
1:A:241:PHE:CE2	1:A:291:MSE:HE1	2.46	0.50
1:A:69:ALA:HA	1:A:83:ASN:ND2	2.21	0.50
1:F:256:GLU:HG3	1:F:257:GLY:H	1.76	0.50
1:C:176:PHE:HB3	1:C:291:MSE:HE1	1.93	0.50
1:C:243:ASN:ND2	1:C:246:ASN:HB3	2.26	0.50
1:F:6:THR:CG2	1:F:68:ALA:CB	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASP:OD1	1:A:115:THR:HB	2.12	0.50
1:F:6:THR:CG2	1:F:68:ALA:HB2	2.41	0.50
1:B:32:ARG:CG	1:B:32:ARG:NH2	2.68	0.50
1:E:157:ARG:O	1:E:263:MSE:HE1	2.11	0.50
1:B:55:ILE:CD1	1:B:96:GLU:HG3	2.42	0.50
1:B:270:GLU:O	1:D:190:ASN:OD1	2.29	0.50
1:C:47:SER:HA	1:C:53:ASP:OD2	2.12	0.50
1:C:152:CYS:HA	1:C:217:SER:HB3	1.93	0.49
1:C:124:LEU:HD12	1:F:124:LEU:CD2	2.40	0.49
1:D:301:LEU:HD23	1:D:301:LEU:H	1.77	0.49
1:C:121:GLU:OE1	1:C:121:GLU:N	2.41	0.49
1:D:6:THR:HG22	1:D:67:LEU:H	1.77	0.49
1:E:171:MSE:HE1	1:E:230:ASN:HD22	1.77	0.49
1:A:288:HIS:C	1:A:290:LEU:H	2.16	0.49
1:A:1:LEU:HB2	1:A:25:ASN:OD1	2.12	0.49
1:C:221:ASN:N	1:C:221:ASN:HD22	2.11	0.49
1:F:167:LYS:O	1:F:168:ASN:CB	2.61	0.48
1:A:130:MSE:HE1	1:B:141:ILE:HG23	1.95	0.48
1:F:195:ARG:NH1	1:F:258:ILE:HD12	2.28	0.48
1:F:242:GLY:C	1:F:243:ASN:HD22	2.15	0.48
1:F:2:LYS:HD3	1:F:28:ILE:HD11	1.95	0.48
1:B:154:LYS:NZ	1:B:210:ALA:O	2.44	0.48
1:B:196:GLU:HA	1:B:226:ASP:O	2.14	0.48
1:D:181:HIS:CE1	1:D:297:VAL:HG23	2.48	0.48
1:F:167:LYS:O	1:F:168:ASN:HB3	2.13	0.48
1:D:164:PHE:CD1	1:D:290:LEU:HB3	2.48	0.48
1:F:6:THR:CG2	1:F:68:ALA:H	2.16	0.48
1:B:86:LEU:C	1:B:86:LEU:HD23	2.34	0.48
1:A:161:LEU:HD12	1:A:161:LEU:H	1.79	0.48
1:A:176:PHE:HE1	1:A:284:VAL:HG13	1.78	0.48
1:A:271:LEU:HG	1:C:271:LEU:CD1	2.43	0.48
1:B:111:TYR:HB2	1:B:119:TRP:CE3	2.49	0.48
1:D:55:ILE:CD1	1:D:96:GLU:HG3	2.44	0.48
1:D:130:MSE:HE1	1:E:141:ILE:CG1	2.31	0.48
1:E:171:MSE:HE1	1:E:230:ASN:ND2	2.29	0.48
1:A:141:ILE:HG12	1:B:130:MSE:CE	2.44	0.47
1:D:285:GLU:O	1:D:289:LEU:HD13	2.14	0.47
1:D:201:LYS:NZ	3:D:316:HOH:O	2.47	0.47
1:D:301:LEU:HD23	1:D:301:LEU:N	2.29	0.47
1:A:162:TYR:CE1	1:A:197:PHE:HB3	2.50	0.47
1:A:184:GLN:HE22	1:A:248:LEU:HD23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:CG	1:E:215:LYS:HB2	2.34	0.47
1:A:283:ALA:O	1:A:287:ILE:HG13	2.13	0.47
1:C:185:LEU:HD22	1:C:238:ASN:OD1	2.14	0.47
1:C:2:LYS:O	1:C:61:VAL:HG13	2.15	0.47
1:A:86:LEU:HD23	1:A:86:LEU:O	2.15	0.47
1:A:184:GLN:NE2	1:A:248:LEU:HD23	2.30	0.47
1:D:123:GLU:HG3	1:D:124:LEU:O	2.15	0.47
1:A:81:HIS:CE1	1:B:84:GLU:OE1	2.65	0.47
1:A:101:ASN:HD22	1:A:154:LYS:HZ1	1.59	0.47
1:A:121:GLU:HG3	1:A:267:LYS:CE	2.44	0.47
1:A:121:GLU:CG	1:A:267:LYS:HE3	2.45	0.47
1:B:11:PHE:HB3	2:B:7517:UDP:O2B	2.15	0.47
1:C:41:ASP:CG	1:C:42:TYR:H	2.18	0.47
1:E:6:THR:HG22	1:E:6:THR:O	2.14	0.47
1:F:65:VAL:HG12	1:F:67:LEU:CD2	2.45	0.47
1:C:184:GLN:NE2	1:C:248:LEU:HB2	2.30	0.46
1:F:136:LEU:HD23	1:F:136:LEU:HA	1.68	0.46
1:F:291:MSE:O	1:F:292:ARG:C	2.54	0.46
1:C:2:LYS:HD3	1:C:28:ILE:HD11	1.98	0.46
1:D:293:GLY:HA2	1:D:294:LEU:HD12	1.98	0.46
1:F:6:THR:HB	1:F:66:HIS:HA	1.97	0.46
1:D:6:THR:O	1:D:67:LEU:HB2	2.16	0.46
1:D:171:MSE:HE1	1:D:230:ASN:CB	2.45	0.46
1:A:196:GLU:OE1	1:A:263:MSE:N	2.41	0.46
1:D:76:LYS:O	1:D:79:GLU:HB2	2.16	0.46
1:D:229:THR:O	1:D:233:VAL:HG23	2.16	0.46
1:F:6:THR:HG23	1:F:68:ALA:CB	2.44	0.46
1:A:97:ASN:HB2	1:A:99:ILE:HD12	1.98	0.46
1:B:175:PHE:CD1	1:B:175:PHE:N	2.84	0.46
1:C:268:ALA:O	1:C:272:LEU:HB2	2.15	0.46
1:D:227:ALA:O	1:D:228:LEU:HD23	2.16	0.46
1:E:16:VAL:HG11	1:E:65:VAL:HG11	1.96	0.46
1:A:184:GLN:CD	1:A:248:LEU:HB2	2.36	0.46
1:B:32:ARG:NH2	2:B:7517:UDP:H2'	2.30	0.46
1:C:156:LEU:HB3	1:C:222:ILE:HG13	1.98	0.46
1:C:248:LEU:HD22	1:C:249:VAL:N	2.30	0.45
1:A:271:LEU:HG	1:C:271:LEU:HG	1.98	0.45
1:A:128:ASP:O	1:B:144:ILE:HD13	2.17	0.45
1:C:243:ASN:ND2	1:C:246:ASN:HD22	2.07	0.45
1:C:287:ILE:O	1:C:291:MSE:HB2	2.16	0.45
1:A:154:LYS:HB2	1:A:154:LYS:HE2	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:TYR:HB3	1:D:155:ASN:ND2	2.27	0.45
1:F:173:ASN:ND2	3:F:321:HOH:O	2.50	0.45
1:A:164:PHE:HB2	1:A:287:ILE:HG23	1.98	0.45
1:D:6:THR:HG23	1:D:68:ALA:HB2	1.98	0.45
1:A:290:LEU:HD12	1:A:290:LEU:O	2.16	0.45
1:C:101:ASN:C	1:C:101:ASN:HD22	2.20	0.45
1:E:145:TYR:HB3	1:E:151:LEU:CD2	2.46	0.45
1:E:166:GLU:O	1:E:168:ASN:N	2.50	0.45
1:E:18:GLU:OE1	1:E:42:TYR:OH	2.35	0.45
1:E:69:ALA:HA	1:E:83:ASN:HD21	1.82	0.45
1:E:172:ILE:HD11	1:E:280:PHE:CZ	2.51	0.45
1:D:86:LEU:HD23	1:D:86:LEU:O	2.16	0.45
1:A:77:ILE:HD13	1:A:130:MSE:HG3	2.00	0.44
1:B:268:ALA:C	1:B:270:GLU:H	2.19	0.44
1:A:12:LEU:HD22	1:A:16:VAL:HG23	1.99	0.44
1:D:180:PHE:CD2	1:D:297:VAL:HG21	2.52	0.44
1:B:114:GLU:OE2	1:B:259:HIS:HD2	2.00	0.44
1:E:26:THR:HA	1:E:27:PRO:HD3	1.86	0.44
1:F:87:THR:CG2	1:F:91:TYR:CE2	3.00	0.44
1:D:202:ASP:HB3	1:D:276:THR:HG22	1.99	0.44
1:F:272:LEU:HD12	1:F:272:LEU:HA	1.83	0.44
1:B:213:GLN:HG3	1:B:272:LEU:HD12	2.00	0.44
1:B:286:GLU:O	1:B:290:LEU:HG	2.18	0.44
1:E:104:TYR:HB3	1:E:155:ASN:HD22	1.83	0.44
1:F:175:PHE:CZ	1:F:284:VAL:HG22	2.53	0.44
1:F:241:PHE:CE2	1:F:291:MSE:HE3	2.53	0.44
1:C:238:ASN:HD22	1:C:238:ASN:HA	1.61	0.43
1:E:108:ILE:C	1:E:110:ALA:H	2.20	0.43
1:F:228:LEU:HB3	1:F:232:GLU:HB2	2.00	0.43
1:C:183:GLU:O	1:C:243:ASN:ND2	2.50	0.43
1:A:124:LEU:HD23	1:B:124:LEU:HD23	1.99	0.43
1:B:77:ILE:HA	1:B:130:MSE:HG3	1.99	0.43
1:C:221:ASN:N	1:C:221:ASN:ND2	2.66	0.43
1:C:101:ASN:HD21	1:C:154:LYS:HZ2	1.65	0.43
1:D:112:SER:OG	1:D:126:LEU:HD23	2.18	0.43
1:A:49:TYR:HB3	1:A:86:LEU:HG	2.01	0.43
1:C:161:LEU:HD12	1:C:161:LEU:H	1.84	0.43
1:F:243:ASN:O	1:F:244:LYS:CB	2.67	0.43
1:A:269:LYS:HE2	1:F:115:THR:OG1	2.17	0.43
1:B:270:GLU:HG3	1:D:231:TYR:CG	2.54	0.43
1:C:11:PHE:O	1:C:15:TYR:HD2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ASN:OD1	1:E:168:ASN:C	2.56	0.43
1:F:175:PHE:CE1	1:F:284:VAL:HG22	2.53	0.43
1:A:164:PHE:O	1:A:165:ASN:HB3	2.18	0.43
1:A:213:GLN:HB3	1:A:216:VAL:CG2	2.49	0.43
1:C:11:PHE:HZ	1:C:163:GLY:HA3	1.84	0.43
1:C:237:ILE:HG23	1:C:241:PHE:CD1	2.53	0.43
1:E:152:CYS:HA	1:E:217:SER:HB3	2.01	0.43
1:F:65:VAL:CG1	1:F:67:LEU:HD21	2.47	0.43
1:C:51:LEU:O	1:C:55:ILE:HG13	2.19	0.42
1:C:163:GLY:HA2	1:C:287:ILE:HD11	2.01	0.42
1:B:215:LYS:HD2	1:B:215:LYS:HA	1.88	0.42
1:D:266:SER:O	1:D:269:LYS:HB3	2.17	0.42
1:F:59:ASN:HA	1:F:97:ASN:OD1	2.19	0.42
1:A:161:LEU:N	1:A:161:LEU:CD1	2.80	0.42
1:A:241:PHE:HE1	1:A:284:VAL:HG12	1.84	0.42
1:D:4:ALA:HA	1:D:28:ILE:O	2.19	0.42
1:D:86:LEU:HD23	1:D:86:LEU:C	2.39	0.42
1:D:168:ASN:OD1	1:D:168:ASN:C	2.57	0.42
1:A:224:SER:OG	1:A:226:ASP:HB3	2.20	0.42
1:B:193:ALA:C	1:B:229:THR:HG22	2.40	0.42
1:F:117:LEU:HD21	1:F:119:TRP:CZ2	2.54	0.42
1:B:230:ASN:N	1:B:230:ASN:ND2	2.66	0.42
1:C:272:LEU:O	1:C:273:ASP:HB2	2.19	0.42
1:E:21:LYS:HD3	1:E:42:TYR:HE1	1.83	0.42
1:E:48:ASP:OD1	1:E:48:ASP:C	2.58	0.42
1:A:195:ARG:NH2	1:A:230:ASN:HD21	2.17	0.42
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.85	0.42
1:F:125:PRO:HB3	1:F:136:LEU:HD11	2.02	0.42
1:F:169:ASN:HB2	1:F:170:TYR:H	1.55	0.42
1:A:145:TYR:O	1:A:149:LYS:HB2	2.19	0.42
1:C:12:LEU:HD13	1:C:67:LEU:HD22	2.02	0.42
1:C:289:LEU:HD12	1:C:290:LEU:N	2.35	0.42
1:D:116:SER:HB3	1:D:119:TRP:CD1	2.54	0.42
1:E:267:LYS:HG3	1:E:271:LEU:HD22	2.02	0.42
1:F:243:ASN:O	1:F:244:LYS:HB2	2.20	0.42
1:A:81:HIS:HB3	1:B:81:HIS:CD2	2.55	0.42
1:A:196:GLU:OE2	1:A:223:GLY:HA3	2.20	0.42
1:C:198:LEU:HD22	1:C:222:ILE:O	2.20	0.42
1:E:47:SER:HA	1:E:53:ASP:OD2	2.20	0.42
1:F:9:THR:O	1:F:9:THR:CG2	2.68	0.42
1:F:238:ASN:HA	1:F:243:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:MSE:HE3	1:A:263:MSE:HB2	1.99	0.41
1:D:115:THR:O	1:D:115:THR:CG2	2.67	0.41
1:F:20:ILE:HA	1:F:208:ILE:HD11	2.01	0.41
1:F:101:ASN:ND2	1:F:214:GLU:HA	2.35	0.41
1:A:136:LEU:HD23	1:A:136:LEU:O	2.21	0.41
1:E:65:VAL:HG12	1:E:67:LEU:HD21	2.02	0.41
1:F:227:ALA:C	1:F:228:LEU:HD23	2.41	0.41
1:A:86:LEU:HD23	1:A:86:LEU:C	2.41	0.41
1:A:241:PHE:HE1	1:A:284:VAL:CG1	2.34	0.41
1:E:224:SER:OG	1:E:226:ASP:HB2	2.21	0.41
1:F:78:SER:HA	1:F:81:HIS:CD2	2.56	0.41
1:B:17:VAL:HG13	1:B:27:PRO:HB3	2.01	0.41
1:B:65:VAL:HG12	1:B:67:LEU:HG	2.03	0.41
1:F:287:ILE:CG2	1:F:291:MSE:HE2	2.49	0.41
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.63	0.41
1:B:6:THR:HG1	1:B:67:LEU:H	1.69	0.41
1:B:233:VAL:O	1:B:237:ILE:HG13	2.20	0.41
1:E:49:TYR:CG	1:E:86:LEU:HD12	2.56	0.41
1:F:102:ILE:HB	1:F:153:ILE:HG12	2.02	0.41
1:A:80:PHE:O	1:A:83:ASN:HB2	2.20	0.41
1:A:185:LEU:HD22	1:A:238:ASN:ND2	2.35	0.41
1:C:230:ASN:HD22	1:C:230:ASN:HA	1.59	0.41
1:E:48:ASP:CG	1:E:50:THR:HG23	2.41	0.41
1:F:66:HIS:CE1	1:F:87:THR:OG1	2.69	0.41
1:F:206:SER:HB3	1:F:274:PHE:CE1	2.56	0.41
1:C:51:LEU:HD12	1:C:55:ILE:HG13	2.03	0.41
1:F:53:ASP:O	1:F:57:GLN:HG2	2.20	0.41
1:A:227:ALA:HB2	1:A:262:TYR:HB3	2.03	0.40
1:B:142:GLY:HA2	1:B:153:ILE:HD13	2.04	0.40
1:F:241:PHE:HZ	1:F:291:MSE:HE3	1.85	0.40
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.81	0.40
1:D:280:PHE:O	1:D:284:VAL:HG23	2.21	0.40
1:F:21:LYS:HD3	1:F:42:TYR:HE1	1.85	0.40
1:F:243:ASN:HB3	1:F:244:LYS:H	1.56	0.40
1:A:59:ASN:HA	1:A:97:ASN:OD1	2.21	0.40
1:A:209:TYR:O	1:A:212:LYS:HB2	2.21	0.40
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.97	0.40
1:E:66:HIS:CE1	1:E:87:THR:OG1	2.60	0.40
1:F:42:TYR:CD2	1:F:42:TYR:N	2.89	0.40
1:A:255:ASN:O	1:A:256:GLU:HB2	2.20	0.40
1:A:271:LEU:HD23	1:C:271:LEU:HD21	2.04	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	281/311 (90%)	254 (90%)	20 (7%)	7 (2%)	5	25
1	B	245/311 (79%)	225 (92%)	17 (7%)	3 (1%)	13	43
1	C	272/311 (88%)	249 (92%)	18 (7%)	5 (2%)	8	33
1	D	283/311 (91%)	266 (94%)	14 (5%)	3 (1%)	14	46
1	E	254/311 (82%)	235 (92%)	14 (6%)	5 (2%)	7	30
1	F	259/311 (83%)	233 (90%)	23 (9%)	3 (1%)	13	43
All	All	1594/1866 (85%)	1462 (92%)	106 (7%)	26 (2%)	9	36

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ASP
1	B	11	PHE
1	C	188	HIS
1	D	294	LEU
1	F	168	ASN
1	D	73	SER
1	D	295	ASP
1	E	167	LYS
1	A	289	LEU
1	B	165	ASN
1	C	68	ALA
1	C	113	ASP
1	E	72	GLY
1	E	109	SER
1	E	113	ASP
1	F	170	TYR
1	F	177	ARG

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Mol	Chain	Res	Type
1	A	112	SER
1	A	165	ASN
1	C	243	ASN
1	E	112	SER
1	A	73	SER
1	A	253	ASN
1	B	112	SER
1	C	192	VAL
1	A	225	GLY

5.3.2 Protein sidechains ⓘ

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	244/262 (93%)	230 (94%)	14 (6%)	20	52
1	B	218/262 (83%)	205 (94%)	13 (6%)	19	50
1	C	240/262 (92%)	226 (94%)	14 (6%)	20	51
1	D	248/262 (95%)	232 (94%)	16 (6%)	17	46
1	E	224/262 (86%)	206 (92%)	18 (8%)	12	37
1	F	223/262 (85%)	205 (92%)	18 (8%)	11	36
All	All	1397/1572 (89%)	1304 (93%)	93 (7%)	16	45

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	34	ILE
1	A	51	LEU
1	A	100	SER
1	A	101	ASN
1	A	116	SER
1	A	130	MSE
1	A	154	LYS
1	A	172	ILE

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Mol	Chain	Res	Type
1	A	177	ARG
1	A	201	LYS
1	A	248	LEU
1	A	271	LEU
1	A	290	LEU
1	B	12	LEU
1	B	32	ARG
1	B	76	LYS
1	B	82	ASP
1	B	116	SER
1	B	130	MSE
1	B	161	LEU
1	B	166	GLU
1	B	169	ASN
1	B	175	PHE
1	B	272	LEU
1	B	275	SER
1	B	289	LEU
1	C	12	LEU
1	C	100	SER
1	C	101	ASN
1	C	116	SER
1	C	130	MSE
1	C	136	LEU
1	C	151	LEU
1	C	169	ASN
1	C	186	THR
1	C	192	VAL
1	C	201	LYS
1	C	215	LYS
1	C	238	ASN
1	C	265	SER
1	D	6	THR
1	D	30	LEU
1	D	82	ASP
1	D	98	ASN
1	D	115	THR
1	D	116	SER
1	D	154	LYS
1	D	187	LEU
1	D	194	LYS
1	D	226	ASP

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Mol	Chain	Res	Type
1	D	247	LEU
1	D	249	VAL
1	D	260	SER
1	D	295	ASP
1	D	297	VAL
1	D	301	LEU
1	E	6	THR
1	E	30	LEU
1	E	32	ARG
1	E	51	LEU
1	E	71	ARG
1	E	86	LEU
1	E	98	ASN
1	E	101	ASN
1	E	115	THR
1	E	116	SER
1	E	124	LEU
1	E	136	LEU
1	E	167	LYS
1	E	211	LEU
1	E	259	HIS
1	E	271	LEU
1	E	272	LEU
1	E	289	LEU
1	F	1	LEU
1	F	9	THR
1	F	31	THR
1	F	42	TYR
1	F	51	LEU
1	F	70	THR
1	F	98	ASN
1	F	100	SER
1	F	115	THR
1	F	116	SER
1	F	192	VAL
1	F	211	LEU
1	F	256	GLU
1	F	258	ILE
1	F	265	SER
1	F	266	SER
1	F	271	LEU
1	F	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	81	HIS
1	A	89	ASN
1	A	101	ASN
1	A	143	ASN
1	A	155	ASN
1	A	169	ASN
1	A	184	GLN
1	A	221	ASN
1	A	230	ASN
1	A	238	ASN
1	B	89	ASN
1	B	101	ASN
1	B	143	ASN
1	B	155	ASN
1	B	160	HIS
1	B	221	ASN
1	B	230	ASN
1	B	238	ASN
1	B	259	HIS
1	C	56	ASN
1	C	81	HIS
1	C	89	ASN
1	C	101	ASN
1	C	143	ASN
1	C	155	ASN
1	C	169	ASN
1	C	184	GLN
1	C	221	ASN
1	C	230	ASN
1	C	238	ASN
1	C	246	ASN
1	D	66	HIS
1	D	89	ASN
1	D	101	ASN
1	D	143	ASN
1	D	155	ASN
1	D	181	HIS
1	D	221	ASN
1	D	230	ASN
1	D	238	ASN

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Mol	Chain	Res	Type
1	E	66	HIS
1	E	89	ASN
1	E	101	ASN
1	E	143	ASN
1	E	155	ASN
1	E	165	ASN
1	E	178	GLN
1	E	221	ASN
1	E	230	ASN
1	E	238	ASN
1	F	66	HIS
1	F	83	ASN
1	F	89	ASN
1	F	101	ASN
1	F	143	ASN
1	F	155	ASN
1	F	221	ASN
1	F	230	ASN
1	F	243	ASN
1	F	259	HIS

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](#)

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	UDP	B	7517	-	25,26,26	3.76	13 (52%)	38,40,40	2.11	13 (34%)

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	UDP	B	7517	-	-	8/16/32/32	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7517	UDP	O4-C4	9.18	1.42	1.24
2	B	7517	UDP	PA-O3A	8.58	1.68	1.59
2	B	7517	UDP	C2-N3	6.39	1.49	1.38
2	B	7517	UDP	PB-O1B	5.57	1.67	1.50
2	B	7517	UDP	PA-O1A	5.08	1.68	1.50
2	B	7517	UDP	C6-N1	4.68	1.49	1.38
2	B	7517	UDP	C6-C5	4.20	1.44	1.35
2	B	7517	UDP	C4-N3	3.58	1.44	1.38
2	B	7517	UDP	PB-O2B	3.08	1.66	1.54
2	B	7517	UDP	PA-O5'	2.84	1.70	1.59
2	B	7517	UDP	C3'-C2'	2.46	1.60	1.53
2	B	7517	UDP	C3'-C4'	2.36	1.59	1.53
2	B	7517	UDP	PB-O3B	-2.13	1.46	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7517	UDP	C4-N3-C2	-5.85	119.34	126.61
2	B	7517	UDP	N3-C2-N1	4.32	120.52	114.89
2	B	7517	UDP	C5-C4-N3	3.74	120.03	114.80
2	B	7517	UDP	O4-C4-C5	-3.34	119.40	125.16
2	B	7517	UDP	O2'-C2'-C1'	3.19	121.07	110.10
2	B	7517	UDP	O5'-C5'-C4'	3.05	119.39	108.99
2	B	7517	UDP	O2'-C2'-C3'	3.01	121.48	111.82
2	B	7517	UDP	O4'-C4'-C5'	2.95	118.79	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7517	UDP	O3'-C3'-C4'	2.80	119.13	111.08
2	B	7517	UDP	O3'-C3'-C2'	2.78	120.72	111.82
2	B	7517	UDP	C5'-C4'-C3'	2.44	124.00	115.21
2	B	7517	UDP	O4'-C4'-C3'	-2.19	100.80	105.15
2	B	7517	UDP	O2-C2-N1	-2.01	120.18	122.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

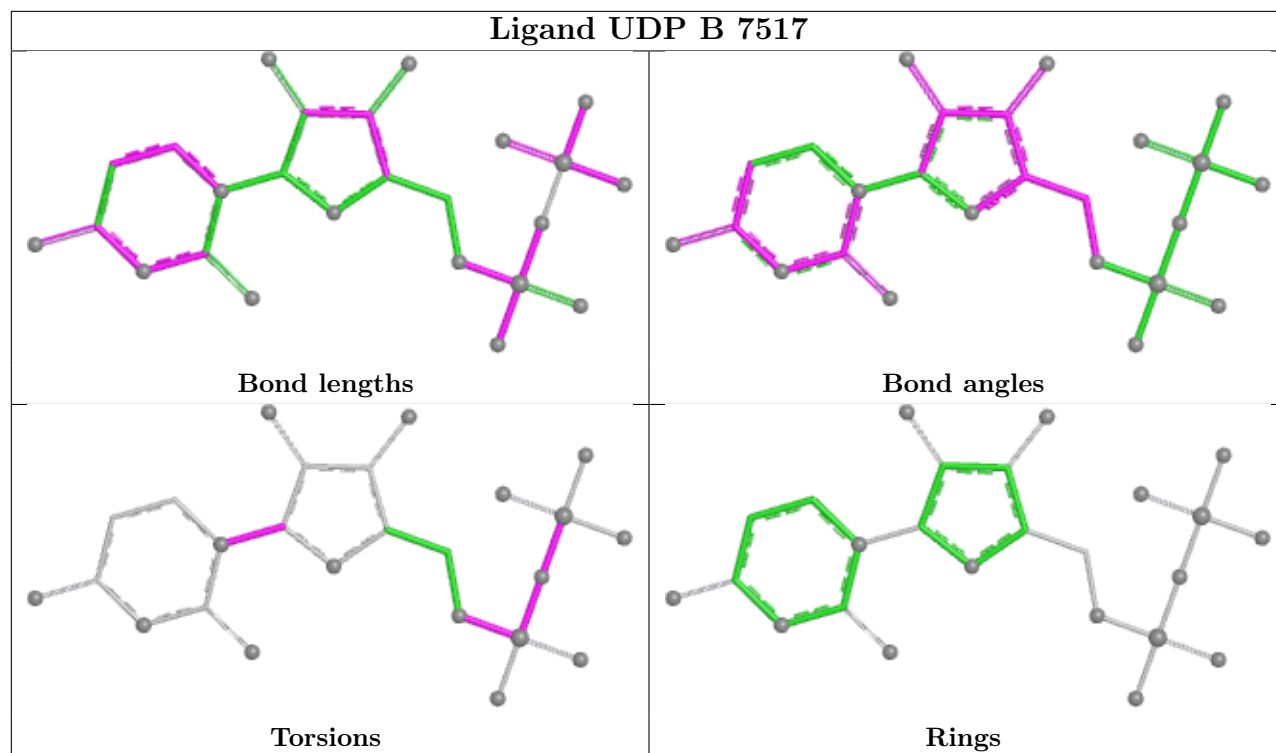
Mol	Chain	Res	Type	Atoms
2	B	7517	UDP	O4'-C1'-N1-C2
2	B	7517	UDP	O4'-C1'-N1-C6
2	B	7517	UDP	PA-O3A-PB-O3B
2	B	7517	UDP	C5'-O5'-PA-O1A
2	B	7517	UDP	PB-O3A-PA-O2A
2	B	7517	UDP	PA-O3A-PB-O2B
2	B	7517	UDP	PB-O3A-PA-O1A
2	B	7517	UDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7517	UDP	4	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 than 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.



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, 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(Å²)	Q<0.9
1	A	283/311 (90%)	0.31	0	100100	32, 40, 59, 71	0
1	B	251/311 (80%)	0.48	5 (1%)	6548	37, 49, 85, 96	0
1	C	276/311 (88%)	0.37	6 (2%)	6245	33, 43, 81, 98	0
1	D	285/311 (91%)	0.31	4 (1%)	7559	26, 39, 54, 72	0
1	E	258/311 (82%)	0.35	3 (1%)	7963	33, 42, 73, 80	0
1	F	263/311 (84%)	0.33	3 (1%)	8065	30, 39, 74, 78	0
All	All	1616/1866 (86%)	0.36	21 (1%)	7761	26, 42, 75, 98	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	PHE	3.3
1	C	172	ILE	2.7
1	C	187	LEU	2.6
1	C	289	LEU	2.5
1	C	237	ILE	2.5
1	C	189	ALA	2.4
1	F	289	LEU	2.4
1	B	241	PHE	2.4
1	D	71	ARG	2.4
1	E	241	PHE	2.3
1	C	70	THR	2.3
1	E	231	TYR	2.2
1	F	280	PHE	2.2
1	D	73	SER	2.2
1	B	169	ASN	2.1
1	B	288	HIS	2.1
1	E	172	ILE	2.1
1	F	165	ASN	2.1
1	D	188	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	243	ASN	2.0
1	D	41	ASP	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](#)

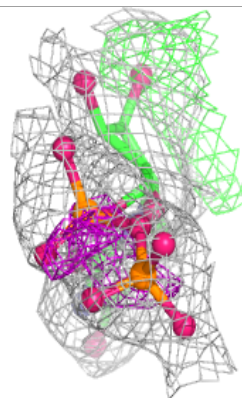
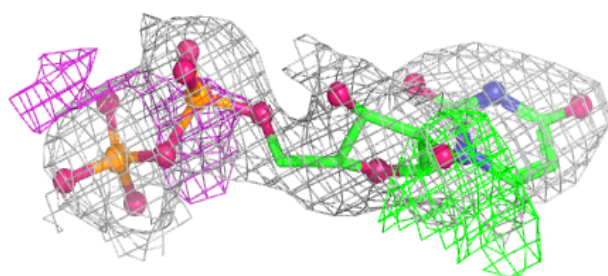
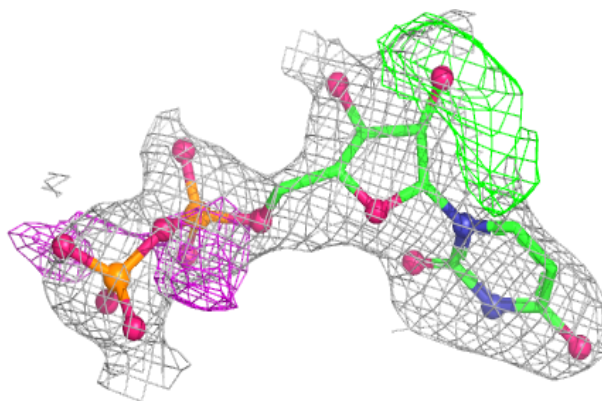
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	UDP	B	7517	25/25	0.85	0.25	51,55,59,62	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 UDP B 7517:

$2mF_o-DF_c$ (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.