



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:20 AM UTC

PDB ID : 1NHE / pdb_00001nhe
Title : Crystal structure of Lactose synthase complex with UDP
Authors : Ramakrishnan, B.; Qasba, P.K.
Deposited on : 2002-12-19
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

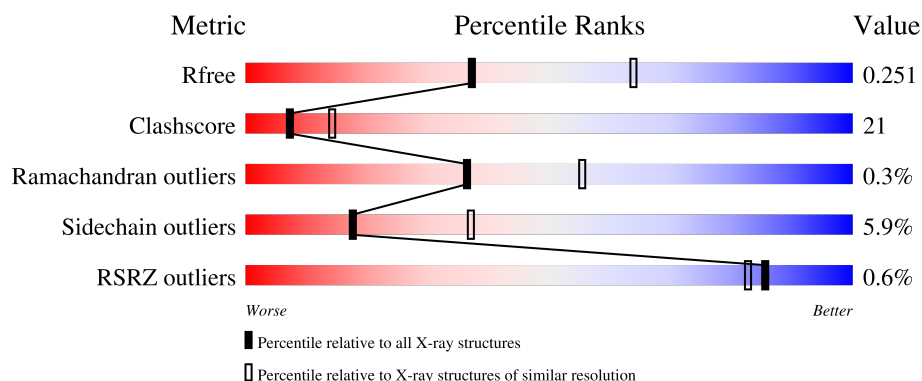
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	123	% 66% 33% .
1	C	123	2% 66% 31% .
2	B	286	55% 34% 6% 5%
2	D	286	56% 31% 7% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6803 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 ALPHA-LACTALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			979	620	156	194	9			
1	C	123	Total	C	N	O	S	0	0	0
			979	620	156	194	9			

- Molecule 2 is a protein called BETA-1,4-GALACTOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	272	Total	C	N	O	S	Se	0	0	0
			2218	1424	382	398	5	9			
2	D	272	Total	C	N	O	S	Se	0	0	0
			2218	1424	382	398	5	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MSE	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MSE	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
B	145	MSE	MET	cloning artifact	UNP P08037
B	174	MSE	MET	cloning artifact	UNP P08037
B	225	MSE	MET	cloning artifact	UNP P08037

Continued on next page...

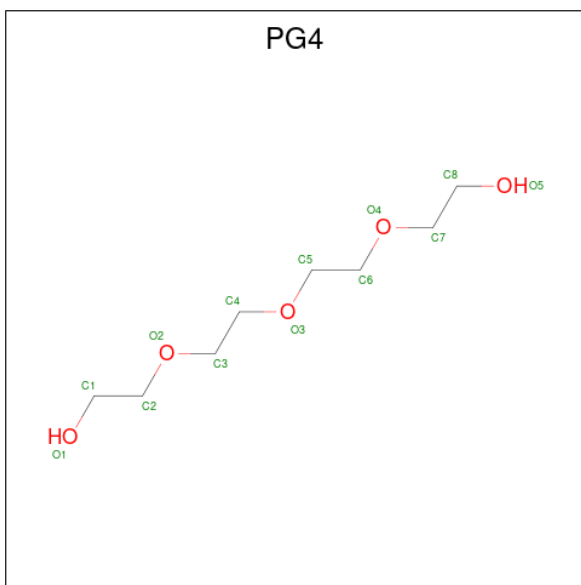
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	258	MSE	MET	cloning artifact	UNP P08037
B	277	MSE	MET	cloning artifact	UNP P08037
B	330	MSE	MET	cloning artifact	UNP P08037
B	344	MSE	MET	cloning artifact	UNP P08037
B	370	MSE	MET	cloning artifact	UNP P08037
B	381	MSE	MET	cloning artifact	UNP P08037
D	117	ALA	-	SEE REMARK 999	UNP P08037
D	118	SER	-	SEE REMARK 999	UNP P08037
D	119	MSE	-	SEE REMARK 999	UNP P08037
D	120	THR	-	SEE REMARK 999	UNP P08037
D	121	GLY	-	SEE REMARK 999	UNP P08037
D	122	GLY	-	SEE REMARK 999	UNP P08037
D	123	GLN	-	SEE REMARK 999	UNP P08037
D	124	GLN	-	SEE REMARK 999	UNP P08037
D	125	MSE	-	SEE REMARK 999	UNP P08037
D	126	GLY	-	SEE REMARK 999	UNP P08037
D	127	ARG	-	SEE REMARK 999	UNP P08037
D	128	GLY	-	SEE REMARK 999	UNP P08037
D	129	SER	-	SEE REMARK 999	UNP P08037
D	145	MSE	MET	cloning artifact	UNP P08037
D	174	MSE	MET	cloning artifact	UNP P08037
D	225	MSE	MET	cloning artifact	UNP P08037
D	258	MSE	MET	cloning artifact	UNP P08037
D	277	MSE	MET	cloning artifact	UNP P08037
D	330	MSE	MET	cloning artifact	UNP P08037
D	344	MSE	MET	cloning artifact	UNP P08037
D	370	MSE	MET	cloning artifact	UNP P08037
D	381	MSE	MET	cloning artifact	UNP P08037

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

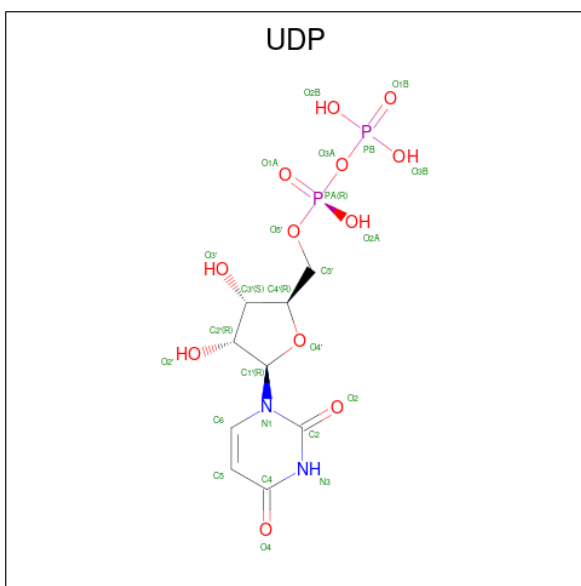
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	C	1	Total C O 13 8 5	0	0

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 25	C 9	N 2	O 12	P 2	0	0
5	D	1	Total 25	C 9	N 2	O 12	P 2	0	0

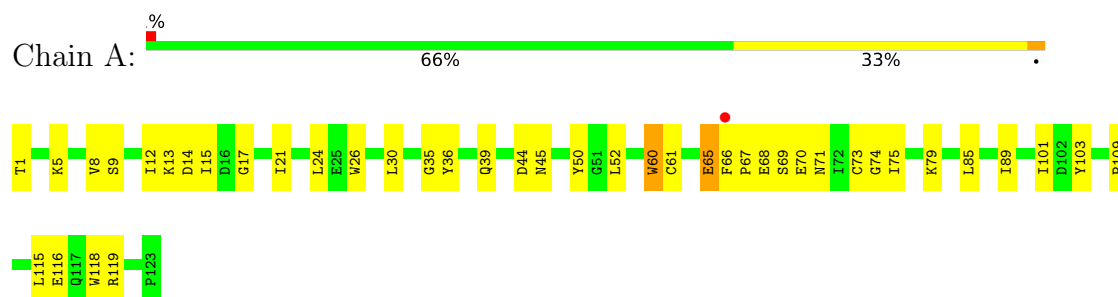
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	55	Total 55	O 55	0	0
6	B	134	Total 134	O 134	0	0
6	C	56	Total 56	O 56	0	0
6	D	86	Total 86	O 86	0	0

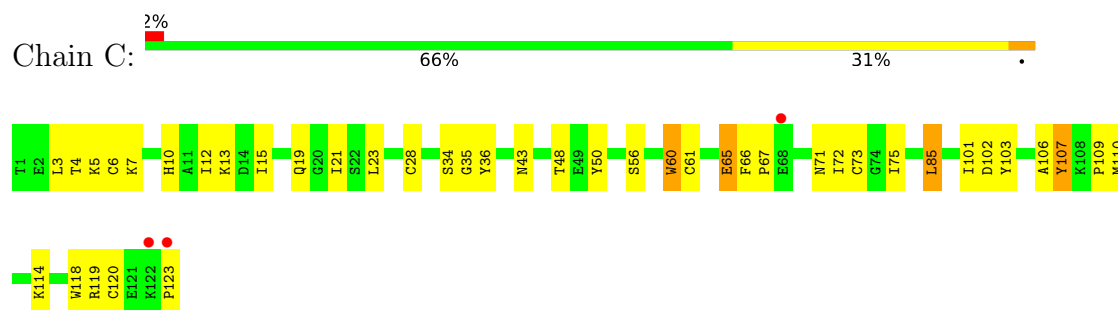
3 Residue-property plots

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.

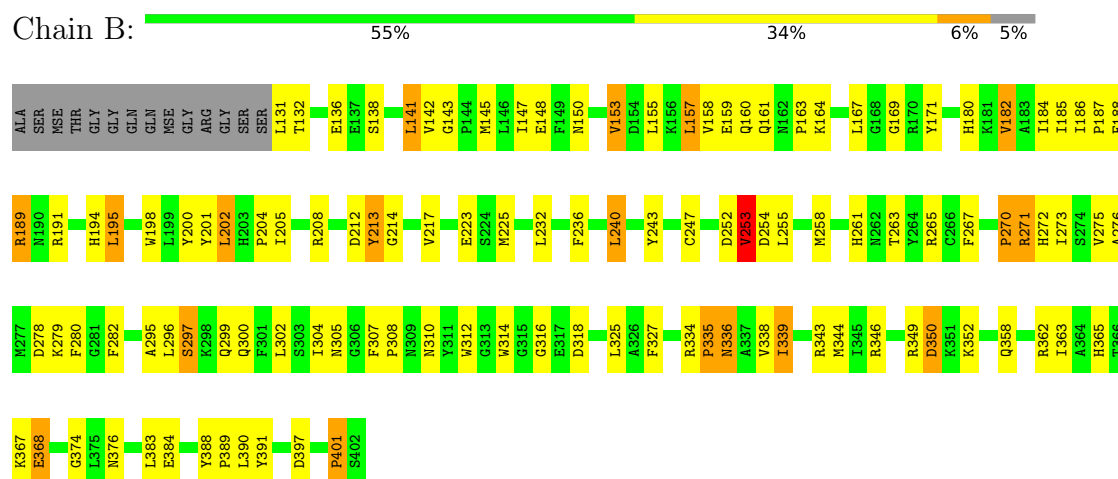
• Molecule 1: ALPHA-LACTALBUMIN



• Molecule 1: ALPHA-LACTALBUMIN

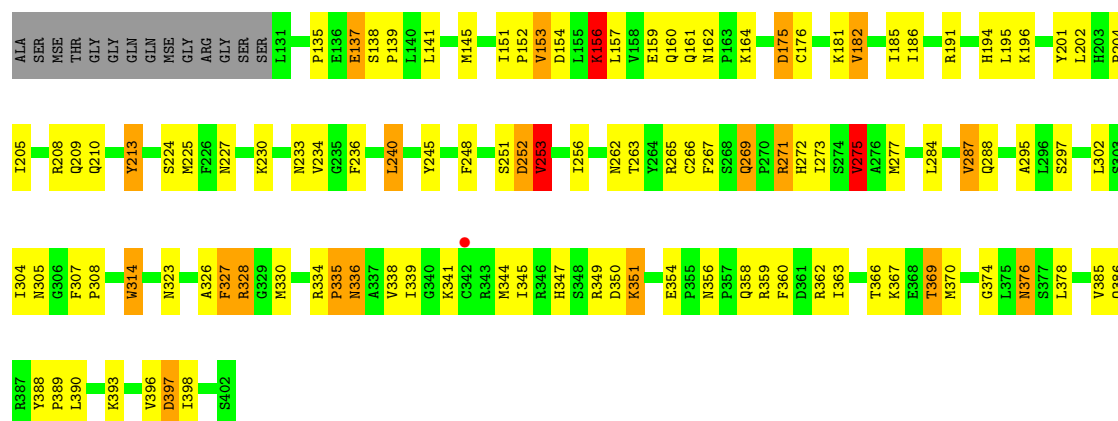


• Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE



• Molecule 2: BETA-1,4-GALACTOSYLTRANSFERASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.17Å 99.01Å 102.38Å 90.00° 103.92° 90.00°	Depositor
Resolution (Å)	19.90 – 2.50 19.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.90-2.50) 99.2 (19.90-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.255 0.194 , 0.251	Depositor DCC
R_{free} test set	3686 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6803	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PG4, 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	0.64	0/1000	1.12	7/1350 (0.5%)
1	C	0.64	0/1000	1.07	7/1350 (0.5%)
2	B	0.64	0/2269	1.09	14/3058 (0.5%)
2	D	0.57	0/2269	1.12	21/3058 (0.7%)
All	All	0.62	0/6538	1.10	49/8816 (0.6%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	TYR	N-CA-C	-9.65	100.84	111.36
2	D	182	VAL	N-CA-C	9.02	121.25	108.36
2	B	182	VAL	N-CA-C	8.28	119.76	108.17
1	C	60	TRP	N-CA-C	8.05	123.64	112.45
1	A	35	GLY	N-CA-C	-7.91	104.30	115.30
2	D	273	ILE	N-CA-C	7.83	118.73	111.45
2	D	275	VAL	N-CA-C	7.74	118.53	110.72
1	A	50	TYR	N-CA-C	7.71	121.97	109.40
2	B	213	TYR	N-CA-C	7.57	120.91	109.41
2	B	297	SER	N-CA-C	-7.38	101.02	110.53
1	A	60	TRP	N-CA-C	7.33	122.50	112.90
2	D	213	TYR	N-CA-C	7.30	120.87	110.14
1	C	120	CYS	N-CA-C	-7.24	100.49	111.56
2	B	188	PHE	N-CA-C	7.21	120.31	108.99
2	D	202	LEU	N-CA-C	7.13	119.06	111.28
2	B	273	ILE	N-CA-C	7.08	118.40	111.67
1	C	50	TYR	N-CA-C	7.03	121.12	109.95
2	B	310	ASN	N-CA-C	6.87	121.26	113.02
2	D	297	SER	N-CA-C	-6.79	102.06	110.41
1	C	103	TYR	N-CA-C	-6.60	104.17	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	314	TRP	N-CA-C	6.42	119.55	110.50
2	D	253	VAL	CB-CA-C	-6.38	101.93	112.26
2	B	263	THR	N-CA-C	6.31	119.50	110.10
2	D	335	PRO	N-CA-C	-6.30	101.74	111.13
2	D	156	LYS	N-CA-C	-6.25	104.38	111.07
2	B	271	ARG	N-CA-C	6.19	118.81	108.73
2	D	162	ASN	CA-C-N	6.14	126.03	119.28
2	D	162	ASN	C-N-CA	6.14	126.03	119.28
2	D	369	THR	N-CA-C	6.03	119.47	111.75
1	A	24	LEU	N-CA-C	-5.87	104.80	111.14
2	B	253	VAL	CB-CA-C	-5.82	102.83	112.26
2	D	314	TRP	N-CA-C	5.79	118.66	110.50
2	B	202	LEU	N-CA-C	5.59	117.38	111.28
1	C	107	TYR	N-CA-C	5.59	117.07	110.97
2	D	385	VAL	N-CA-C	-5.59	100.43	108.48
2	B	335	PRO	N-CA-C	-5.57	103.06	111.41
2	D	356	ASN	CA-C-N	5.53	125.20	119.56
2	D	356	ASN	C-N-CA	5.53	125.20	119.56
1	C	56	SER	N-CA-C	5.47	118.84	110.20
2	D	201	TYR	N-CA-C	5.45	118.04	111.40
1	A	109	PRO	N-CA-C	5.43	120.68	113.57
2	B	350	ASP	N-CA-C	5.18	117.74	110.23
2	B	185	ILE	N-CA-C	5.17	115.30	107.80
1	C	85	LEU	N-CA-C	5.17	119.43	113.18
1	A	14	ASP	N-CA-C	5.16	119.06	112.87
2	D	251	SER	N-CA-C	5.12	117.80	109.24
2	D	271	ARG	N-CA-C	5.10	117.27	109.07
2	D	388	TYR	N-CA-C	-5.07	101.31	109.82
2	D	252	ASP	N-CA-C	-5.05	103.37	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	979	0	936	32	0
1	C	979	0	936	36	0
2	B	2218	0	2185	84	0
2	D	2218	0	2185	116	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	13	0	18	3	0
4	C	13	0	18	3	0
5	B	25	0	11	2	0
5	D	25	0	11	5	0
6	A	55	0	0	2	0
6	B	134	0	0	6	0
6	C	56	0	0	2	0
6	D	86	0	0	3	0
All	All	6803	0	6300	263	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 21.

All (263) 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)
2:D:336:ASN:HD21	2:D:339:ILE:H	1.04	0.98
2:D:336:ASN:ND2	2:D:339:ILE:H	1.66	0.93
2:D:335:PRO:HB2	2:D:339:ILE:HD11	1.53	0.89
2:D:336:ASN:C	2:D:336:ASN:HD22	1.81	0.88
2:B:155:LEU:O	2:B:159:GLU:HG3	1.73	0.88
2:D:151:ILE:HD12	2:D:152:PRO:HD2	1.60	0.82
2:B:336:ASN:HD22	2:B:338:VAL:H	1.31	0.78
2:D:275:VAL:HG22	2:D:334:ARG:HD3	1.67	0.77
1:C:23:LEU:HD12	1:C:123:PRO:HB3	1.66	0.76
2:D:287:VAL:HG12	2:D:288:GLN:OE1	1.85	0.76
2:B:225:MSE:HE2	2:B:352:LYS:HE3	1.67	0.75
1:C:10:HIS:HA	1:C:13:LYS:HE2	1.68	0.75
2:D:154:ASP:OD2	2:D:156:LYS:HB2	1.87	0.75
2:B:336:ASN:ND2	2:B:338:VAL:H	1.85	0.75
2:B:336:ASN:HD22	2:B:336:ASN:C	1.96	0.74
2:D:336:ASN:HD21	2:D:339:ILE:N	1.83	0.74
1:A:71:ASN:HD21	1:A:75:ILE:H	1.35	0.73
1:A:61:CYS:HA	1:A:71:ASN:HD22	1.54	0.72
2:D:267:PHE:CE1	2:D:271:ARG:HD2	2.26	0.71
2:B:191:ARG:HH11	2:B:194:HIS:HD2	1.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:ILE:HD12	2:D:152:PRO:CD	2.22	0.70
2:B:180:HIS:CE1	2:B:265:ARG:HD2	2.27	0.70
2:D:275:VAL:CG2	2:D:334:ARG:HD3	2.21	0.70
2:D:191:ARG:HH11	2:D:194:HIS:HD2	1.40	0.69
1:C:21:ILE:HG13	1:C:101:ILE:HD13	1.72	0.69
2:D:233:ASN:HB3	2:D:378:LEU:HD22	1.73	0.69
1:C:71:ASN:HD21	1:C:75:ILE:H	1.41	0.69
2:B:305:ASN:HD21	2:B:376:ASN:H	1.41	0.68
1:A:61:CYS:HA	1:A:71:ASN:ND2	2.08	0.68
2:B:186:ILE:HG21	2:B:253:VAL:HG13	1.76	0.68
2:B:252:ASP:HB3	5:B:809:UDP:O3'	1.92	0.67
2:D:191:ARG:NH1	2:D:194:HIS:HD2	1.92	0.67
2:B:136:GLU:HB3	6:B:1011:HOH:O	1.94	0.67
2:D:307:PHE:HB3	2:D:308:PRO:HD2	1.77	0.67
2:B:307:PHE:HB3	2:B:308:PRO:HD2	1.76	0.66
2:D:153:VAL:HG22	2:D:196:LYS:HB3	1.78	0.66
2:D:358:GLN:O	2:D:362:ARG:HG3	1.96	0.66
2:D:284:LEU:HD21	2:D:334:ARG:CZ	2.27	0.65
2:D:225:MSE:HE1	2:D:354:GLU:OE1	1.95	0.65
2:D:339:ILE:C	2:D:339:ILE:HD12	2.22	0.64
2:B:160:GLN:O	2:B:163:PRO:HD3	1.98	0.64
2:D:186:ILE:HG21	2:D:253:VAL:HG13	1.80	0.64
2:D:137:GLU:CD	2:D:137:GLU:H	2.06	0.64
2:B:316:GLY:HA2	2:B:363:ILE:HD11	1.80	0.64
1:A:12:ILE:HD13	1:A:89:ILE:HD11	1.80	0.63
2:D:138:SER:HA	2:D:210:GLN:NE2	2.13	0.63
2:D:386:GLN:HE22	2:D:393:LYS:HD3	1.64	0.63
2:B:169:GLY:O	2:B:214:GLY:HA2	1.99	0.62
1:C:3:LEU:HD22	1:C:7:LYS:HE2	1.82	0.61
1:C:119:ARG:HE	1:C:123:PRO:HD3	1.63	0.61
2:D:230:LYS:HE2	2:D:398:ILE:HB	1.82	0.61
1:C:4:THR:H	1:C:7:LYS:HD3	1.65	0.61
1:C:85:LEU:HD22	1:C:85:LEU:N	2.16	0.61
2:D:205:ILE:O	2:D:209:GLN:HG3	2.00	0.60
2:D:386:GLN:NE2	2:D:393:LYS:HD3	2.15	0.60
1:A:116:GLU:OE2	1:A:119:ARG:NH2	2.33	0.60
2:B:187:PRO:HD3	2:B:232:LEU:HD21	1.83	0.60
2:D:209:GLN:NE2	2:D:263:THR:HA	2.15	0.60
1:A:66:PHE:HD2	1:A:69:SER:HB2	1.66	0.60
2:D:336:ASN:ND2	2:D:336:ASN:C	2.48	0.60
2:D:339:ILE:HD12	2:D:339:ILE:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:C	1:A:67:PRO:HD3	2.27	0.59
2:B:141:LEU:HD23	2:B:261:HIS:CD2	2.37	0.58
2:D:253:VAL:HG22	5:D:810:UDP:O2'	2.03	0.58
2:D:145:MSE:SE	2:D:208:ARG:HH22	2.37	0.57
2:D:252:ASP:HB3	5:D:810:UDP:O3'	2.05	0.57
2:D:307:PHE:O	2:D:374:GLY:HA2	2.04	0.57
2:D:351:LYS:HB3	2:D:351:LYS:HZ2	1.69	0.57
2:B:191:ARG:NH1	2:B:194:HIS:HD2	2.00	0.57
2:B:336:ASN:HD22	2:B:338:VAL:N	2.00	0.57
1:A:1:THR:N	1:A:39:GLN:HG3	2.20	0.57
2:D:269:GLN:HE21	2:D:269:GLN:HA	1.69	0.57
2:D:272:HIS:HB3	2:D:334:ARG:HG2	1.87	0.57
2:D:326:ALA:C	2:D:328:ARG:H	2.13	0.57
2:B:365:HIS:O	2:B:368:GLU:HG2	2.04	0.56
2:D:138:SER:HB3	2:D:141:LEU:CD1	2.35	0.56
2:D:327:PHE:CD2	2:D:367:LYS:HD3	2.40	0.56
2:D:328:ARG:CZ	2:D:370:MSE:HE2	2.35	0.56
2:D:137:GLU:CD	2:D:137:GLU:N	2.64	0.56
2:B:145:MSE:HE3	2:B:147:ILE:HD11	1.88	0.56
2:B:223:GLU:O	2:B:352:LYS:HE2	2.06	0.56
2:D:336:ASN:ND2	2:D:338:VAL:HG12	2.21	0.56
1:C:4:THR:OG1	1:C:7:LYS:HG3	2.07	0.55
4:C:814:PG4:H51	2:D:314:TRP:CH2	2.41	0.55
2:D:305:ASN:ND2	2:D:376:ASN:ND2	2.55	0.55
2:D:277:MSE:CE	2:D:344:MSE:HE3	2.37	0.55
1:A:66:PHE:N	1:A:67:PRO:HD3	2.22	0.55
1:C:65:GLU:C	1:C:67:PRO:HD3	2.32	0.54
2:D:153:VAL:HA	6:D:1189:HOH:O	2.07	0.54
2:D:327:PHE:CZ	2:D:367:LYS:HB2	2.43	0.54
1:C:34:SER:HA	4:C:814:PG4:H32	1.90	0.54
2:B:388:TYR:HB3	2:B:389:PRO:HD2	1.90	0.54
2:B:191:ARG:HD2	2:B:194:HIS:CD2	2.43	0.54
2:D:153:VAL:CG2	2:D:196:LYS:HB3	2.38	0.54
1:A:116:GLU:HB2	6:A:997:HOH:O	2.06	0.54
1:C:10:HIS:O	1:C:13:LYS:HG2	2.08	0.53
1:C:85:LEU:HD22	1:C:85:LEU:H	1.73	0.53
1:A:1:THR:H3	1:A:39:GLN:HG3	1.73	0.53
2:D:336:ASN:OD1	2:D:338:VAL:HG12	2.08	0.53
1:A:17:GLY:HA2	6:A:933:HOH:O	2.07	0.53
2:B:316:GLY:CA	2:B:363:ILE:HD11	2.39	0.53
2:D:336:ASN:CG	2:D:338:VAL:HG12	2.33	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:MSE:HE2	2:B:352:LYS:CE	2.36	0.52
2:B:358:GLN:O	2:B:362:ARG:HG3	2.10	0.52
2:D:336:ASN:HD21	2:D:338:VAL:CG1	2.23	0.52
1:A:8:VAL:HG21	1:A:36:TYR:CD1	2.45	0.52
1:A:12:ILE:CG2	1:A:15:ILE:HG22	2.39	0.52
2:B:184:ILE:N	2:B:184:ILE:HD12	2.25	0.51
2:B:336:ASN:ND2	2:B:336:ASN:C	2.63	0.51
2:D:359:ARG:O	2:D:363:ILE:HG23	2.10	0.51
2:B:270:PRO:HG2	2:B:325:LEU:HD22	1.91	0.51
2:B:147:ILE:O	2:B:343:ARG:HD2	2.10	0.51
2:B:254:ASP:O	2:B:344:MSE:HA	2.10	0.51
1:C:61:CYS:HA	1:C:71:ASN:ND2	2.25	0.51
1:A:71:ASN:OD1	1:A:74:GLY:HA2	2.10	0.51
1:C:119:ARG:HE	1:C:123:PRO:CD	2.24	0.51
2:D:157:LEU:O	2:D:160:GLN:HB3	2.10	0.51
2:D:266:CYS:C	2:D:267:PHE:CD1	2.89	0.51
2:B:191:ARG:NH1	2:B:194:HIS:CD2	2.79	0.50
2:B:253:VAL:HG22	5:B:809:UDP:O2'	2.10	0.50
2:B:186:ILE:CG2	2:B:253:VAL:HG13	2.42	0.50
2:D:277:MSE:HE3	2:D:344:MSE:HE3	1.93	0.50
2:D:204:PRO:O	2:D:208:ARG:HB2	2.12	0.50
2:D:181:LYS:O	2:D:245:TYR:HB3	2.11	0.50
1:A:70:GLU:O	1:A:71:ASN:C	2.54	0.49
2:D:138:SER:HA	2:D:210:GLN:HE21	1.76	0.49
1:C:110:MET:SD	2:D:363:ILE:HD12	2.52	0.49
1:A:9:SER:O	1:A:13:LYS:HE2	2.13	0.49
2:D:186:ILE:CG2	2:D:253:VAL:HG13	2.43	0.49
2:D:139:PRO:HD2	2:D:210:GLN:NE2	2.27	0.49
2:B:225:MSE:HA	2:B:352:LYS:O	2.11	0.49
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.47	0.49
2:D:233:ASN:O	2:D:236:PHE:HB3	2.13	0.49
1:A:12:ILE:O	1:A:12:ILE:HG22	2.12	0.49
4:C:814:PG4:H51	2:D:314:TRP:HH2	1.78	0.49
2:D:236:PHE:O	2:D:240:LEU:HD23	2.12	0.49
2:B:258:MSE:SE	2:B:343:ARG:HG3	2.62	0.48
2:B:279:LYS:HA	2:B:346:ARG:HH22	1.78	0.48
2:B:145:MSE:HE1	2:B:205:ILE:HD11	1.95	0.48
4:A:813:PG4:H72	2:B:349:ARG:HH22	1.78	0.48
2:D:138:SER:HB3	2:D:141:LEU:HD11	1.95	0.48
2:B:295:ALA:C	2:B:296:LEU:HD12	2.37	0.48
2:B:191:ARG:NH2	2:B:350:ASP:OD2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:ASP:HA	6:B:1222:HOH:O	2.13	0.48
4:A:813:PG4:H12	2:B:280:PHE:HE2	1.79	0.48
2:B:157:LEU:HD13	2:B:161:GLN:HG3	1.96	0.48
2:D:327:PHE:CE1	2:D:367:LYS:HB2	2.49	0.48
1:C:12:ILE:O	1:C:15:ILE:HG22	2.14	0.47
1:C:13:LYS:HD3	1:C:23:LEU:HD11	1.96	0.47
2:D:336:ASN:ND2	2:D:338:VAL:H	2.12	0.47
2:B:153:VAL:HA	6:B:1134:HOH:O	2.15	0.47
2:D:157:LEU:O	2:D:161:GLN:HG3	2.15	0.47
2:B:180:HIS:NE2	2:B:265:ARG:HD2	2.28	0.47
1:C:35:GLY:O	1:C:36:TYR:HB2	2.14	0.47
2:D:345:ILE:O	2:D:347:HIS:HD2	1.97	0.47
2:B:182:VAL:HG22	2:B:247:CYS:HB3	1.97	0.47
2:B:390:LEU:O	2:B:391:TYR:HB3	2.15	0.47
1:C:19:GLN:O	1:C:19:GLN:HG3	2.14	0.47
2:D:185:ILE:HD12	2:D:185:ILE:N	2.30	0.47
2:D:335:PRO:CB	2:D:339:ILE:HD11	2.35	0.47
2:B:145:MSE:SE	2:B:208:ARG:HH22	2.48	0.47
1:C:101:ILE:O	1:C:101:ILE:HG13	2.14	0.47
2:D:338:VAL:O	2:D:341:LYS:HG3	2.14	0.47
2:D:389:PRO:HG2	6:D:956:HOH:O	2.15	0.47
1:C:60:TRP:O	1:C:73:CYS:HB2	2.15	0.47
2:B:198:TRP:CZ2	2:B:202:LEU:HG	2.50	0.46
4:A:813:PG4:H12	2:B:279:LYS:HE2	1.98	0.46
2:B:389:PRO:HG2	6:B:1026:HOH:O	2.15	0.46
1:C:72:ILE:HG22	1:C:72:ILE:O	2.15	0.46
1:A:115:LEU:O	1:A:116:GLU:C	2.57	0.46
1:C:106:ALA:HB2	2:D:360:PHE:CZ	2.51	0.46
2:B:236:PHE:O	2:B:240:LEU:HD22	2.16	0.46
2:D:336:ASN:HD21	2:D:338:VAL:HG12	1.81	0.46
2:D:335:PRO:HB2	2:D:339:ILE:CD1	2.34	0.46
1:A:68:GLU:OE2	1:A:68:GLU:N	2.48	0.46
2:B:145:MSE:HE3	2:B:145:MSE:HB2	1.93	0.46
2:D:397:ASP:C	2:D:397:ASP:OD1	2.59	0.46
2:B:336:ASN:ND2	2:B:338:VAL:N	2.58	0.45
2:D:248:PHE:O	2:D:295:ALA:HA	2.15	0.45
2:D:157:LEU:O	2:D:161:GLN:N	2.43	0.45
2:B:171:TYR:HB3	2:B:213:TYR:CE2	2.51	0.45
2:D:358:GLN:HB2	2:D:362:ARG:HD2	1.98	0.45
1:C:6:CYS:O	1:C:10:HIS:CD2	2.69	0.45
2:D:135:PRO:HG3	2:D:139:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:CG2	1:A:12:ILE:O	2.64	0.45
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.99	0.45
2:B:307:PHE:O	2:B:374:GLY:HA2	2.17	0.45
1:C:107:TYR:HB3	6:C:927:HOH:O	2.17	0.45
1:A:60:TRP:O	1:A:73:CYS:HB2	2.17	0.45
1:C:102:ASP:HB2	6:C:943:HOH:O	2.17	0.45
2:D:182:VAL:O	2:D:213:TYR:HA	2.17	0.45
2:D:151:ILE:HG13	2:D:152:PRO:O	2.17	0.44
2:D:230:LYS:CE	2:D:398:ILE:HB	2.47	0.44
2:D:256:ILE:HD12	2:D:256:ILE:N	2.32	0.44
2:D:336:ASN:ND2	2:D:339:ILE:N	2.48	0.44
1:A:116:GLU:OE1	1:A:116:GLU:HA	2.16	0.44
1:C:109:PRO:HB2	2:D:363:ILE:CD1	2.47	0.44
1:A:21:ILE:HG13	1:A:101:ILE:HD13	1.99	0.44
2:B:198:TRP:CE2	2:B:202:LEU:HG	2.52	0.44
1:C:3:LEU:HD22	1:C:7:LYS:CE	2.48	0.44
1:C:28:CYS:HB2	1:C:118:TRP:CD1	2.53	0.44
2:B:212:ASP:OD2	2:B:243:TYR:OH	2.26	0.44
2:B:131:LEU:HB2	6:B:1107:HOH:O	2.16	0.44
1:A:12:ILE:HG23	1:A:15:ILE:HG22	1.99	0.43
2:B:158:VAL:HG22	2:B:200:TYR:HD1	1.82	0.43
1:C:43:ASN:ND2	1:C:48:THR:OG1	2.51	0.43
2:D:234:VAL:HG11	2:D:396:VAL:HG11	2.00	0.43
1:A:26:TRP:O	1:A:30:LEU:HG	2.19	0.43
2:D:271:ARG:HG3	2:D:272:HIS:N	2.32	0.43
2:B:195:LEU:HD11	2:B:217:VAL:HG21	2.00	0.43
2:B:358:GLN:HG2	6:B:1152:HOH:O	2.19	0.43
2:B:155:LEU:C	2:B:159:GLU:HG3	2.38	0.43
1:C:21:ILE:N	1:C:21:ILE:HD13	2.32	0.43
2:B:318:ASP:OD1	2:B:318:ASP:N	2.46	0.43
1:C:66:PHE:N	1:C:67:PRO:HD3	2.34	0.43
1:A:66:PHE:CD2	1:A:69:SER:HB2	2.49	0.43
2:B:278:ASP:OD1	2:B:279:LYS:N	2.51	0.43
1:A:12:ILE:HG23	1:A:15:ILE:CG2	2.48	0.43
1:C:114:LYS:HD3	2:D:287:VAL:HG11	2.01	0.43
2:D:336:ASN:ND2	2:D:338:VAL:N	2.67	0.43
2:D:369:THR:HB	6:D:1064:HOH:O	2.18	0.43
2:D:262:ASN:HB2	2:D:339:ILE:O	2.19	0.42
2:D:253:VAL:HG22	5:D:810:UDP:H2'	2.00	0.42
2:B:147:ILE:HB	2:B:343:ARG:HD2	2.00	0.42
2:D:159:GLU:HA	2:D:390:LEU:HD21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:LEU:CD2	2:B:344:MSE:HB2	2.50	0.42
2:B:201:TYR:O	2:B:204:PRO:HD2	2.19	0.42
2:D:304:ILE:HG23	2:D:330:MSE:HE1	2.02	0.42
2:D:326:ALA:C	2:D:328:ARG:N	2.76	0.42
2:D:253:VAL:CG2	5:D:810:UDP:H2'	2.50	0.42
2:B:138:SER:HB3	2:B:141:LEU:HD13	2.02	0.42
2:B:312:TRP:CD2	2:B:401:PRO:HG3	2.55	0.41
2:D:191:ARG:NH1	2:D:194:HIS:CD2	2.81	0.41
2:D:344:MSE:O	2:D:345:ILE:C	2.62	0.41
2:B:297:SER:OG	2:B:300:GLN:HG3	2.20	0.41
2:D:265:ARG:NH2	2:D:266:CYS:O	2.53	0.41
2:B:267:PHE:CD1	2:B:271:ARG:HD3	2.55	0.41
1:C:109:PRO:HB2	2:D:363:ILE:HD11	2.02	0.41
2:D:236:PHE:O	2:D:240:LEU:CD2	2.68	0.41
2:B:143:GLY:O	2:B:145:MSE:HG3	2.21	0.41
2:B:276:ALA:HB1	2:B:282:PHE:O	2.21	0.41
2:D:141:LEU:CD1	2:D:141:LEU:H	2.33	0.41
2:B:336:ASN:ND2	2:B:339:ILE:H	2.19	0.41
2:D:175:ASP:HB2	2:D:176:CYS:H	1.61	0.41
2:D:323:ASN:HB2	2:D:366:THR:HG21	2.02	0.41
2:B:159:GLU:HG2	2:B:390:LEU:HD11	2.02	0.41
2:B:304:ILE:O	2:B:305:ASN:HB3	2.21	0.41
1:C:4:THR:O	1:C:5:LYS:C	2.64	0.41
2:D:138:SER:CB	2:D:210:GLN:HE21	2.34	0.41
2:D:227:ASN:OD1	2:D:230:LYS:HB2	2.21	0.41
2:D:240:LEU:HD21	2:D:248:PHE:CZ	2.56	0.41
2:D:338:VAL:HG13	2:D:339:ILE:N	2.36	0.41
2:D:349:ARG:HG3	2:D:350:ASP:N	2.36	0.41
2:B:335:PRO:HB2	2:B:339:ILE:HG12	2.03	0.40
2:B:383:LEU:O	2:B:384:GLU:HB2	2.20	0.40
2:D:253:VAL:HG22	5:D:810:UDP:C2'	2.51	0.40
1:A:36:TYR:HA	1:A:52:LEU:CD1	2.52	0.40
2:B:189:ARG:O	2:B:191:ARG:HG2	2.21	0.40
1:A:5:LYS:HD2	1:A:118:TRP:O	2.22	0.40
1:A:101:ILE:O	1:A:101:ILE:HG13	2.21	0.40
2:D:209:GLN:HE22	2:D:263:THR:HA	1.83	0.40
2:D:326:ALA:O	2:D:328:ARG:N	2.55	0.40
1:A:44:ASP:HB3	1:A:45:ASN:H	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
1	C	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
2	B	270/286 (94%)	255 (94%)	14 (5%)	1 (0%)	30	49
2	D	270/286 (94%)	247 (92%)	22 (8%)	1 (0%)	30	49
All	All	782/818 (96%)	725 (93%)	55 (7%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	327	PHE
2	B	401	PRO

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	109/109 (100%)	106 (97%)	3 (3%)	38	66
1	C	109/109 (100%)	108 (99%)	1 (1%)	70	87
2	B	245/243 (101%)	225 (92%)	20 (8%)	10	23
2	D	245/243 (101%)	227 (93%)	18 (7%)	13	27
All	All	708/704 (101%)	666 (94%)	42 (6%)	18	37

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	79	LYS
1	A	85	LEU
2	B	132	THR
2	B	141	LEU
2	B	142	VAL
2	B	148	GLU
2	B	150	ASN
2	B	153	VAL
2	B	157	LEU
2	B	164	LYS
2	B	167	LEU
2	B	189	ARG
2	B	195	LEU
2	B	240	LEU
2	B	253	VAL
2	B	270	PRO
2	B	275	VAL
2	B	299	GLN
2	B	302	LEU
2	B	336	ASN
2	B	339	ILE
2	B	368	GLU
1	C	65	GLU
2	D	137	GLU
2	D	153	VAL
2	D	156	LYS
2	D	164	LYS
2	D	175	ASP
2	D	195	LEU
2	D	224	SER
2	D	240	LEU
2	D	253	VAL
2	D	269	GLN
2	D	275	VAL
2	D	287	VAL
2	D	302	LEU
2	D	328	ARG
2	D	336	ASN
2	D	351	LYS
2	D	376	ASN
2	D	397	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	71	ASN
2	B	160	GLN
2	B	162	ASN
2	B	194	HIS
2	B	305	ASN
2	B	310	ASN
2	B	336	ASN
1	C	32	HIS
1	C	43	ASN
1	C	71	ASN
2	D	150	ASN
2	D	160	GLN
2	D	180	HIS
2	D	194	HIS
2	D	210	GLN
2	D	305	ASN
2	D	310	ASN
2	D	336	ASN
2	D	347	HIS
2	D	386	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PG4	A	813	-	12,12,12	0.64	0	11,11,11	0.30	0
5	UDP	B	809	-	25,26,26	2.28	4 (16%)	38,40,40	1.45	7 (18%)
5	UDP	D	810	-	25,26,26	2.52	4 (16%)	38,40,40	1.41	8 (21%)
4	PG4	C	814	-	12,12,12	0.52	0	11,11,11	0.22	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
4	PG4	A	813	-	-	5/10/10/10	-
5	UDP	B	809	-	-	5/16/32/32	0/2/2/2
5	UDP	D	810	-	-	1/16/32/32	0/2/2/2
4	PG4	C	814	-	-	4/10/10/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	810	UDP	PA-O3A	10.60	1.70	1.59
5	B	809	UDP	PA-O3A	9.38	1.69	1.59
5	D	810	UDP	PB-O1B	3.97	1.62	1.50
5	B	809	UDP	PB-O1B	3.72	1.62	1.50
5	D	810	UDP	C2-N1	2.44	1.42	1.38
5	B	809	UDP	C4-N3	2.33	1.42	1.38
5	D	810	UDP	C1'-N1	2.10	1.53	1.47
5	B	809	UDP	C2-N1	2.03	1.41	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	809	UDP	O3B-PB-O1B	3.69	125.22	110.83
5	D	810	UDP	O3B-PB-O1B	3.68	125.17	110.83
5	B	809	UDP	O5'-C5'-C4'	3.20	119.88	108.99
5	B	809	UDP	O2-C2-N1	-3.01	118.87	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	810	UDP	O4'-C4'-C3'	-2.94	99.32	105.15
5	B	809	UDP	O2-C2-N3	2.61	126.30	121.49
5	B	809	UDP	C2'-C1'-N1	2.61	120.50	113.25
5	D	810	UDP	C2'-C1'-N1	2.46	120.11	113.25
5	D	810	UDP	O5'-C5'-C4'	2.44	117.31	108.99
5	B	809	UDP	O4'-C4'-C3'	-2.43	100.32	105.15
5	D	810	UDP	O4'-C1'-N1	-2.30	103.15	108.36
5	D	810	UDP	O2-C2-N1	-2.28	119.83	122.80
5	D	810	UDP	O2-C2-N3	2.20	125.55	121.49
5	D	810	UDP	O3A-PB-O1B	-2.13	99.81	111.04
5	B	809	UDP	O3A-PB-O1B	-2.12	99.90	111.04

There are no chirality outliers.

All (15) torsion outliers are listed below:

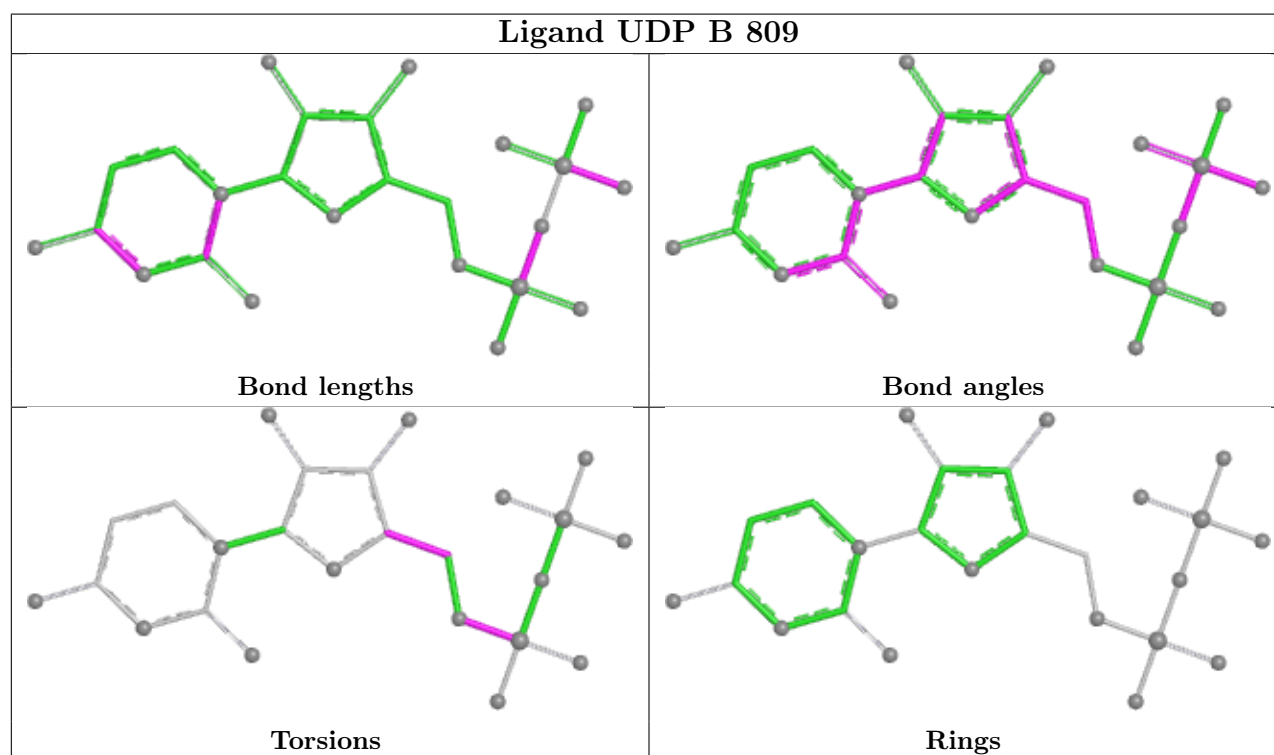
Mol	Chain	Res	Type	Atoms
5	B	809	UDP	C5'-O5'-PA-O1A
5	B	809	UDP	C5'-O5'-PA-O2A
5	B	809	UDP	C5'-O5'-PA-O3A
5	B	809	UDP	O4'-C4'-C5'-O5'
4	A	813	PG4	O2-C3-C4-O3
4	A	813	PG4	O3-C5-C6-O4
5	B	809	UDP	C3'-C4'-C5'-O5'
4	A	813	PG4	O1-C1-C2-O2
4	C	814	PG4	O4-C7-C8-O5
5	D	810	UDP	C3'-C4'-C5'-O5'
4	C	814	PG4	C1-C2-O2-C3
4	A	813	PG4	C3-C4-O3-C5
4	C	814	PG4	O1-C1-C2-O2
4	A	813	PG4	O4-C7-C8-O5
4	C	814	PG4	O3-C5-C6-O4

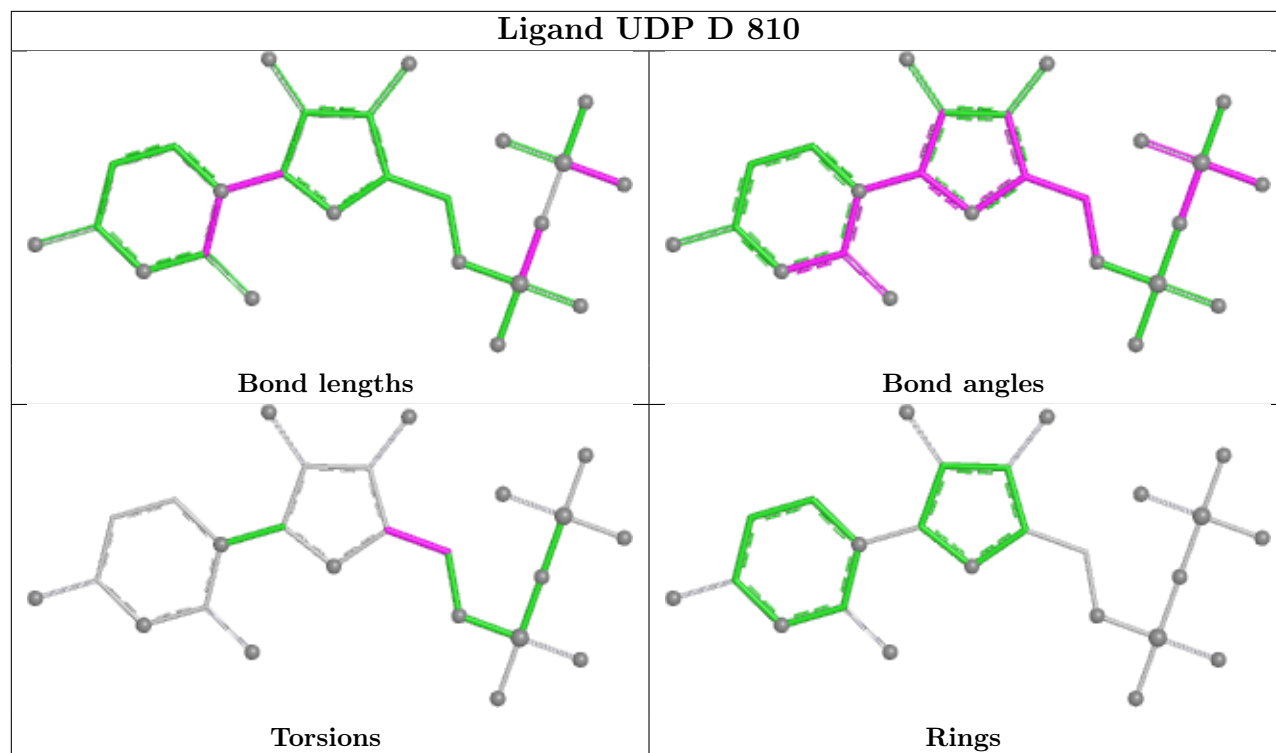
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	813	PG4	3	0
5	B	809	UDP	2	0
5	D	810	UDP	5	0
4	C	814	PG4	3	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 [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	123/123 (100%)	-0.20	1 (0%) 82 80	24, 42, 70, 85	0
1	C	123/123 (100%)	-0.33	3 (2%) 59 55	23, 37, 70, 101	0
2	B	263/286 (91%)	-0.41	0 100 100	20, 38, 66, 82	0
2	D	263/286 (91%)	-0.29	1 (0%) 88 86	30, 44, 68, 80	0
All	All	772/818 (94%)	-0.32	5 (0%) 85 83	20, 41, 69, 101	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	PRO	3.6
1	C	68	GLU	2.6
1	C	122	LYS	2.5
1	A	66	PHE	2.4
2	D	342	CYS	2.2

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 oligosaccharides in this entry.

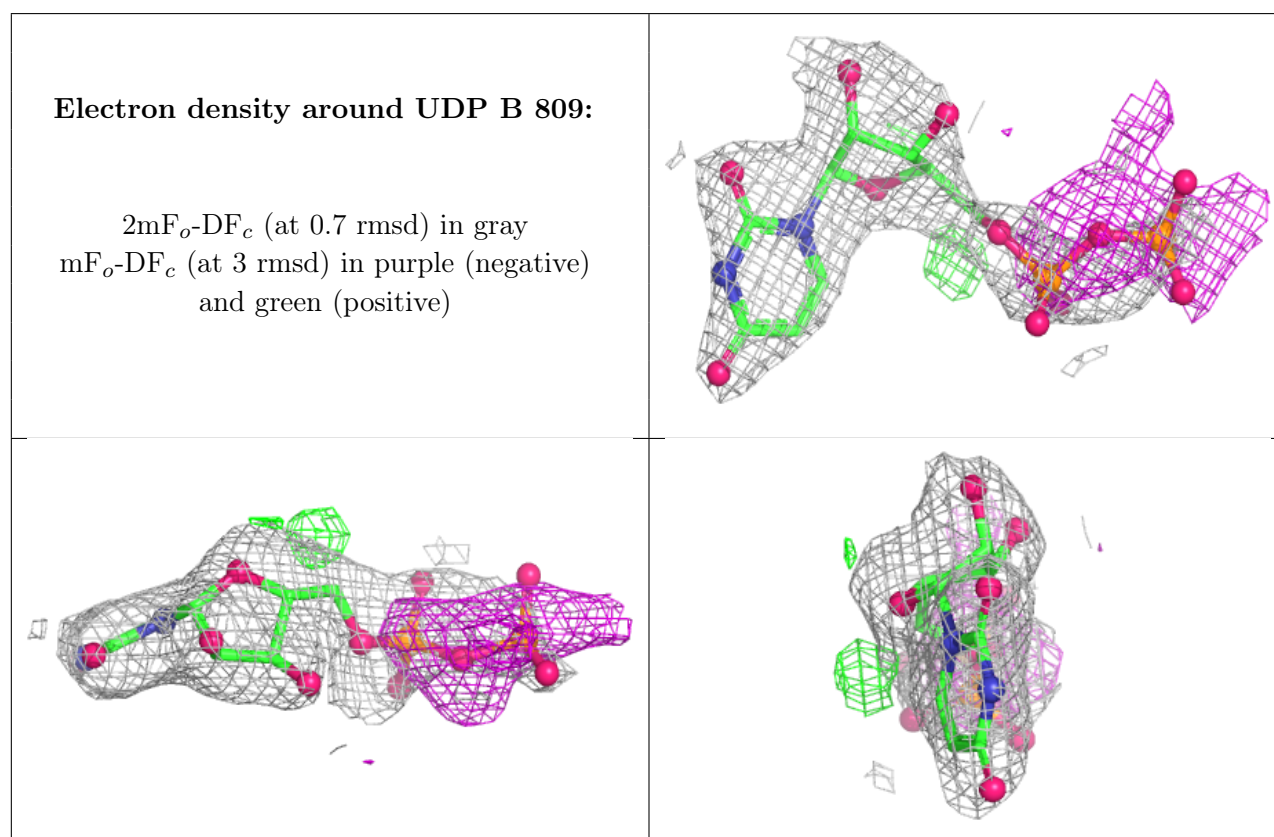
6.4 Ligands [i](#)

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.

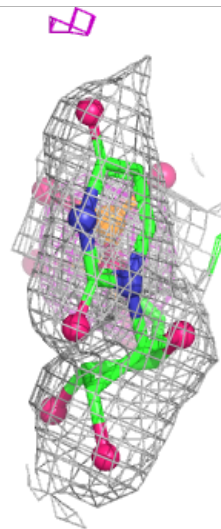
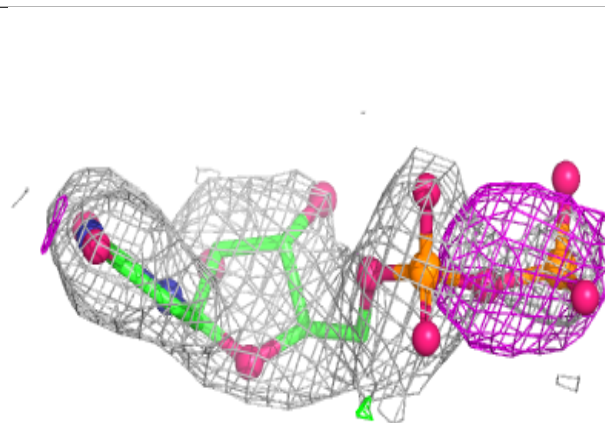
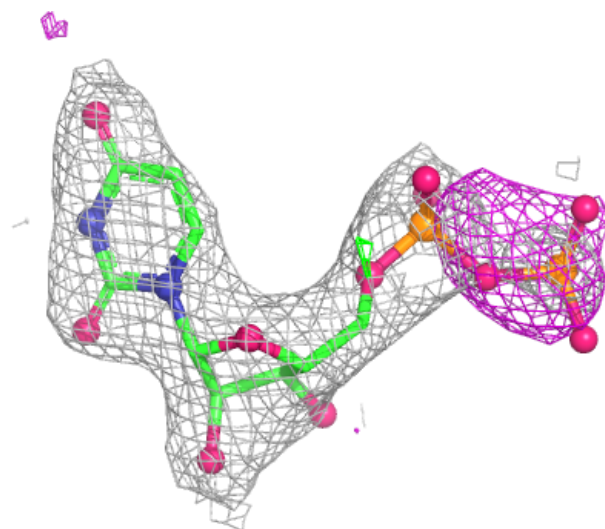
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	UDP	B	809	25/25	0.76	0.17	71,79,110,110	0
5	UDP	D	810	25/25	0.82	0.15	58,68,104,104	0
4	PG4	A	813	13/13	0.87	0.12	51,53,58,58	0
4	PG4	C	814	13/13	0.90	0.11	64,66,67,67	0
3	CA	A	805	1/1	0.98	0.03	40,40,40,40	0
3	CA	C	806	1/1	0.98	0.02	35,35,35,35	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 D 810:

$2mF_o-DF_c$ (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.