



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:49 AM UTC

PDB ID : 8F30 / pdb_00008f30
Title : LSD1-CoREST in complex with AW2, long soaking
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2022-11-09
Resolution : 3.10 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

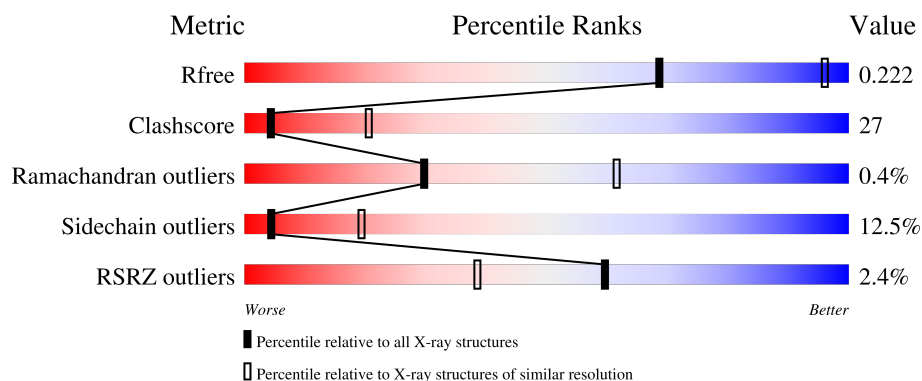
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	871	
2	B	144	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6349 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5204	3316	904	964	20			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O60341
A	-17	SER	-	expression tag	UNP O60341
A	-16	SER	-	expression tag	UNP O60341
A	-15	HIS	-	expression tag	UNP O60341
A	-14	HIS	-	expression tag	UNP O60341
A	-13	HIS	-	expression tag	UNP O60341
A	-12	HIS	-	expression tag	UNP O60341
A	-11	HIS	-	expression tag	UNP O60341
A	-10	HIS	-	expression tag	UNP O60341
A	-9	SER	-	expression tag	UNP O60341
A	-8	SER	-	expression tag	UNP O60341
A	-7	GLY	-	expression tag	UNP O60341
A	-6	LEU	-	expression tag	UNP O60341
A	-5	VAL	-	expression tag	UNP O60341
A	-4	PRO	-	expression tag	UNP O60341
A	-3	ARG	-	expression tag	UNP O60341
A	-2	GLY	-	expression tag	UNP O60341
A	-1	SER	-	expression tag	UNP O60341
A	0	HIS	-	expression tag	UNP O60341

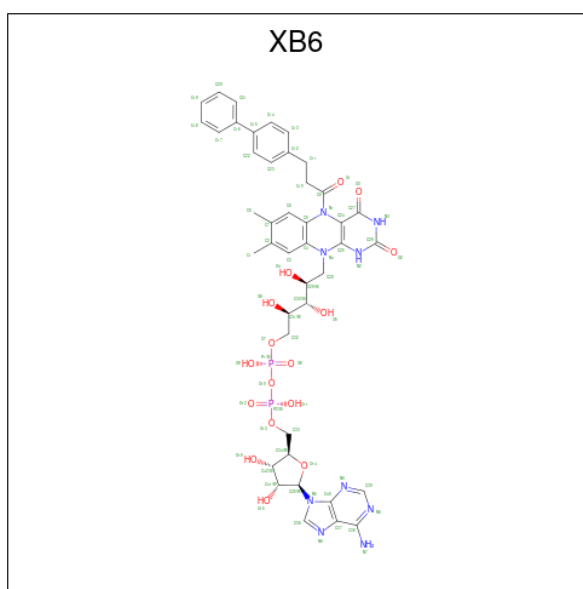
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

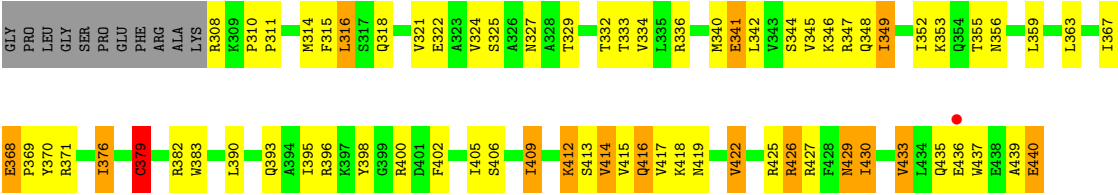
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag	UNP Q9UKL0
B	304	PHE	-	expression tag	UNP Q9UKL0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2R,3S,4S)-5-{5-[3-([1,1'-biphenyl]-4-yl)propanoyl]-7,8-dimethyl-2,4-dioxo-1,3,4,5-tetrahydrobenzo[g]pteridin-10(2H)-yl]-2,3,4-trihydroxypentyl dihydrogen diphosphate (non-preferred name) (CCD ID: XB6) (formula: C₄₂H₄₇N₉O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			69	42	9	16		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.21Å 179.76Å 234.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 3.10 47.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.57-3.10) 99.5 (47.57-3.10)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.202 , 0.223 0.218 , 0.222	Depositor DCC
R_{free} test set	887 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6349	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: XB6

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	0.96	8/5317 (0.2%)	1.15	9/7213 (0.1%)
2	B	0.89	1/1091 (0.1%)	1.30	2/1471 (0.1%)
All	All	0.95	9/6408 (0.1%)	1.18	11/8684 (0.1%)

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	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	808	PRO	C-O	-7.76	1.13	1.23
1	A	470	PRO	C-O	-7.26	1.18	1.24
1	A	361	PRO	C-O	-6.47	1.16	1.23
1	A	760	SER	CA-CB	-5.80	1.45	1.53
1	A	794	PRO	C-O	-5.65	1.17	1.23
1	A	782	PRO	C-O	-5.62	1.17	1.23
2	B	310	PRO	C-O	-5.49	1.18	1.24
1	A	755	PRO	C-O	-5.20	1.18	1.24
1	A	644	PRO	C-O	-5.03	1.17	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	ASP	CB-CA-C	-9.94	93.78	110.68
1	A	308	GLU	N-CA-CB	-7.19	98.46	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	PRO	CB-CA-C	-6.43	103.00	111.23
1	A	575	PRO	CB-CA-C	-6.03	103.00	113.20
1	A	525	ASP	CB-CA-C	-5.77	102.07	110.96
1	A	308	GLU	CB-CG-CD	-5.61	103.07	112.60
1	A	469	LYS	CA-C-N	5.50	123.62	119.66
1	A	469	LYS	C-N-CA	5.50	123.62	119.66
1	A	343	ALA	N-CA-C	-5.22	105.48	111.07
2	B	329	THR	CB-CA-C	-5.06	102.01	110.56
2	B	416	GLN	N-CA-C	-5.02	105.80	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	470	PRO	Peptide

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	5204	0	5239	278	2
2	B	1076	0	1091	99	2
3	A	69	0	0	6	0
All	All	6349	0	6330	340	2

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 27.

All (340) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:MET:CE	1:A:497:LEU:HB3	1.68	1.21
1:A:448:MET:HE2	1:A:497:LEU:HB3	1.28	1.10
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.15	1.05
1:A:668:ARG:HA	1:A:668:ARG:HH21	1.21	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ASP:OD1	1:A:755:PRO:HD2	1.58	1.03
2:B:376:ILE:HD12	2:B:376:ILE:H	1.20	1.03
1:A:732:LYS:HG2	1:A:740:VAL:CG1	1.91	1.01
1:A:332:MET:SD	1:A:661:LYS:NZ	2.33	1.01
1:A:352:GLU:HG2	1:A:568:ARG:HB2	1.41	1.00
1:A:668:ARG:HA	1:A:668:ARG:NH2	1.78	0.98
1:A:332:MET:CE	1:A:661:LYS:HZ1	1.77	0.98
2:B:383:TRP:CZ2	2:B:412:LYS:HD3	1.97	0.98
1:A:448:MET:HE2	1:A:497:LEU:CB	1.92	0.98
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.47	0.96
1:A:448:MET:HE3	1:A:497:LEU:HB3	1.46	0.96
1:A:435:VAL:CG1	2:B:349:ILE:HG12	1.96	0.95
1:A:526:ARG:HG2	1:A:526:ARG:HH21	1.30	0.94
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.03	0.93
2:B:426:ARG:HG2	2:B:426:ARG:HH11	1.32	0.93
1:A:732:LYS:HG2	1:A:740:VAL:HG11	1.48	0.93
1:A:332:MET:CE	1:A:661:LYS:NZ	2.33	0.92
1:A:441:LEU:HD23	2:B:356:ASN:OD1	1.67	0.92
1:A:458:LEU:HD22	1:A:487:LEU:HB2	1.53	0.91
1:A:319:THR:CB	1:A:572:SER:HB3	2.02	0.89
1:A:316:ARG:HG2	1:A:316:ARG:HH11	1.37	0.89
1:A:332:MET:HE2	1:A:661:LYS:HZ1	1.38	0.89
1:A:358:GLN:O	1:A:358:GLN:NE2	2.07	0.88
1:A:319:THR:HB	1:A:572:SER:HB3	1.53	0.87
1:A:448:MET:HE1	1:A:498:ALA:N	1.90	0.86
2:B:318:GLN:O	2:B:318:GLN:NE2	2.08	0.86
1:A:344:VAL:HG12	1:A:348:GLN:OE1	1.76	0.86
1:A:434:ILE:HG22	2:B:349:ILE:CD1	2.07	0.85
1:A:448:MET:CE	1:A:497:LEU:CB	2.50	0.84
1:A:448:MET:CE	1:A:497:LEU:C	2.50	0.84
1:A:435:VAL:HG12	2:B:349:ILE:CD1	2.09	0.83
1:A:435:VAL:HG12	2:B:349:ILE:CG1	2.08	0.82
1:A:231:PHE:HE1	1:A:249:VAL:CG1	1.92	0.81
1:A:341:PRO:HG3	1:A:816:LEU:HD21	1.63	0.81
2:B:426:ARG:HG2	2:B:426:ARG:NH1	1.94	0.80
1:A:310:ARG:NH2	1:A:754:ASP:OD2	2.12	0.79
1:A:732:LYS:CG	1:A:740:VAL:HG11	2.11	0.79
1:A:312:ARG:HH11	1:A:312:ARG:HG3	1.46	0.78
1:A:448:MET:HE1	1:A:497:LEU:C	2.10	0.76
1:A:308:GLU:HB3	1:A:585:LYS:O	1.86	0.76
2:B:316:LEU:O	2:B:316:LEU:HD12	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.68	0.75
2:B:383:TRP:CE2	2:B:412:LYS:HD3	2.20	0.75
1:A:441:LEU:CD2	2:B:356:ASN:OD1	2.33	0.75
1:A:569:ASN:OD1	1:A:569:ASN:N	2.19	0.75
1:A:506:GLU:OE1	1:A:506:GLU:N	2.19	0.75
1:A:754:ASP:OD1	1:A:755:PRO:CD	2.34	0.75
1:A:260:GLY:O	1:A:264:PHE:CD2	2.39	0.75
2:B:440:GLU:O	2:B:440:GLU:HG3	1.85	0.75
1:A:445:LEU:N	1:A:445:LEU:HD23	2.00	0.75
1:A:677:LEU:N	1:A:677:LEU:HD23	2.03	0.74
1:A:329:LEU:N	1:A:329:LEU:HD12	2.02	0.74
1:A:691:LEU:CD2	1:A:727:CYS:SG	2.76	0.74
1:A:316:ARG:HG2	1:A:316:ARG:NH1	2.02	0.74
1:A:289:SER:OG	3:A:901:XB6:O9	2.07	0.72
1:A:668:ARG:HH21	1:A:668:ARG:CA	2.01	0.72
2:B:396:ARG:O	2:B:437:TRP:HD1	1.71	0.72
2:B:398:TYR:C	2:B:437:TRP:NE1	2.48	0.71
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.21	0.71
2:B:409:ILE:HD12	2:B:409:ILE:N	2.06	0.71
1:A:308:GLU:HG2	1:A:586:LEU:HD23	1.71	0.71
1:A:668:ARG:HH21	1:A:668:ARG:HG2	1.56	0.70
1:A:392:LEU:C	1:A:392:LEU:HD23	2.16	0.70
1:A:276:LYS:HD3	1:A:276:LYS:N	2.05	0.70
1:A:656:PHE:CE1	1:A:759:GLY:HA3	2.27	0.70
1:A:434:ILE:CG2	2:B:349:ILE:CD1	2.70	0.69
1:A:438:GLN:HE22	2:B:353:LYS:HG2	1.57	0.69
1:A:690:GLU:OE2	1:A:715:MET:HE3	1.92	0.69
1:A:316:ARG:HH11	1:A:316:ARG:CG	2.03	0.69
1:A:659:LEU:HD12	1:A:659:LEU:C	2.18	0.69
1:A:533:PHE:O	1:A:537:GLU:HG3	1.92	0.68
1:A:691:LEU:HD23	1:A:727:CYS:SG	2.34	0.68
2:B:376:ILE:HD12	2:B:376:ILE:N	2.03	0.68
2:B:376:ILE:H	2:B:376:ILE:CD1	1.98	0.68
1:A:321:ARG:NH2	1:A:569:ASN:O	2.27	0.68
1:A:668:ARG:HH21	1:A:668:ARG:CG	2.07	0.68
1:A:235:LEU:HD21	1:A:246:THR:HG22	1.75	0.67
1:A:260:GLY:O	1:A:264:PHE:HD2	1.76	0.67
1:A:312:ARG:HG3	1:A:312:ARG:NH1	2.07	0.67
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.76	0.67
1:A:434:ILE:HG22	2:B:349:ILE:HD11	1.75	0.67
1:A:435:VAL:CG1	2:B:349:ILE:CG1	2.66	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLN:HB3	2:B:352:ILE:HG21	1.75	0.66
1:A:435:VAL:CG1	2:B:349:ILE:CD1	2.74	0.66
1:A:574:VAL:HB	1:A:575:PRO:HD3	1.77	0.66
1:A:667:ASP:HB3	1:A:744:LYS:HE3	1.78	0.66
1:A:690:GLU:CD	1:A:715:MET:HE3	2.21	0.65
2:B:409:ILE:HD12	2:B:409:ILE:H	1.59	0.65
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.32	0.64
1:A:442:LYS:CB	2:B:356:ASN:HD21	2.11	0.64
1:A:449:VAL:HG23	2:B:363:LEU:CD2	2.27	0.64
1:A:238:LEU:HD21	1:A:242:TYR:HB2	1.78	0.64
1:A:793:ILE:HG22	1:A:794:PRO:HD2	1.79	0.64
2:B:398:TYR:C	2:B:437:TRP:HE1	2.05	0.64
1:A:437:THR:OG1	1:A:508:LEU:HD21	1.99	0.63
1:A:308:GLU:HG2	1:A:586:LEU:CD2	2.28	0.63
1:A:438:GLN:HB3	2:B:352:ILE:CG2	2.29	0.63
1:A:732:LYS:O	1:A:736:GLY:N	2.32	0.62
2:B:414:VAL:O	2:B:418:LYS:N	2.30	0.62
1:A:380:GLN:O	1:A:384:ARG:HG3	2.00	0.62
1:A:238:LEU:HD22	1:A:243:ASN:HB3	1.80	0.62
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.34	0.62
1:A:526:ARG:HH21	1:A:526:ARG:CG	2.09	0.61
1:A:668:ARG:NH2	1:A:668:ARG:HG2	2.14	0.61
1:A:740:VAL:O	1:A:740:VAL:HG13	2.00	0.61
1:A:294:ALA:CB	1:A:306:LEU:HD11	2.31	0.60
1:A:442:LYS:HB2	2:B:356:ASN:HD21	1.66	0.60
1:A:669:VAL:HG22	1:A:669:VAL:O	2.01	0.60
1:A:392:LEU:HD21	1:A:398:PHE:HD2	1.66	0.60
2:B:429:ASN:HD22	2:B:429:ASN:N	1.98	0.60
2:B:395:ILE:HG22	2:B:433:VAL:HG11	1.83	0.60
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.82	0.60
1:A:793:ILE:HG22	1:A:794:PRO:CD	2.31	0.59
1:A:449:VAL:HG23	2:B:363:LEU:HD21	1.83	0.59
1:A:320:PHE:HB2	1:A:329:LEU:HD11	1.83	0.59
2:B:368:GLU:N	2:B:369:PRO:HD2	2.18	0.59
1:A:362:LEU:HD11	1:A:531:TRP:CD2	2.38	0.58
1:A:427:GLN:O	1:A:431:TRP:HD1	1.85	0.58
1:A:468:VAL:HG12	1:A:468:VAL:O	2.02	0.58
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.85	0.58
2:B:402:PHE:CE1	2:B:418:LYS:HG3	2.39	0.58
1:A:663:VAL:CG1	1:A:747:VAL:HB	2.33	0.58
2:B:426:ARG:HH11	2:B:426:ARG:CG	2.11	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG12	1:A:317:VAL:O	2.04	0.58
1:A:435:VAL:CG1	2:B:349:ILE:HD11	2.34	0.58
2:B:409:ILE:H	2:B:409:ILE:CD1	2.17	0.57
1:A:719:SER:HB2	1:A:722:VAL:HG23	1.86	0.57
1:A:418:LEU:HD11	2:B:324:VAL:HG21	1.84	0.57
1:A:356:ILE:HG22	1:A:356:ILE:O	2.03	0.57
1:A:267:TYR:CD1	1:A:267:TYR:N	2.73	0.57
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.87	0.57
1:A:392:LEU:HD21	1:A:398:PHE:CD2	2.40	0.57
2:B:395:ILE:CG2	2:B:433:VAL:HG11	2.35	0.57
2:B:348:GLN:OE1	2:B:348:GLN:HA	2.03	0.57
2:B:383:TRP:CH2	2:B:412:LYS:HD3	2.36	0.57
1:A:690:GLU:CD	1:A:715:MET:CE	2.78	0.57
2:B:396:ARG:O	2:B:396:ARG:HD2	2.04	0.57
1:A:266:ILE:HG22	1:A:266:ILE:O	2.05	0.57
1:A:677:LEU:HD23	1:A:677:LEU:H	1.69	0.57
1:A:625:LEU:HD22	1:A:629:VAL:HG11	1.87	0.56
1:A:691:LEU:HA	1:A:706:LEU:O	2.06	0.56
2:B:400:ARG:HB3	2:B:402:PHE:HE2	1.70	0.56
2:B:405:ILE:O	2:B:409:ILE:HD13	2.05	0.56
1:A:442:LYS:HG3	2:B:356:ASN:HD21	1.69	0.56
2:B:341:GLU:HG3	2:B:341:GLU:O	2.02	0.56
1:A:656:PHE:CD1	1:A:759:GLY:HA3	2.41	0.56
1:A:526:ARG:HG2	1:A:526:ARG:NH2	2.09	0.56
1:A:441:LEU:O	1:A:444:LEU:N	2.34	0.55
1:A:442:LYS:CG	2:B:356:ASN:HD21	2.19	0.55
1:A:670:PHE:CD1	1:A:670:PHE:C	2.84	0.55
1:A:694:PHE:HA	1:A:704:LEU:O	2.07	0.55
1:A:781:THR:HG23	1:A:793:ILE:C	2.31	0.55
1:A:335:THR:O	1:A:335:THR:OG1	2.20	0.55
1:A:352:GLU:HG2	1:A:568:ARG:CB	2.27	0.55
1:A:690:GLU:OE2	1:A:715:MET:CE	2.55	0.55
1:A:319:THR:HB	1:A:572:SER:CB	2.31	0.55
1:A:724:VAL:O	1:A:727:CYS:HB2	2.07	0.55
1:A:435:VAL:HG13	2:B:349:ILE:HD11	1.89	0.54
1:A:448:MET:HE3	1:A:497:LEU:C	2.32	0.54
1:A:448:MET:HE1	1:A:498:ALA:CA	2.37	0.54
1:A:640:VAL:HG12	1:A:640:VAL:O	2.06	0.54
2:B:336:ARG:O	2:B:340:MET:HG3	2.07	0.54
1:A:494:TYR:OH	2:B:363:LEU:HD12	2.06	0.54
1:A:264:PHE:CD1	1:A:264:PHE:C	2.84	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PHE:CE1	1:A:747:VAL:HG21	2.43	0.54
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.88	0.54
2:B:396:ARG:O	2:B:437:TRP:CD1	2.58	0.54
1:A:332:MET:CE	1:A:661:LYS:HZ3	2.17	0.53
2:B:383:TRP:CH2	2:B:412:LYS:CD	2.92	0.53
1:A:456:LYS:HG2	2:B:370:TYR:CE1	2.44	0.53
1:A:666:PHE:CD1	1:A:743:PRO:HA	2.44	0.53
1:A:781:THR:HG23	1:A:793:ILE:O	2.09	0.53
1:A:188:MET:CE	1:A:200:ILE:HB	2.39	0.52
1:A:276:LYS:N	1:A:276:LYS:CD	2.73	0.52
2:B:412:LYS:HG2	2:B:416:GLN:HG3	1.90	0.52
1:A:663:VAL:HG12	1:A:747:VAL:HB	1.91	0.52
2:B:395:ILE:CG2	2:B:433:VAL:CG1	2.88	0.52
1:A:677:LEU:N	1:A:677:LEU:CD2	2.72	0.52
2:B:311:PRO:HG2	2:B:314:MET:HB2	1.91	0.52
1:A:427:GLN:O	1:A:431:TRP:CD1	2.63	0.52
1:A:329:LEU:N	1:A:329:LEU:CD1	2.73	0.52
2:B:409:ILE:N	2:B:409:ILE:CD1	2.73	0.52
1:A:362:LEU:HD11	1:A:531:TRP:CE2	2.45	0.51
1:A:448:MET:HE2	1:A:497:LEU:HB2	1.89	0.51
1:A:319:THR:OG1	1:A:572:SER:HB3	2.10	0.51
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.93	0.51
1:A:438:GLN:HE22	2:B:353:LYS:CG	2.24	0.51
1:A:445:LEU:HB2	2:B:359:LEU:HD23	1.92	0.51
1:A:494:TYR:CD1	2:B:367:ILE:HD13	2.46	0.50
1:A:381:GLU:HA	1:A:384:ARG:HD3	1.93	0.50
1:A:297:LEU:HB2	1:A:304:VAL:HG11	1.93	0.50
2:B:383:TRP:CZ2	2:B:412:LYS:CD	2.85	0.50
1:A:415:VAL:O	1:A:419:GLN:HG2	2.11	0.50
1:A:724:VAL:O	1:A:728:LEU:HG	2.11	0.50
1:A:732:LYS:CG	1:A:740:VAL:CG1	2.75	0.50
1:A:284:ILE:HG12	1:A:590:VAL:HG21	1.94	0.49
1:A:656:PHE:CE1	1:A:759:GLY:CA	2.95	0.49
1:A:718:ILE:CG2	1:A:723:ILE:HG13	2.42	0.49
1:A:231:PHE:CE1	1:A:249:VAL:CG1	2.81	0.49
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.44	0.49
2:B:402:PHE:H	2:B:402:PHE:HD2	1.60	0.49
1:A:666:PHE:O	1:A:701:PRO:HG2	2.13	0.49
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.95	0.49
1:A:670:PHE:HD1	1:A:670:PHE:O	1.95	0.49
1:A:307:LEU:HD12	1:A:590:VAL:CG2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HE1	1:A:661:LYS:NZ	2.27	0.49
1:A:205:GLN:O	1:A:209:VAL:HG23	2.12	0.48
1:A:458:LEU:O	1:A:458:LEU:HD23	2.13	0.48
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.94	0.48
1:A:680:HIS:ND1	1:A:680:HIS:C	2.71	0.48
1:A:198:ASP:OD1	1:A:198:ASP:N	2.45	0.48
1:A:379:GLU:O	1:A:382:PHE:HB3	2.14	0.48
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.48	0.48
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.78	0.48
1:A:275:THR:O	1:A:275:THR:OG1	2.25	0.48
1:A:434:ILE:HG21	2:B:349:ILE:HD12	1.96	0.48
1:A:257:GLU:HG3	1:A:263:ASN:HD22	1.79	0.48
1:A:836:LEU:N	1:A:836:LEU:HD23	2.29	0.47
2:B:315:PHE:N	2:B:315:PHE:CD2	2.81	0.47
2:B:406:SER:HB2	2:B:417:VAL:HG21	1.94	0.47
1:A:337:LEU:HD23	1:A:337:LEU:N	2.29	0.47
1:A:192:GLU:OE1	1:A:214:ARG:NH1	2.48	0.47
1:A:270:ILE:O	1:A:272:PRO:HD3	2.15	0.47
2:B:318:GLN:HE21	2:B:318:GLN:C	2.17	0.47
1:A:498:ALA:HA	1:A:501:GLN:HB3	1.96	0.47
1:A:800:GLY:O	1:A:803:THR:OG1	2.30	0.47
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.97	0.47
1:A:666:PHE:CE1	1:A:743:PRO:HB3	2.50	0.47
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.15	0.47
1:A:836:LEU:N	1:A:836:LEU:CD2	2.78	0.47
2:B:379:CYS:SG	2:B:413:SER:HB3	2.55	0.47
1:A:319:THR:HA	1:A:328:ASP:HA	1.96	0.46
3:A:901:XB6:C11	3:A:901:XB6:C24	2.93	0.46
1:A:427:GLN:HB3	2:B:342:LEU:HD11	1.97	0.46
1:A:659:LEU:HD23	1:A:761:TYR:OH	2.15	0.46
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.98	0.46
1:A:349:VAL:HG21	1:A:577:ALA:CB	2.45	0.46
1:A:381:GLU:O	1:A:384:ARG:HB2	2.16	0.46
1:A:671:TRP:O	1:A:673:PRO:HD3	2.15	0.46
2:B:318:GLN:HE22	2:B:322:GLU:HG3	1.80	0.46
1:A:232:GLU:CD	1:A:232:GLU:H	2.24	0.46
1:A:474:ILE:HG23	2:B:393:GLN:OE1	2.16	0.46
1:A:492:LYS:HD2	1:A:492:LYS:N	2.30	0.46
1:A:526:ARG:O	1:A:529:LEU:HB3	2.16	0.46
1:A:537:GLU:HG2	1:A:544:LEU:HG	1.98	0.46
1:A:235:LEU:CD2	1:A:246:THR:HG22	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ASN:HA	1:A:692:PHE:CE2	2.51	0.45
1:A:632:GLN:CD	1:A:758:ARG:HE	2.24	0.45
1:A:485:ARG:HD3	1:A:485:ARG:C	2.42	0.45
2:B:318:GLN:NE2	2:B:318:GLN:C	2.73	0.45
2:B:400:ARG:O	2:B:402:PHE:HD2	1.99	0.45
1:A:358:GLN:NE2	1:A:358:GLN:C	2.72	0.45
1:A:474:ILE:HD12	1:A:477:GLU:HB3	1.99	0.45
1:A:310:ARG:HG3	3:A:901:XB6:O15	2.17	0.45
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.52	0.45
1:A:670:PHE:CD1	1:A:670:PHE:O	2.70	0.45
2:B:400:ARG:HB3	2:B:402:PHE:CE2	2.52	0.45
1:A:238:LEU:HD21	1:A:242:TYR:CB	2.47	0.45
1:A:449:VAL:CG2	2:B:363:LEU:CD2	2.95	0.45
1:A:358:GLN:C	1:A:358:GLN:CD	2.85	0.45
1:A:435:VAL:HG11	2:B:349:ILE:HG12	1.91	0.44
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.53	0.44
1:A:659:LEU:HD12	1:A:660:ASN:N	2.32	0.44
1:A:794:PRO:HD2	1:A:828:GLN:NE2	2.33	0.44
1:A:526:ARG:CG	1:A:526:ARG:NH2	2.72	0.44
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.63	0.44
1:A:811:VAL:H	3:A:901:XB6:C26	2.27	0.44
2:B:318:GLN:O	2:B:321:VAL:HG12	2.18	0.44
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.71	0.43
2:B:414:VAL:HA	2:B:417:VAL:HB	1.98	0.43
1:A:294:ALA:HB2	1:A:306:LEU:HD11	2.00	0.43
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.53	0.43
1:A:715:MET:HE1	1:A:726:ARG:NH1	2.33	0.43
1:A:666:PHE:HD1	1:A:743:PRO:HA	1.80	0.43
1:A:331:ALA:HB1	3:A:901:XB6:C27	2.48	0.43
1:A:370:VAL:HG21	1:A:528:ILE:HD13	2.00	0.43
1:A:691:LEU:HD21	1:A:727:CYS:SG	2.55	0.43
1:A:442:LYS:HB2	2:B:356:ASN:ND2	2.30	0.43
1:A:729:ALA:HA	1:A:732:LYS:HE2	2.00	0.43
1:A:296:GLN:O	1:A:299:SER:HB3	2.18	0.43
1:A:362:LEU:N	1:A:362:LEU:CD2	2.82	0.43
1:A:645:GLU:C	1:A:645:GLU:CD	2.87	0.43
1:A:207:GLN:O	1:A:211:LEU:HD12	2.19	0.43
1:A:320:PHE:CE1	1:A:747:VAL:CG2	3.02	0.43
1:A:419:GLN:OE1	2:B:315:PHE:O	2.37	0.43
1:A:291:LEU:HD12	1:A:291:LEU:HA	1.86	0.42
1:A:275:THR:N	1:A:276:LYS:HE2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.49	0.42
1:A:506:GLU:OE1	1:A:506:GLU:CA	2.68	0.42
2:B:322:GLU:HA	2:B:325:SER:OG	2.19	0.42
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.83	0.42
1:A:312:ARG:NH1	1:A:312:ARG:CG	2.72	0.42
1:A:362:LEU:N	1:A:362:LEU:HD22	2.34	0.42
2:B:437:TRP:CE3	2:B:437:TRP:C	2.98	0.42
1:A:286:SER:O	1:A:286:SER:OG	2.21	0.42
1:A:507:LYS:HB2	1:A:507:LYS:HE2	1.34	0.42
1:A:693:LEU:HD12	1:A:694:PHE:H	1.84	0.42
1:A:353:LEU:HG	1:A:565:LEU:HD12	2.01	0.42
2:B:318:GLN:NE2	2:B:322:GLU:HG3	2.34	0.42
1:A:647:LYS:O	1:A:647:LYS:HG3	2.20	0.42
1:A:392:LEU:HD21	1:A:398:PHE:HB3	2.01	0.42
1:A:392:LEU:CD2	1:A:398:PHE:HB3	2.50	0.42
1:A:412:LEU:HD13	1:A:533:PHE:CE2	2.55	0.42
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.91	0.42
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.71	0.42
2:B:405:ILE:O	2:B:409:ILE:CD1	2.68	0.42
1:A:175:GLU:HG3	1:A:185:HIS:CG	2.55	0.42
1:A:691:LEU:N	1:A:691:LEU:HD12	2.35	0.42
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.01	0.42
1:A:435:VAL:HG12	2:B:349:ILE:HD13	2.00	0.42
1:A:504:LEU:N	1:A:504:LEU:HD23	2.35	0.42
2:B:437:TRP:CE3	2:B:437:TRP:O	2.73	0.42
1:A:665:CYS:HB2	1:A:745:GLU:O	2.19	0.42
2:B:426:ARG:HD3	2:B:427:ARG:H	1.85	0.41
1:A:804:ILE:HG23	1:A:804:ILE:O	2.20	0.41
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.85	0.41
3:A:901:XB6:O3	3:A:901:XB6:C9	2.68	0.41
2:B:419:ASN:HA	2:B:422:VAL:HG23	2.01	0.41
1:A:361:PRO:O	1:A:361:PRO:HG2	2.20	0.41
1:A:442:LYS:HE2	2:B:355:THR:HG21	2.02	0.41
1:A:782:PRO:O	1:A:792:PRO:HG2	2.21	0.41
1:A:294:ALA:HB1	1:A:306:LEU:HD11	2.02	0.41
1:A:353:LEU:HD12	1:A:566:THR:O	2.20	0.41
1:A:448:MET:CE	1:A:498:ALA:N	2.69	0.41
1:A:574:VAL:CB	1:A:575:PRO:HD3	2.46	0.41
1:A:609:SER:C	1:A:611:SER:H	2.29	0.41
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.56	0.41
1:A:266:ILE:H	1:A:348:GLN:NE2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:MET:HB3	1:A:654:MET:HE2	1.82	0.41
2:B:425:ARG:HA	2:B:430:ILE:HG13	2.03	0.41
1:A:471:PRO:O	1:A:471:PRO:CG	2.70	0.40
1:A:574:VAL:HB	1:A:575:PRO:CD	2.48	0.40
1:A:732:LYS:HG3	1:A:740:VAL:HG11	1.99	0.40
1:A:296:GLN:HA	1:A:299:SER:HB3	2.03	0.40
1:A:316:ARG:NH1	1:A:760:SER:O	2.55	0.40
1:A:718:ILE:HG22	1:A:718:ILE:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ARG:NH1	2:B:347:ARG:NH2[8_455]	1.69	0.51
1:A:718:ILE:CG1	2:B:436:GLU:OE1[7_555]	2.13	0.07

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	662/871 (76%)	625 (94%)	36 (5%)	1 (0%)	43 73
2	B	131/144 (91%)	123 (94%)	6 (5%)	2 (2%)	8 32
All	All	793/1015 (78%)	748 (94%)	42 (5%)	3 (0%)	30 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	439	ALA
2	B	379	CYS
1	A	225	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	564/715 (79%)	506 (90%)	58 (10%)	7	27
2	B	117/125 (94%)	90 (77%)	27 (23%)	1	4
All	All	681/840 (81%)	596 (88%)	85 (12%)	4	19

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	THR
1	A	249	VAL
1	A	266	ILE
1	A	267	TYR
1	A	268	LYS
1	A	276	LYS
1	A	282	ILE
1	A	291	LEU
1	A	316	ARG
1	A	328	ASP
1	A	352	GLU
1	A	353	LEU
1	A	356	ILE
1	A	364	GLU
1	A	392	LEU
1	A	434	ILE
1	A	436	LYS
1	A	441	LEU
1	A	442	LYS
1	A	445	LEU
1	A	446	ASN
1	A	448	MET
1	A	449	VAL
1	A	452	LYS
1	A	453	GLU
1	A	454	LYS
1	A	463	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	468	VAL
1	A	471	PRO
1	A	472	ARG
1	A	474	ILE
1	A	500	THR
1	A	505	GLU
1	A	506	GLU
1	A	507	LYS
1	A	508	LEU
1	A	524	ARG
1	A	526	ARG
1	A	528	ILE
1	A	538	PHE
1	A	569	ASN
1	A	575	PRO
1	A	659	LEU
1	A	661	LYS
1	A	668	ARG
1	A	669	VAL
1	A	680	HIS
1	A	685	THR
1	A	718	ILE
1	A	719	SER
1	A	727	CYS
1	A	748	VAL
1	A	780	ILE
1	A	785	SER
1	A	793	ILE
1	A	811	VAL
1	A	815	LEU
1	A	836	LEU
2	B	308	ARG
2	B	316	LEU
2	B	327	ASN
2	B	332	THR
2	B	333	THR
2	B	334	VAL
2	B	341	GLU
2	B	344	SER
2	B	345	VAL
2	B	346	LYS
2	B	349	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	368	GLU
2	B	371	ARG
2	B	376	ILE
2	B	379	CYS
2	B	382	ARG
2	B	409	ILE
2	B	412	LYS
2	B	414	VAL
2	B	415	VAL
2	B	422	VAL
2	B	426	ARG
2	B	429	ASN
2	B	430	ILE
2	B	433	VAL
2	B	435	GLN
2	B	440	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	228	GLN
1	A	399	ASN
1	A	410	GLN
1	A	417	GLN
1	A	438	GLN
1	A	446	ASN
1	A	460	GLN
1	A	828	GLN
2	B	318	GLN
2	B	356	ASN
2	B	377	GLN
2	B	429	ASN

5.3.3 RNA ⓘ

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](#)

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$
3	XB6	A	901	-	75,76,76	1.46	9 (12%)	100,114,114	1.04	7 (7%)

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
3	XB6	A	901	-	-	19/47/63/63	0/8/8/8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	XB6	C5-N1	-6.20	1.34	1.42
3	A	901	XB6	P2-O10	-5.06	1.54	1.59
3	A	901	XB6	P1-O10	-3.71	1.55	1.59
3	A	901	XB6	C24-C27	-3.43	1.34	1.43
3	A	901	XB6	O4-C29	-3.27	1.36	1.43
3	A	901	XB6	C6-C7	-2.36	1.36	1.39
3	A	901	XB6	O5-C30	-2.16	1.37	1.43
3	A	901	XB6	C28-C29	-2.03	1.49	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	XB6	P2-O11	-2.03	1.46	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	XB6	O11-P2-O12	3.63	129.31	112.44
3	A	901	XB6	C24-C27-N3	3.60	117.28	110.94
3	A	901	XB6	O10-P2-O12	-3.52	100.11	110.70
3	A	901	XB6	C42-C41-C35	-2.98	95.82	101.46
3	A	901	XB6	O11-P2-O10	-2.32	101.00	107.27
3	A	901	XB6	C6-C5-N1	-2.03	119.65	122.70
3	A	901	XB6	C27-N3-C26	-2.01	123.61	126.37

There are no chirality outliers.

All (19) torsion outliers are listed below:

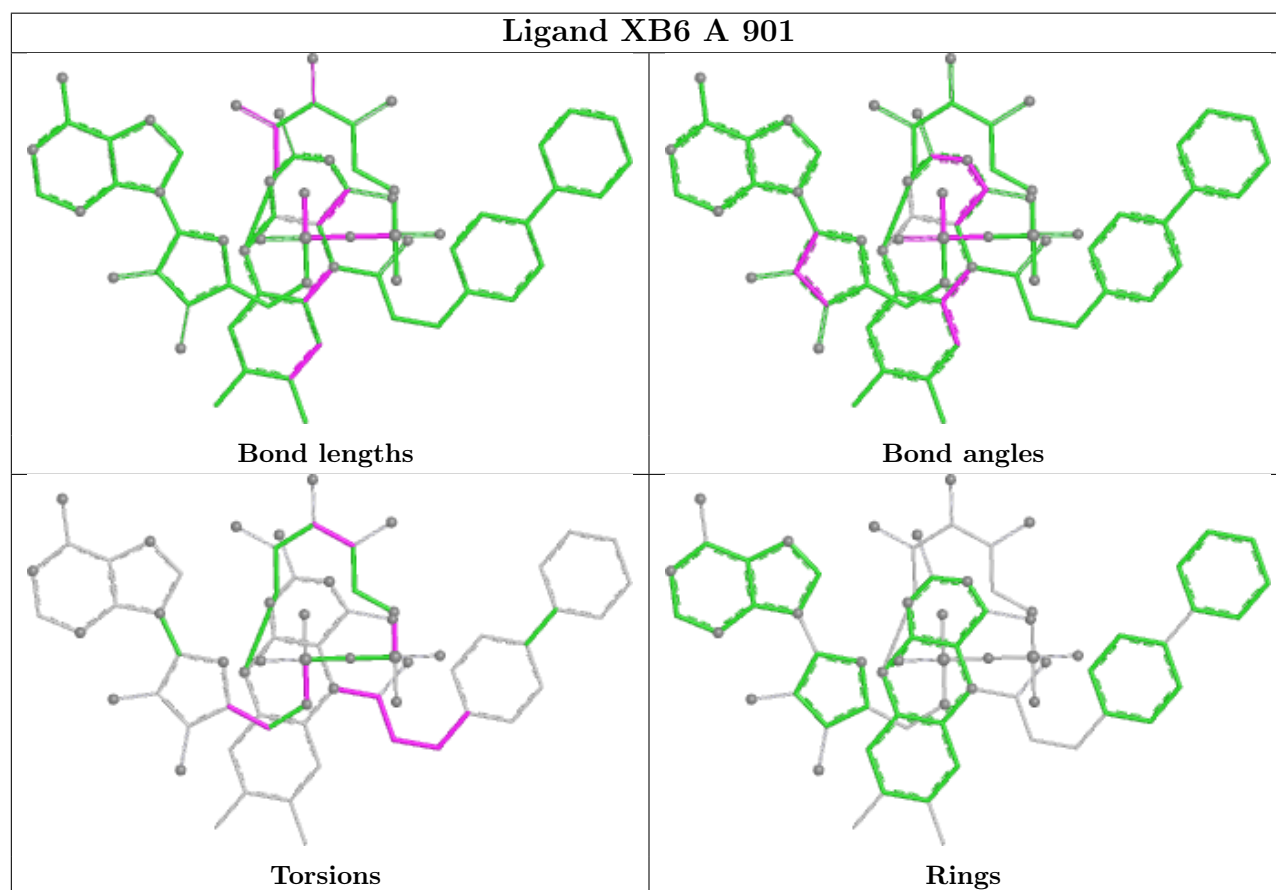
Mol	Chain	Res	Type	Atoms
3	A	901	XB6	C9-C10-C11-C12
3	A	901	XB6	C11-C10-C9-N1
3	A	901	XB6	C10-C9-N1-C5
3	A	901	XB6	C10-C9-N1-C24
3	A	901	XB6	O1-C9-N1-C5
3	A	901	XB6	O1-C9-N1-C24
3	A	901	XB6	C33-O13-P2-O10
3	A	901	XB6	C33-O13-P2-O12
3	A	901	XB6	C32-O7-P1-O10
3	A	901	XB6	C32-O7-P1-O8
3	A	901	XB6	C11-C10-C9-O1
3	A	901	XB6	O5-C30-C31-C32
3	A	901	XB6	O5-C30-C31-O6
3	A	901	XB6	C29-C30-C31-O6
3	A	901	XB6	C32-O7-P1-O9
3	A	901	XB6	C10-C11-C12-C23
3	A	901	XB6	C10-C11-C12-C13
3	A	901	XB6	C29-C30-C31-C32
3	A	901	XB6	O13-C33-C34-O14

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	XB6	6	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 ⓘ

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	664/871 (76%)	0.07	18 (2%) 56 35	61, 93, 125, 146	0
2	B	133/144 (92%)	0.40	1 (0%) 82 65	94, 121, 139, 150	0
All	All	797/1015 (78%)	0.13	19 (2%) 59 38	61, 99, 130, 150	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	6.2
2	B	436	GLU	4.1
1	A	668	ARG	2.8
1	A	453	GLU	2.7
1	A	508	LEU	2.7
1	A	556	ASP	2.5
1	A	660	ASN	2.5
1	A	269	ARG	2.5
1	A	645	GLU	2.4
1	A	350	ASN	2.4
1	A	835	THR	2.3
1	A	509	GLN	2.3
1	A	699	LYS	2.1
1	A	557	ASP	2.1
1	A	833	MET	2.1
1	A	785	SER	2.1
1	A	373	GLU	2.1
1	A	364	GLU	2.0
1	A	511	LEU	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](#)

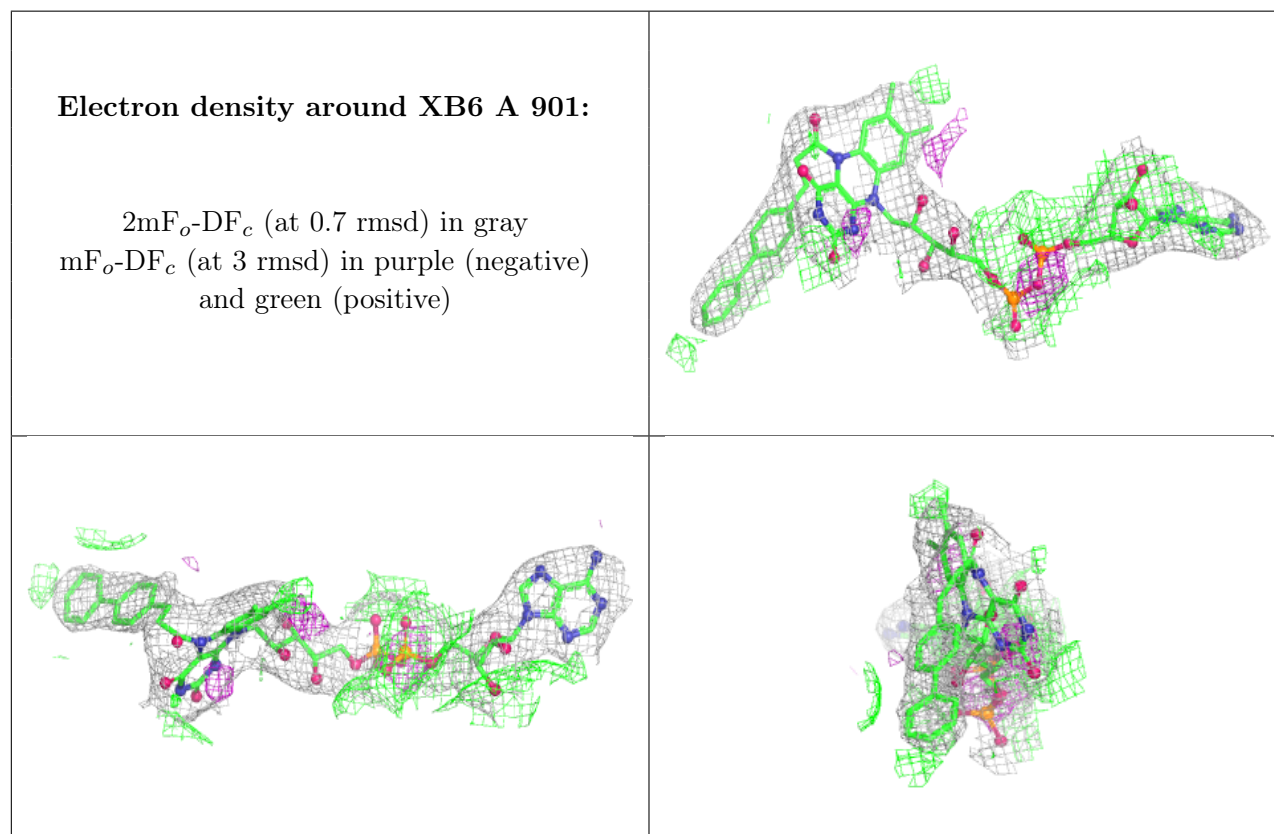
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	XB6	A	901	69/69	0.95	0.11	61,77,104,115	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.