



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:19 AM UTC

PDB ID : 2VUE / pdb_00002vue
Title : Human serum albumin complexed with 4Z,15E-bilirubin-IX-alpha
Authors : Zunszain, P.A.; Ghuman, J.; Curry, S.
Deposited on : 2008-05-24
Resolution : 2.42 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

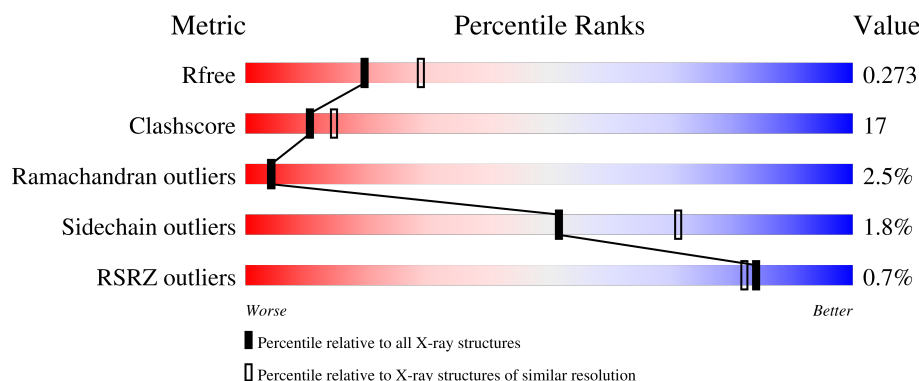
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	585	% 65% 29% ..
1	B	585	59% 34% ..

2 Entry composition [i](#)

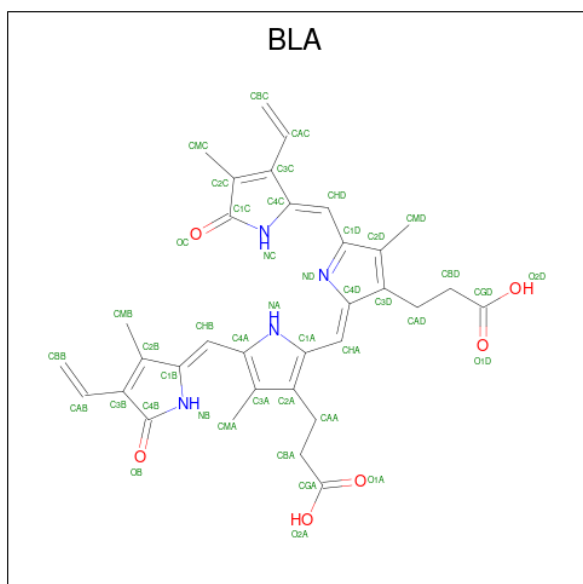
There are 3 unique types of molecules in this entry. The entry contains 8835 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4379	2768	732	839	40			
1	B	559	Total	C	N	O	S	0	0	0
			4355	2749	730	836	40			

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		

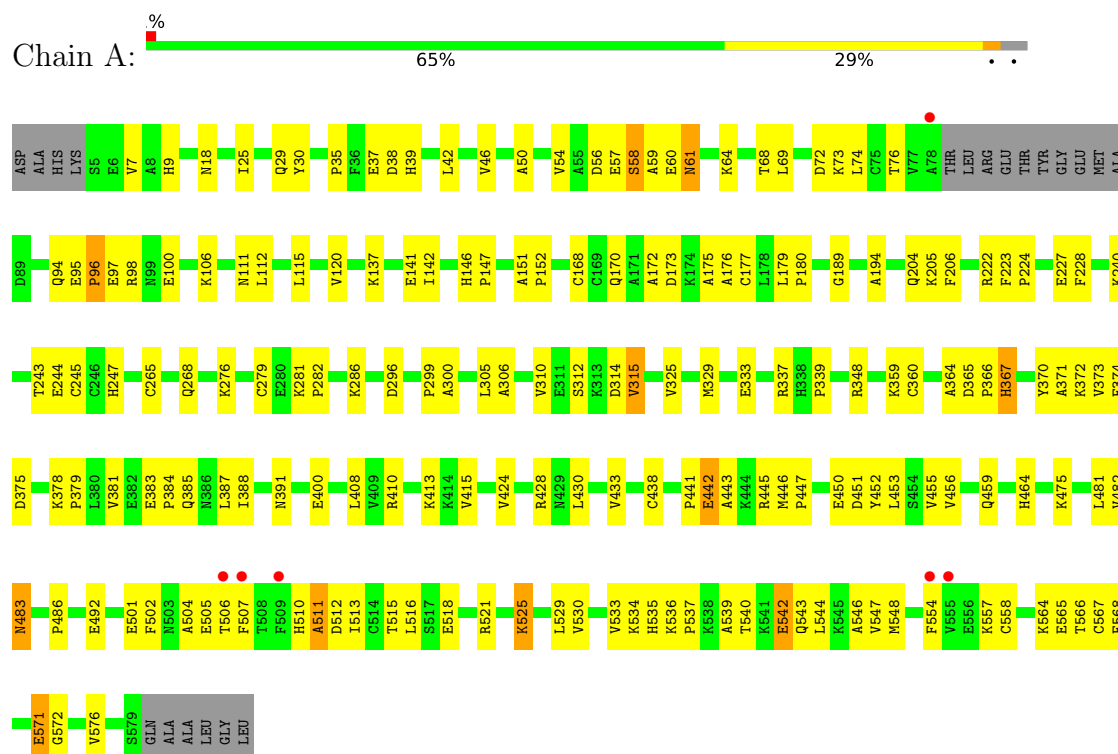
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	7	Total 7	O 7	0	0

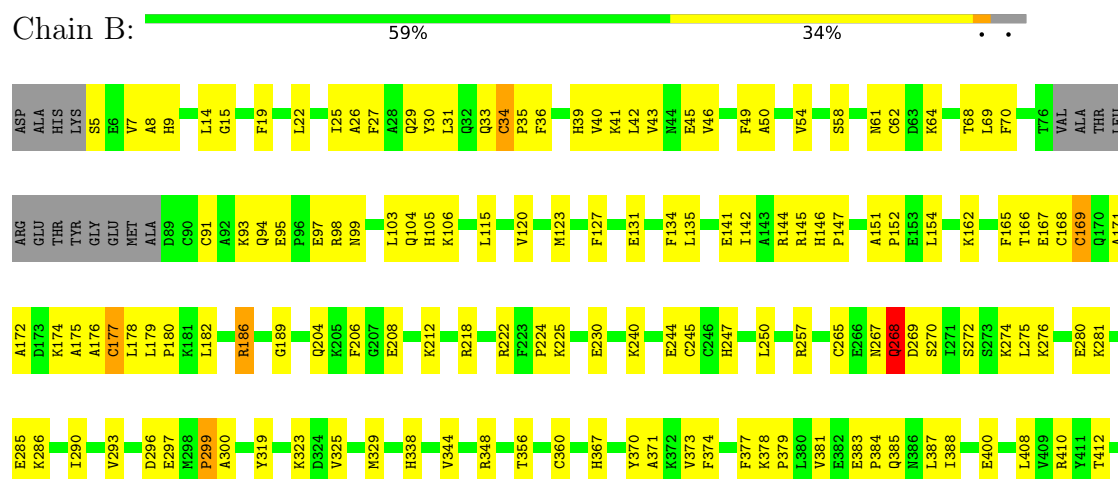
3 Residue-property plots

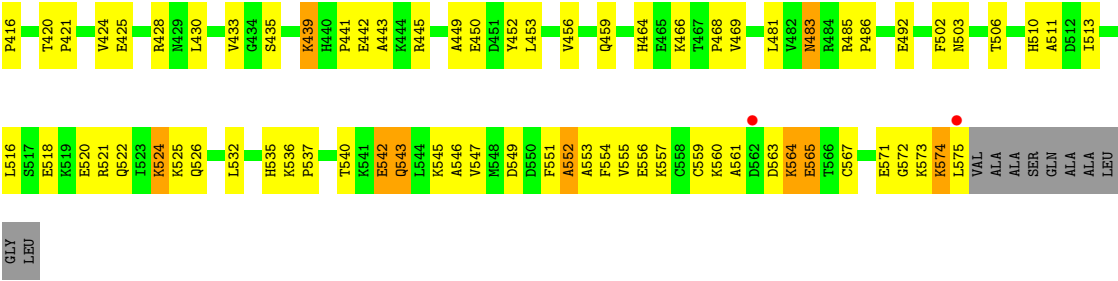
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SERUM ALBUMIN



• Molecule 1: SERUM ALBUMIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.09Å 55.54Å 119.83Å 81.22° 90.70° 65.42°	Depositor
Resolution (Å)	35.07 – 2.42 35.07 – 2.42	Depositor EDS
% Data completeness (in resolution range)	94.9 (35.07-2.42) 95.0 (35.07-2.42)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.42Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.218 , 0.273 0.218 , 0.273	Depositor DCC
R_{free} test set	2418 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8835	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	12/4465 (0.3%)	1.03	29/6047 (0.5%)
1	B	0.58	9/4437 (0.2%)	0.95	15/6001 (0.2%)
All	All	0.59	21/8902 (0.2%)	0.99	44/12048 (0.4%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLN	CD-OE1	5.55	1.34	1.23
1	A	18	ASN	CG-OD1	5.52	1.34	1.23
1	B	204	GLN	CD-OE1	5.51	1.34	1.23
1	A	464	HIS	ND1-CE1	5.43	1.38	1.32
1	B	338	HIS	ND1-CE1	5.38	1.38	1.32
1	B	9	HIS	ND1-CE1	5.37	1.38	1.32
1	A	247	HIS	ND1-CE1	5.36	1.38	1.32
1	A	483	ASN	CG-OD1	5.36	1.33	1.23
1	A	367	HIS	ND1-CE1	5.36	1.38	1.32
1	A	39	HIS	ND1-CE1	5.34	1.37	1.32
1	A	111	ASN	CG-OD1	5.33	1.33	1.23
1	B	483	ASN	CG-OD1	5.32	1.33	1.23
1	B	33	GLN	CD-OE1	5.27	1.33	1.23
1	B	268	GLN	CD-OE1	5.26	1.33	1.23
1	A	9	HIS	ND1-CE1	5.26	1.37	1.32
1	B	543	GLN	CD-OE1	5.24	1.33	1.23
1	A	61	ASN	CG-OD1	5.23	1.33	1.23
1	A	391	ASN	CG-OD1	5.18	1.33	1.23
1	B	464	HIS	ND1-CE1	5.12	1.37	1.32
1	B	385	GLN	CD-OE1	5.11	1.33	1.23
1	A	483	ASN	CG-ND2	-5.01	1.22	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLU	CA-C-N	-12.63	104.05	119.84
1	A	95	GLU	C-N-CA	-12.63	104.05	119.84
1	A	96	PRO	CA-N-CD	-8.99	99.41	112.00
1	B	204	GLN	N-CA-C	6.93	119.85	111.82
1	A	146	HIS	CA-C-N	6.91	126.59	119.82
1	A	146	HIS	C-N-CA	6.91	126.59	119.82
1	A	39	HIS	CB-CG-CD2	-6.69	122.50	131.20
1	A	367	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	B	338	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	A	112	LEU	CA-C-N	6.62	126.97	119.83
1	A	112	LEU	C-N-CA	6.62	126.97	119.83
1	B	9	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	415	VAL	CA-C-N	6.58	126.27	119.56
1	A	415	VAL	C-N-CA	6.58	126.27	119.56
1	A	247	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	B	464	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	A	9	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	A	204	GLN	N-CA-C	6.43	120.33	112.23
1	A	464	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	30	TYR	N-CA-C	-6.39	105.38	113.43
1	B	177	CYS	N-CA-C	-6.36	107.37	114.62
1	A	400	GLU	N-CA-C	6.05	118.40	111.02
1	A	365	ASP	CA-C-N	5.92	125.40	119.24
1	A	365	ASP	C-N-CA	5.92	125.40	119.24
1	B	34	CYS	CA-C-N	5.90	125.86	119.78
1	B	34	CYS	C-N-CA	5.90	125.86	119.78
1	B	9	HIS	CB-CG-ND1	5.75	131.32	122.70
1	A	39	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	367	HIS	CB-CG-ND1	5.67	131.20	122.70
1	B	338	HIS	CB-CG-ND1	5.64	131.16	122.70
1	A	247	HIS	CB-CG-ND1	5.63	131.15	122.70
1	A	9	HIS	CB-CG-ND1	5.60	131.10	122.70
1	B	464	HIS	CB-CG-ND1	5.58	131.07	122.70
1	A	339	PRO	N-CA-C	-5.54	107.43	114.35
1	A	464	HIS	CB-CG-ND1	5.53	131.00	122.70
1	B	552	ALA	N-CA-C	-5.42	105.45	111.36
1	B	400	GLU	N-CA-C	5.35	117.55	111.02
1	B	146	HIS	CA-C-N	5.34	126.52	119.84
1	B	146	HIS	C-N-CA	5.34	126.52	119.84
1	A	450	GLU	N-CA-C	5.30	117.06	111.28
1	A	95	GLU	N-CA-C	5.22	121.34	109.81
1	A	438	CYS	N-CA-C	5.19	118.71	112.38
1	B	445	ARG	N-CA-C	5.09	116.64	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	ARG	N-CA-C	5.08	116.89	111.36

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	4379	0	4183	115	0
1	B	4355	0	4184	164	0
2	A	43	0	34	10	0
2	B	43	0	34	18	0
3	A	8	0	0	1	0
3	B	7	0	0	0	0
All	All	8835	0	8435	289	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 17.

All (289) 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:B:2001:BLA:HMA2	2:B:2001:BLA:HMB2	1.26	1.15
1:B:123:MET:HA	2:B:2001:BLA:HBB2	1.45	0.98
1:B:410:ARG:HH22	1:B:492:GLU:HA	1.41	0.86
1:B:123:MET:HE2	1:B:165:PHE:HZ	1.37	0.86
1:B:325:VAL:HG12	1:B:329:MET:HE2	1.56	0.86
1:B:123:MET:HA	2:B:2001:BLA:CBB	2.07	0.85
2:B:2001:BLA:HMA2	2:B:2001:BLA:CMB	2.07	0.84
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.43	0.83
1:B:120:VAL:HG21	1:B:175:ALA:CB	2.11	0.81
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.16	0.80
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.64	0.79
1:A:424:VAL:O	1:A:428:ARG:HG3	1.84	0.77
1:B:152:PRO:HB2	1:B:257:ARG:HH11	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.20	0.77
1:B:120:VAL:HG21	1:B:175:ALA:HB1	1.67	0.76
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.70	0.74
1:A:240:LYS:O	1:A:244:GLU:HG3	1.88	0.74
1:B:134:PHE:HE1	2:B:2001:BLA:HAB	1.54	0.73
1:B:39:HIS:O	1:B:43:VAL:HG23	1.87	0.73
1:B:134:PHE:CE1	2:B:2001:BLA:HAB	2.23	0.73
2:B:2001:BLA:HMB2	2:B:2001:BLA:CMA	2.11	0.72
1:A:25:ILE:O	1:A:29:GLN:HG2	1.89	0.72
1:B:36:PHE:O	1:B:40:VAL:HG23	1.90	0.71
2:B:2001:BLA:HBD2	2:B:2001:BLA:HMD3	1.71	0.71
1:A:430:LEU:O	1:A:433:VAL:HG23	1.91	0.71
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.72	0.70
1:A:359:LYS:HG3	1:A:360:CYS:N	2.06	0.70
1:B:290:ILE:O	1:B:293:VAL:HG12	1.91	0.70
1:B:274:LYS:HE3	1:B:296:ASP:HA	1.74	0.70
1:A:502:PHE:HE1	1:A:506:THR:HG21	1.56	0.70
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.74	0.69
1:B:441:PRO:O	1:B:443:ALA:N	2.25	0.69
1:B:424:VAL:O	1:B:428:ARG:HG3	1.93	0.69
1:B:123:MET:HE2	1:B:165:PHE:CZ	2.26	0.68
1:A:115:LEU:HD21	2:A:2001:BLA:C3A	2.23	0.68
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.74	0.68
1:A:513:ILE:HG13	1:A:516:LEU:HD12	1.74	0.68
1:B:521:ARG:HG2	1:B:525:LYS:NZ	2.09	0.68
1:A:142:ILE:HG23	2:A:2001:BLA:HBC1	1.77	0.67
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.77	0.66
1:B:25:ILE:O	1:B:29:GLN:HG3	1.94	0.66
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.76	0.66
1:A:483:ASN:C	1:A:486:PRO:HD2	2.21	0.66
1:B:115:LEU:HD13	1:B:145:ARG:NH2	2.10	0.66
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.76	0.65
1:A:115:LEU:HD21	2:A:2001:BLA:C4A	2.26	0.65
1:A:115:LEU:CD2	2:A:2001:BLA:C4A	2.75	0.65
1:A:94:GLN:O	1:A:98:ARG:CB	2.45	0.64
1:A:543:GLN:O	1:A:547:VAL:HG23	1.97	0.64
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.62	0.64
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.62	0.63
1:B:441:PRO:C	1:B:443:ALA:H	2.06	0.63
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.28	0.63
1:B:572:GLY:O	1:B:575:LEU:HD13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:OE1	1:A:37:GLU:N	2.24	0.63
1:A:433:VAL:HG21	1:A:453:LEU:HD21	1.80	0.63
1:B:410:ARG:NH2	1:B:492:GLU:HA	2.11	0.63
2:B:2001:BLA:O1D	2:B:2001:BLA:HMD2	1.99	0.63
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.81	0.62
1:B:115:LEU:HD22	1:B:145:ARG:NH1	2.13	0.62
1:B:175:ALA:C	1:B:177:CYS:H	2.07	0.62
1:B:120:VAL:HG21	1:B:175:ALA:HB2	1.80	0.62
1:B:520:GLU:O	1:B:524:LYS:HG2	1.99	0.62
1:A:35:PRO:HD2	1:A:38:ASP:OD2	2.00	0.62
1:A:115:LEU:HD23	2:A:2001:BLA:C1A	2.29	0.62
1:B:68:THR:HA	1:B:98:ARG:NH2	2.15	0.62
1:B:532:LEU:HD11	1:B:547:VAL:HG11	1.81	0.61
1:B:68:THR:HA	1:B:98:ARG:HH21	1.66	0.61
1:A:408:LEU:HD21	1:A:424:VAL:HA	1.84	0.60
1:B:556:GLU:O	1:B:560:LYS:HG2	2.02	0.60
1:B:387:LEU:HD23	1:B:388:ILE:HD13	1.83	0.60
1:B:384:PRO:O	1:B:388:ILE:HG12	2.02	0.59
1:A:557:LYS:HG3	1:A:558:CYS:N	2.18	0.59
1:B:15:GLY:O	1:B:19:PHE:HB2	2.03	0.59
1:A:42:LEU:O	1:A:46:VAL:HG23	2.03	0.59
1:B:208:GLU:OE2	1:B:212:LYS:NZ	2.35	0.59
1:B:388:ILE:HD12	1:B:449:ALA:CB	2.33	0.59
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.85	0.59
1:A:364:ALA:O	1:A:366:PRO:HD3	2.02	0.59
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.85	0.59
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.85	0.58
1:B:115:LEU:HD13	1:B:145:ARG:HH22	1.66	0.58
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.85	0.58
1:B:535:HIS:C	1:B:537:PRO:HD3	2.29	0.58
1:B:574:LYS:C	1:B:575:LEU:HD12	2.28	0.58
1:A:50:ALA:O	1:A:54:VAL:HG23	2.04	0.57
1:A:189:GLY:HA3	2:A:2001:BLA:HAC	1.85	0.57
1:B:564:LYS:HD2	1:B:564:LYS:N	2.20	0.57
1:A:502:PHE:CE1	1:A:506:THR:HG21	2.39	0.57
1:B:545:LYS:O	1:B:545:LYS:HD3	2.05	0.57
1:B:168:CYS:SG	1:B:177:CYS:C	2.88	0.56
1:B:240:LYS:O	1:B:244:GLU:HG3	2.05	0.56
2:B:2001:BLA:CMB	2:B:2001:BLA:CMA	2.77	0.56
1:A:525:LYS:O	1:A:548:MET:HE1	2.06	0.56
1:A:413:LYS:HE2	1:A:537:PRO:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.37	0.55
1:B:281:LYS:HD2	1:B:285:GLU:OE1	2.05	0.55
2:B:2001:BLA:ND	2:B:2001:BLA:HAA1	2.22	0.55
1:A:265:CYS:O	1:A:268:GLN:HG3	2.07	0.55
1:B:25:ILE:HD13	1:B:154:LEU:HD23	1.88	0.55
1:A:325:VAL:HG12	1:A:329:MET:CE	2.37	0.55
1:B:388:ILE:HD12	1:B:449:ALA:HB1	1.87	0.55
1:B:50:ALA:O	1:B:54:VAL:HG23	2.07	0.55
1:A:168:CYS:SG	1:A:177:CYS:C	2.90	0.54
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.48	0.54
1:B:319:TYR:CE1	1:B:323:LYS:HB2	2.42	0.54
1:B:435:SER:O	1:B:439:LYS:HE2	2.07	0.54
1:B:483:ASN:C	1:B:486:PRO:HD2	2.32	0.54
1:B:103:LEU:C	1:B:105:HIS:H	2.14	0.54
1:A:564:LYS:C	1:A:566:THR:H	2.14	0.54
1:B:275:LEU:HD22	1:B:290:ILE:HG22	1.90	0.54
1:B:561:ALA:HB3	1:B:563:ASP:OD1	2.08	0.54
1:A:483:ASN:O	1:A:486:PRO:HD2	2.07	0.53
1:B:521:ARG:NH1	1:B:521:ARG:HB2	2.23	0.53
1:A:433:VAL:HG22	1:A:452:TYR:CE2	2.43	0.53
1:B:573:LYS:C	1:B:575:LEU:H	2.16	0.53
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.42	0.53
1:B:123:MET:HE3	2:B:2001:BLA:HMB3	1.91	0.53
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.91	0.53
2:A:2001:BLA:HAA1	2:A:2001:BLA:ND	2.24	0.53
1:B:511:ALA:C	1:B:513:ILE:H	2.17	0.53
1:A:512:ASP:O	1:A:515:THR:HG22	2.09	0.52
1:B:441:PRO:C	1:B:443:ALA:N	2.67	0.52
1:A:530:VAL:O	1:A:534:LYS:HG3	2.08	0.52
1:B:513:ILE:HG13	1:B:516:LEU:HD12	1.90	0.52
2:B:2001:BLA:HBD2	2:B:2001:BLA:CMD	2.38	0.52
1:A:572:GLY:O	1:A:576:VAL:HG23	2.10	0.51
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.93	0.51
1:A:557:LYS:HE3	1:A:571:GLU:HG2	1.93	0.51
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.93	0.51
1:A:372:LYS:O	1:A:375:ASP:HB2	2.11	0.51
1:B:265:CYS:SG	1:B:286:LYS:HD2	2.50	0.51
1:B:377:PHE:O	1:B:381:VAL:HG23	2.11	0.51
1:A:37:GLU:H	1:A:37:GLU:CD	2.14	0.51
1:B:127:PHE:O	1:B:131:GLU:HB3	2.11	0.51
1:B:218:ARG:HH21	1:B:222:ARG:HH21	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASN:OD1	1:A:64:LYS:HE3	2.10	0.50
1:A:173:ASP:HB3	1:A:176:ALA:HB3	1.94	0.50
1:B:42:LEU:O	1:B:46:VAL:HG23	2.11	0.50
1:B:141:GLU:HA	1:B:141:GLU:OE2	2.11	0.50
1:B:433:VAL:HG21	1:B:453:LEU:HD21	1.94	0.50
1:B:49:PHE:CE2	1:B:69:LEU:HD21	2.46	0.50
1:A:115:LEU:HG	2:A:2001:BLA:NA	2.26	0.50
1:B:123:MET:HG2	2:B:2001:BLA:CBB	2.42	0.50
1:A:367:HIS:O	1:A:371:ALA:HB2	2.12	0.49
1:B:165:PHE:C	1:B:167:GLU:N	2.69	0.49
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.94	0.49
1:A:370:TYR:CD1	1:A:370:TYR:C	2.91	0.49
1:B:186:ARG:HG2	2:B:2001:BLA:CHD	2.42	0.49
1:B:168:CYS:SG	1:B:177:CYS:O	2.70	0.49
1:B:536:LYS:N	1:B:537:PRO:HD3	2.28	0.49
1:A:554:PHE:HZ	1:A:568:PHE:HA	1.77	0.49
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.94	0.49
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.47	0.49
1:A:518:GLU:HA	1:A:521:ARG:NH1	2.28	0.48
1:B:30:TYR:O	1:B:31:LEU:HG	2.13	0.48
1:B:178:LEU:HG	1:B:182:LEU:CD1	2.43	0.48
1:B:430:LEU:O	1:B:433:VAL:HG23	2.13	0.48
1:A:69:LEU:O	1:A:73:LYS:HG2	2.14	0.48
1:A:222:ARG:HG2	1:A:223:PHE:CE1	2.49	0.48
1:A:410:ARG:NH2	1:A:492:GLU:O	2.46	0.48
1:B:5:SER:N	1:B:62:CYS:O	2.46	0.48
1:B:218:ARG:NH2	1:B:222:ARG:HH21	2.12	0.48
1:B:567:CYS:HA	1:B:571:GLU:HG2	1.96	0.48
1:B:319:TYR:O	1:B:323:LYS:HB3	2.14	0.48
1:A:97:GLU:HA	1:A:100:GLU:HG2	1.96	0.48
1:A:56:ASP:C	1:A:58:SER:H	2.22	0.48
1:A:279:CYS:HA	1:A:286:LYS:HD3	1.96	0.47
1:B:274:LYS:CE	1:B:296:ASP:HA	2.41	0.47
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.97	0.47
1:B:142:ILE:HG23	2:B:2001:BLA:HBC1	1.96	0.47
1:B:152:PRO:CB	1:B:257:ARG:HH11	2.22	0.47
1:A:115:LEU:CD2	2:A:2001:BLA:C3A	2.91	0.47
1:B:175:ALA:O	1:B:177:CYS:N	2.41	0.47
1:B:483:ASN:O	1:B:486:PRO:HD2	2.15	0.47
1:B:543:GLN:O	1:B:546:ALA:HB3	2.14	0.47
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:CYS:HA	1:A:571:GLU:H	1.79	0.47
1:A:115:LEU:HG	2:A:2001:BLA:C4A	2.45	0.47
1:A:433:VAL:HG21	1:A:453:LEU:CD2	2.45	0.46
1:B:466:LYS:O	1:B:468:PRO:HD3	2.16	0.46
1:A:384:PRO:O	1:A:388:ILE:HD13	2.15	0.46
1:B:152:PRO:HB2	1:B:257:ARG:NH1	2.25	0.46
1:A:387:LEU:HD23	1:A:388:ILE:HD12	1.97	0.46
1:B:94:GLN:O	1:B:97:GLU:HB2	2.15	0.46
1:A:544:LEU:C	1:A:546:ALA:H	2.23	0.46
1:B:135:LEU:HD11	1:B:162:LYS:HB2	1.97	0.46
1:B:178:LEU:HG	1:B:182:LEU:HD11	1.98	0.46
1:B:367:HIS:O	1:B:371:ALA:HB2	2.15	0.46
1:B:410:ARG:HH22	1:B:492:GLU:CA	2.22	0.46
1:B:516:LEU:O	1:B:521:ARG:NH2	2.49	0.45
1:B:412:THR:O	1:B:416:PRO:HG3	2.16	0.45
1:B:225:LYS:NZ	1:B:297:GLU:HB3	2.32	0.45
1:A:510:HIS:C	1:A:512:ASP:H	2.25	0.45
1:A:536:LYS:CB	1:A:539:ALA:HB2	2.47	0.45
1:B:208:GLU:CD	1:B:212:LYS:NZ	2.75	0.45
1:B:356:THR:O	1:B:360:CYS:HB2	2.16	0.45
1:B:370:TYR:CD1	1:B:370:TYR:C	2.95	0.45
1:A:501:GLU:OE1	1:A:501:GLU:HA	2.17	0.45
1:B:165:PHE:O	1:B:167:GLU:N	2.50	0.45
1:A:502:PHE:CE2	1:A:576:VAL:HG11	2.51	0.45
1:B:433:VAL:HG21	1:B:453:LEU:CD2	2.46	0.45
1:B:456:VAL:O	1:B:459:GLN:HB2	2.17	0.45
1:B:513:ILE:HG12	1:B:513:ILE:O	2.17	0.44
1:B:27:PHE:HE1	1:B:70:PHE:CD2	2.35	0.44
1:B:560:LYS:O	1:B:560:LYS:HG3	2.17	0.44
1:A:535:HIS:C	1:A:537:PRO:HD3	2.42	0.44
1:B:41:LYS:HG2	1:B:45:GLU:OE2	2.17	0.44
1:B:95:GLU:OE2	1:B:99:ASN:HB2	2.17	0.44
1:B:540:THR:C	1:B:542:GLU:N	2.74	0.44
1:B:25:ILE:CD1	1:B:154:LEU:HD23	2.47	0.44
1:B:172:ALA:C	1:B:174:LYS:N	2.75	0.44
1:B:189:GLY:C	2:B:2001:BLA:HAC	2.43	0.44
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.43	0.44
1:B:230:GLU:OE1	1:B:230:GLU:HA	2.17	0.44
1:B:521:ARG:HG2	1:B:525:LYS:HZ1	1.80	0.44
1:A:168:CYS:C	1:A:170:GLN:H	2.25	0.43
1:A:456:VAL:O	1:A:459:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLN:O	1:B:526:GLN:HG3	2.18	0.43
1:A:506:THR:HG23	1:A:507:PHE:N	2.33	0.43
1:B:549:ASP:O	1:B:552:ALA:HB3	2.18	0.43
1:B:344:VAL:O	1:B:348:ARG:HB2	2.18	0.43
1:B:521:ARG:HG2	1:B:525:LYS:HZ2	1.84	0.43
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.99	0.43
1:B:268:GLN:C	1:B:270:SER:H	2.25	0.43
1:B:420:THR:N	1:B:421:PRO:CD	2.82	0.43
1:A:518:GLU:HA	1:A:521:ARG:HH11	1.84	0.43
1:A:557:LYS:NZ	1:A:571:GLU:HG2	2.34	0.43
1:B:7:VAL:HG13	1:B:8:ALA:N	2.34	0.43
1:B:268:GLN:C	1:B:270:SER:N	2.77	0.43
1:B:165:PHE:HD1	1:B:169:CYS:SG	2.42	0.43
1:B:502:PHE:CD1	1:B:502:PHE:C	2.96	0.43
1:B:565:GLU:HG3	1:B:565:GLU:O	2.19	0.43
1:A:120:VAL:HG21	1:A:175:ALA:HA	2.00	0.42
1:B:410:ARG:NH2	1:B:492:GLU:OE1	2.51	0.42
1:B:553:ALA:C	1:B:555:VAL:H	2.27	0.42
1:A:205:LYS:NZ	3:A:2002:HOH:O	2.52	0.42
1:A:314:ASP:O	1:A:315:VAL:C	2.62	0.42
1:A:447:PRO:O	1:A:451:ASP:HB2	2.19	0.42
1:A:74:LEU:C	1:A:76:THR:H	2.27	0.42
1:A:206:PHE:CD2	1:A:481:LEU:HD22	2.54	0.42
1:A:441:PRO:O	1:A:442:GLU:C	2.62	0.42
1:A:511:ALA:HB3	1:A:565:GLU:OE2	2.19	0.42
1:B:165:PHE:O	1:B:166:THR:C	2.62	0.42
1:A:227:GLU:O	1:A:228:PHE:C	2.62	0.42
1:B:545:LYS:NZ	1:B:549:ASP:HB2	2.35	0.42
1:A:513:ILE:HA	1:A:516:LEU:HD12	2.02	0.42
1:A:68:THR:HG22	1:A:72:ASP:OD2	2.18	0.42
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.83	0.42
1:B:553:ALA:HB1	1:B:557:LYS:HD2	2.02	0.42
1:A:475:LYS:HE3	1:A:475:LYS:HB3	1.91	0.42
1:B:267:ASN:O	1:B:270:SER:HB3	2.20	0.42
1:B:551:PHE:O	1:B:555:VAL:HG23	2.19	0.42
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.50	0.42
1:A:381:VAL:O	1:A:384:PRO:HD2	2.20	0.42
1:A:536:LYS:O	1:A:537:PRO:C	2.63	0.42
1:A:542:GLU:N	1:A:542:GLU:OE1	2.52	0.42
1:B:172:ALA:C	1:B:174:LYS:H	2.27	0.42
1:B:268:GLN:O	1:B:270:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:LEU:HD21	1:B:424:VAL:HA	2.02	0.42
1:A:441:PRO:O	1:A:443:ALA:N	2.53	0.42
1:A:504:ALA:C	1:A:506:THR:H	2.27	0.42
1:B:518:GLU:HA	1:B:521:ARG:NH1	2.34	0.42
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.41
1:B:276:LYS:O	1:B:280:GLU:HG2	2.20	0.41
2:B:2001:BLA:CMD	2:B:2001:BLA:CB	2.97	0.41
1:B:91:CYS:C	1:B:93:LYS:N	2.78	0.41
1:A:61:ASN:HB3	1:A:64:LYS:HG3	2.02	0.41
1:A:529:LEU:O	1:A:533:VAL:HG23	2.20	0.41
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.85	0.41
1:A:279:CYS:HA	1:A:286:LYS:CD	2.49	0.41
1:B:540:THR:C	1:B:542:GLU:H	2.28	0.41
1:B:175:ALA:C	1:B:177:CYS:N	2.72	0.41
1:A:137:LYS:O	1:A:141:GLU:HG2	2.21	0.41
1:A:168:CYS:SG	1:A:177:CYS:O	2.79	0.41
1:A:385:GLN:HG2	1:A:446:MET:HE2	2.03	0.41
1:A:540:THR:OG1	1:A:543:GLN:HG2	2.21	0.41
1:B:103:LEU:C	1:B:105:HIS:N	2.78	0.41
1:B:103:LEU:HD11	1:B:247:HIS:O	2.21	0.41
1:B:555:VAL:O	1:B:559:CYS:SG	2.78	0.41
1:B:14:LEU:HD13	1:B:22:LEU:HD12	2.02	0.41
1:B:503:ASN:O	1:B:506:THR:HB	2.21	0.41
1:B:296:ASP:CG	1:B:297:GLU:N	2.79	0.40
1:B:513:ILE:HA	1:B:516:LEU:HD12	2.03	0.40
1:B:141:GLU:OE2	1:B:144:ARG:HD3	2.20	0.40
1:B:567:CYS:HA	1:B:571:GLU:CG	2.51	0.40
1:B:374:PHE:O	1:B:377:PHE:HB2	2.21	0.40
1:B:378:LYS:CB	1:B:379:PRO:HD3	2.45	0.40
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.52	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	561/585 (96%)	500 (89%)	48 (9%)	13 (2%)	5	5
1	B	555/585 (95%)	495 (89%)	45 (8%)	15 (3%)	4	3
All	All	1116/1170 (95%)	995 (89%)	93 (8%)	28 (2%)	4	4

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	ALA
1	A	276	LYS
1	A	300	ALA
1	B	61	ASN
1	B	64	LYS
1	B	268	GLN
1	B	300	ALA
1	B	442	GLU
1	B	510	HIS
1	B	565	GLU
1	A	59	ALA
1	A	511	ALA
1	A	60	GLU
1	A	96	PRO
1	A	312	SER
1	A	315	VAL
1	A	442	GLU
1	A	505	GLU
1	B	104	GLN
1	B	171	ALA
1	B	176	ALA
1	B	269	ASP
1	A	57	GLU
1	A	58	SER
1	B	169	CYS
1	B	554	PHE
1	B	574	LYS
1	B	299	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	467/511 (91%)	461 (99%)	6 (1%)	61	78
1	B	466/511 (91%)	455 (98%)	11 (2%)	43	63
All	All	933/1022 (91%)	916 (98%)	17 (2%)	51	71

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	243	THR
1	A	245	CYS
1	A	525	LYS
1	A	542	GLU
1	A	571	GLU
1	B	58	SER
1	B	186	ARG
1	B	245	CYS
1	B	299	PRO
1	B	425	GLU
1	B	439	LYS
1	B	450	GLU
1	B	469	VAL
1	B	524	LYS
1	B	542	GLU
1	B	564	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	242	HIS
1	B	29	GLN
1	B	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	BLA	A	2001	-	46,46,46	1.79	13 (28%)	66,67,67	1.64	13 (19%)
2	BLA	B	2001	-	46,46,46	1.77	13 (28%)	66,67,67	1.65	13 (19%)

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	BLA	A	2001	-	-	19/26/74/74	0/4/4/4
2	BLA	B	2001	-	-	19/26/74/74	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	BLA	C3C-C4C	4.01	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	BLA	C3C-C4C	3.57	1.52	1.45
2	A	2001	BLA	CHA-C4D	3.55	1.45	1.38
2	B	2001	BLA	C1A-C2A	3.45	1.50	1.42
2	B	2001	BLA	CBC-CAC	3.41	1.46	1.30
2	A	2001	BLA	C1B-C2B	3.40	1.51	1.45
2	A	2001	BLA	CBC-CAC	3.38	1.46	1.30
2	B	2001	BLA	C1B-C2B	3.26	1.50	1.45
2	A	2001	BLA	C1A-C2A	3.25	1.50	1.42
2	B	2001	BLA	C4A-C3A	3.14	1.49	1.41
2	B	2001	BLA	CHA-C4D	3.11	1.44	1.38
2	A	2001	BLA	C4A-C3A	3.10	1.48	1.41
2	B	2001	BLA	CAB-C3B	-2.62	1.40	1.47
2	A	2001	BLA	CHA-C1A	2.62	1.46	1.40
2	A	2001	BLA	CAB-C3B	-2.60	1.40	1.47
2	B	2001	BLA	CHA-C1A	2.55	1.46	1.40
2	B	2001	BLA	O2A-CGA	2.43	1.38	1.30
2	A	2001	BLA	O2A-CGA	2.31	1.38	1.30
2	B	2001	BLA	CMD-C2D	2.31	1.55	1.50
2	A	2001	BLA	CMD-C2D	2.24	1.55	1.50
2	A	2001	BLA	O2D-CGD	2.20	1.38	1.30
2	A	2001	BLA	CBD-CAD	2.10	1.59	1.51
2	B	2001	BLA	CHB-C1B	2.07	1.42	1.37
2	A	2001	BLA	CBB-CAB	2.05	1.40	1.30
2	B	2001	BLA	CBB-CAB	2.04	1.40	1.30
2	B	2001	BLA	O2D-CGD	2.01	1.37	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	BLA	C3B-C4B-NB	6.14	113.84	106.13
2	A	2001	BLA	C3B-C4B-NB	6.06	113.74	106.13
2	B	2001	BLA	C1B-NB-C4B	-4.63	104.98	110.66
2	A	2001	BLA	C1B-NB-C4B	-4.59	105.03	110.66
2	B	2001	BLA	C4C-NC-C1C	-3.04	106.92	110.66
2	A	2001	BLA	O2D-CGD-O1D	-2.99	115.63	123.33
2	B	2001	BLA	O2D-CGD-O1D	-2.96	115.71	123.33
2	A	2001	BLA	C4C-NC-C1C	-2.81	107.21	110.66
2	A	2001	BLA	C2B-C1B-NB	2.75	110.98	106.97
2	A	2001	BLA	CHB-C1B-NB	-2.74	120.22	126.06
2	B	2001	BLA	C2B-C1B-NB	2.73	110.95	106.97
2	B	2001	BLA	O2D-CGD-CBD	2.72	122.59	114.00
2	A	2001	BLA	O2D-CGD-CBD	2.65	122.39	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	BLA	C4B-C3B-C2B	-2.58	104.61	107.92
2	B	2001	BLA	CHB-C1B-NB	-2.54	120.64	126.06
2	A	2001	BLA	C4B-C3B-C2B	-2.54	104.67	107.92
2	A	2001	BLA	C2C-C1C-NC	2.43	111.99	106.55
2	B	2001	BLA	C2C-C1C-NC	2.43	111.98	106.55
2	A	2001	BLA	CMB-C2B-C1B	2.33	127.00	124.16
2	B	2001	BLA	C1A-C2A-C3A	-2.26	104.99	107.62
2	A	2001	BLA	C1A-C2A-C3A	-2.22	105.04	107.62
2	B	2001	BLA	CMB-C2B-C1B	2.18	126.81	124.16
2	A	2001	BLA	C3B-C2B-C1B	-2.10	105.58	107.92
2	B	2001	BLA	C3B-C2B-C1B	-2.07	105.61	107.92
2	A	2001	BLA	C2A-C1A-NA	2.06	110.16	107.57
2	B	2001	BLA	OB-C4B-C3B	-2.02	124.84	129.71

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	BLA	ND-C4D-CHA-C1A
2	A	2001	BLA	C3D-C4D-CHA-C1A
2	A	2001	BLA	NB-C1B-CHB-C4A
2	A	2001	BLA	C2B-C1B-CHB-C4A
2	A	2001	BLA	C2B-C3B-CAB-CBB
2	A	2001	BLA	C4B-C3B-CAB-CBB
2	A	2001	BLA	C2C-C3C-CAC-CBC
2	A	2001	BLA	C3D-CAD-CBD-CGD
2	B	2001	BLA	ND-C4D-CHA-C1A
2	B	2001	BLA	C3D-C4D-CHA-C1A
2	B	2001	BLA	C2B-C3B-CAB-CBB
2	B	2001	BLA	C2C-C3C-CAC-CBC
2	B	2001	BLA	C2D-C3D-CAD-CBD
2	A	2001	BLA	NA-C1A-CHA-C4D
2	B	2001	BLA	NA-C1A-CHA-C4D
2	B	2001	BLA	NA-C4A-CHB-C1B
2	A	2001	BLA	C2A-C1A-CHA-C4D
2	B	2001	BLA	C2A-C1A-CHA-C4D
2	B	2001	BLA	C3A-C4A-CHB-C1B
2	B	2001	BLA	C4D-C3D-CAD-CBD
2	B	2001	BLA	C2B-C1B-CHB-C4A
2	A	2001	BLA	NA-C4A-CHB-C1B
2	A	2001	BLA	C3A-C4A-CHB-C1B
2	B	2001	BLA	NB-C1B-CHB-C4A

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Mol	Chain	Res	Type	Atoms
2	B	2001	BLA	C4B-C3B-CAB-CBB
2	A	2001	BLA	C4D-C3D-CAD-CBD
2	A	2001	BLA	C2D-C3D-CAD-CBD
2	A	2001	BLA	C4C-C3C-CAC-CBC
2	B	2001	BLA	C4C-C3C-CAC-CBC
2	B	2001	BLA	ND-C1D-CHD-C4C
2	A	2001	BLA	CAD-CBD-CGD-O1D
2	A	2001	BLA	CAA-CBA-CGA-O1A
2	A	2001	BLA	CAD-CBD-CGD-O2D
2	A	2001	BLA	CAA-CBA-CGA-O2A
2	B	2001	BLA	CAD-CBD-CGD-O1D
2	B	2001	BLA	CAD-CBD-CGD-O2D
2	B	2001	BLA	C2D-C1D-CHD-C4C
2	B	2001	BLA	NC-C4C-CHD-C1D

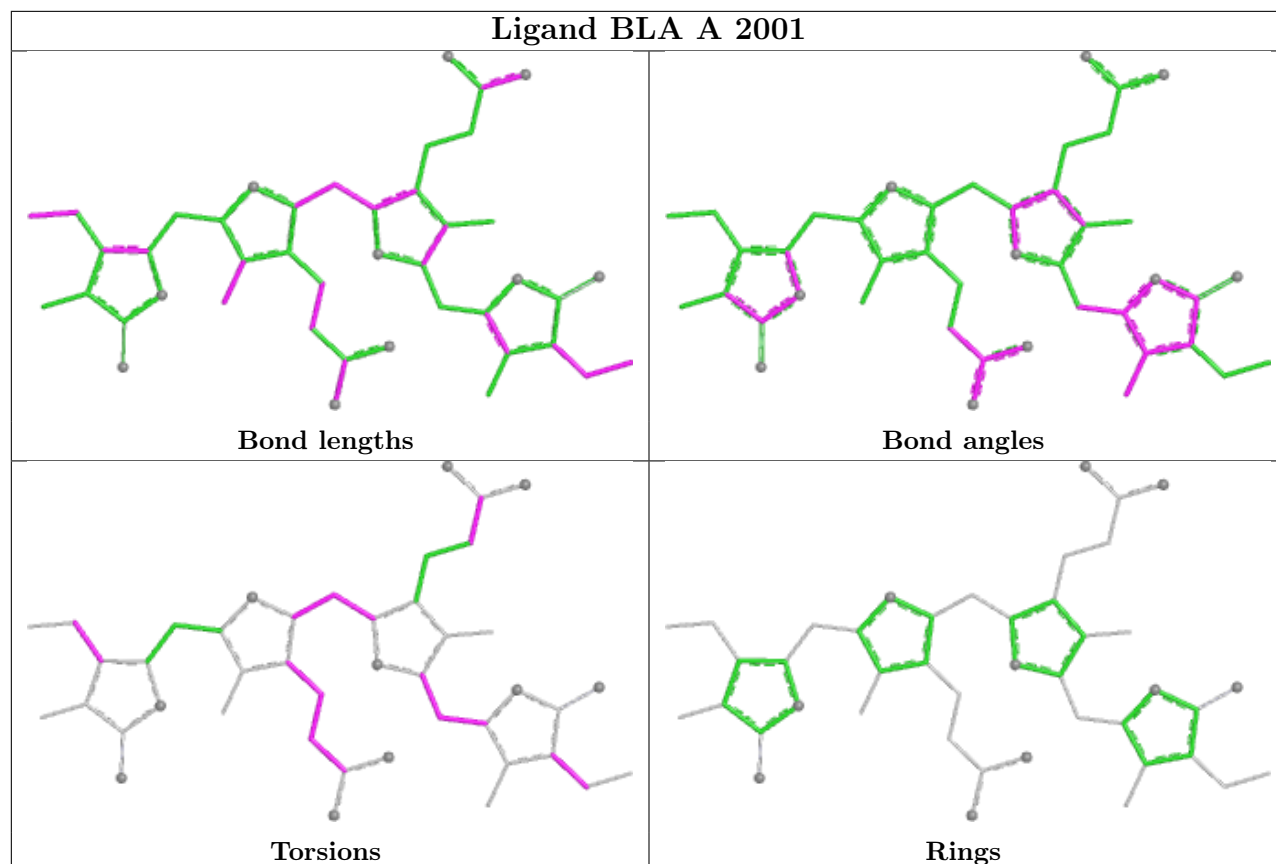
There are no ring outliers.

2 monomers are involved in 28 short contacts:

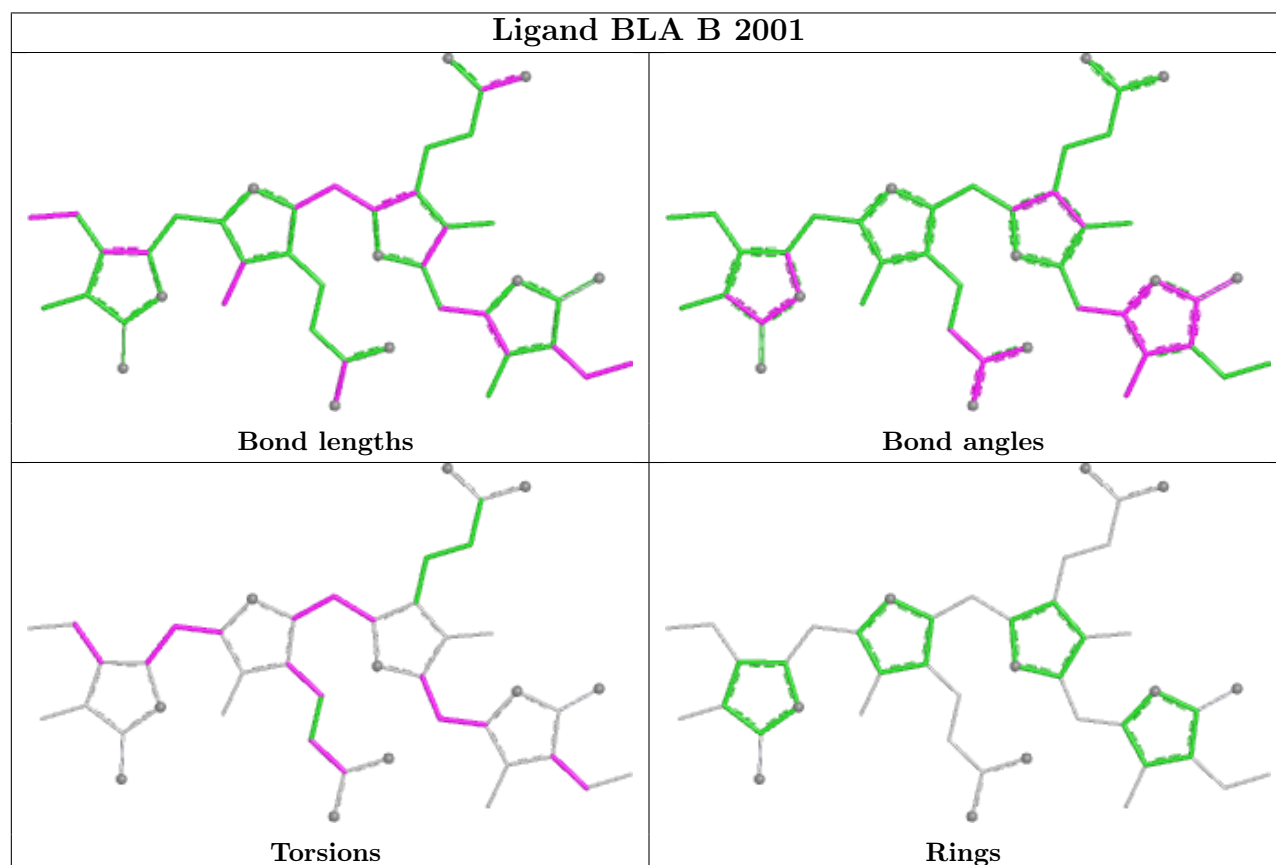
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	BLA	10	0
2	B	2001	BLA	18	0

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.

Ligand BLA A 2001



Ligand BLA B 2001



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	565/585 (96%)	-0.15	6 (1%)	78 75	38, 72, 136, 156	0
1	B	559/585 (95%)	-0.09	2 (0%)	88 87	40, 76, 139, 164	0
All	All	1124/1170 (96%)	-0.12	8 (0%)	84 82	38, 73, 138, 164	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	LEU	3.0
1	A	555	VAL	3.0
1	A	506	THR	2.7
1	A	78	ALA	2.4
1	A	509	PHE	2.3
1	A	554	PHE	2.2
1	A	507	PHE	2.2
1	B	562	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 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,

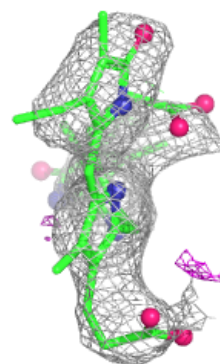
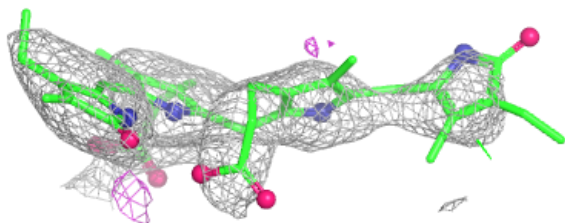
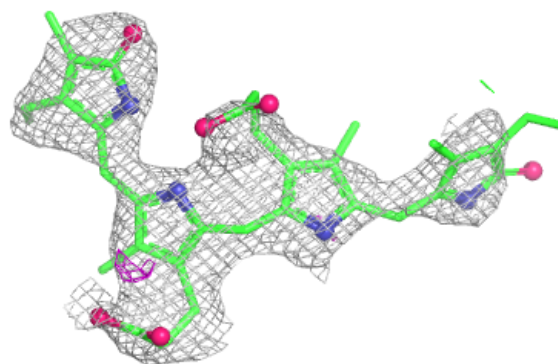
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

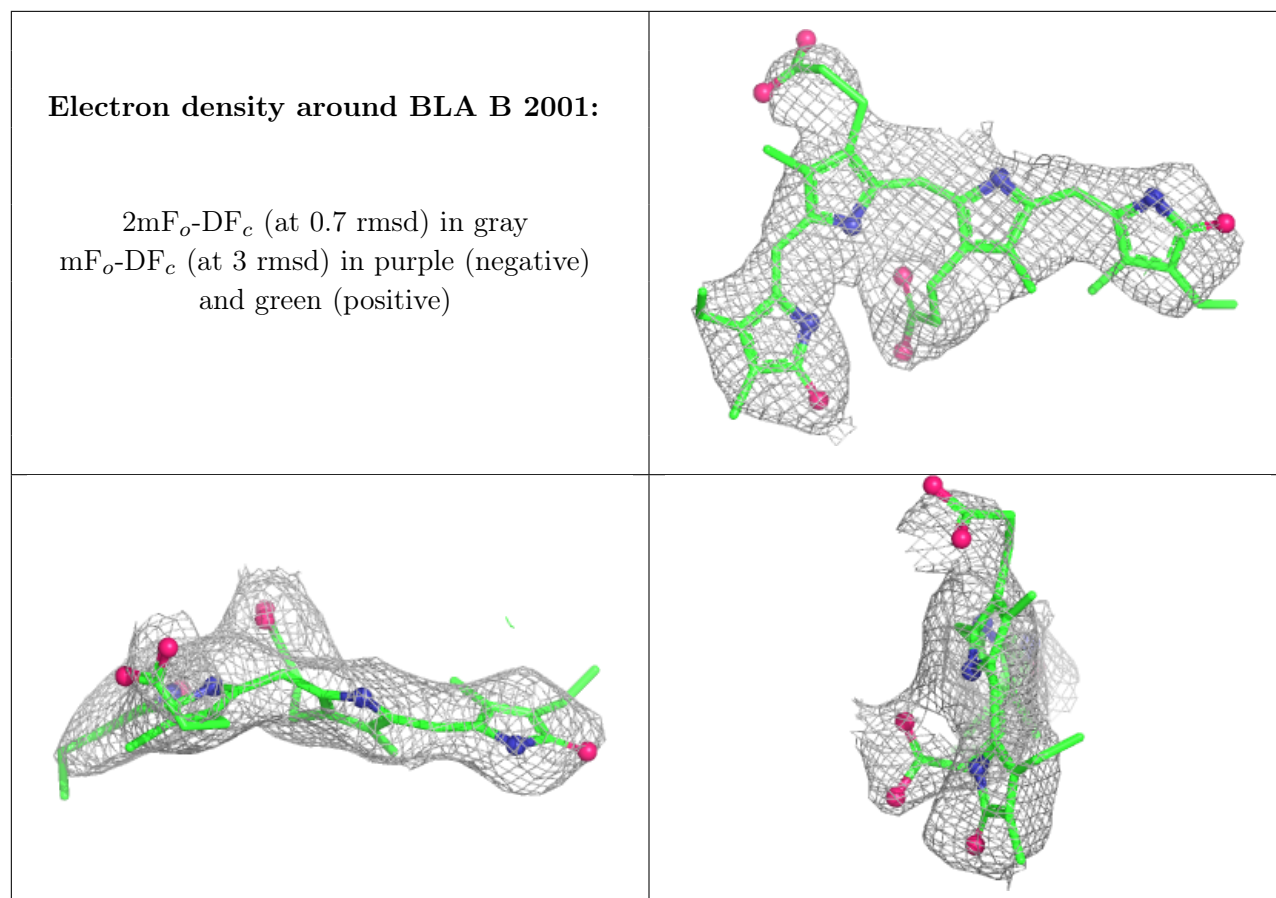
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BLA	A	2001	43/43	0.90	0.13	87,110,120,120	0
2	BLA	B	2001	43/43	0.91	0.11	83,106,120,121	0

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 BLA A 2001:

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 ⓘ

There are no such residues in this entry.