



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:07 PM UTC

PDB ID : 5URK / pdb_00005urk
Title : Crystal structure of human BRR2 in complex with T-3935799
Authors : Qin, L.; Tjhen, R.; Klein, M.G.
Deposited on : 2017-02-10
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

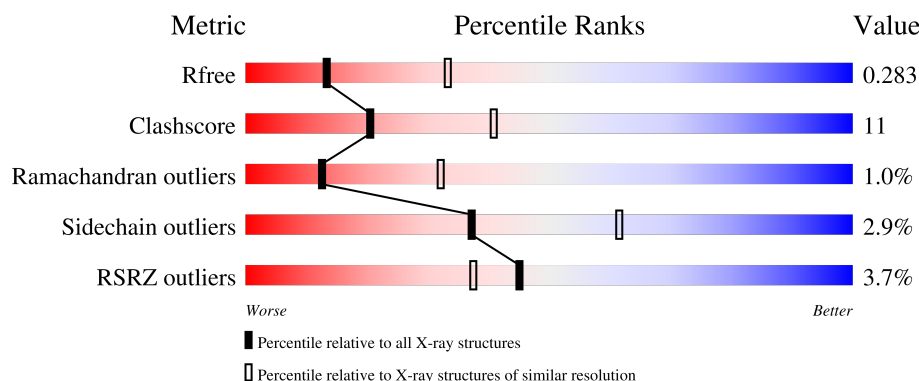
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	1738	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13657 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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1706	13618	8710	2320	2520	68	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

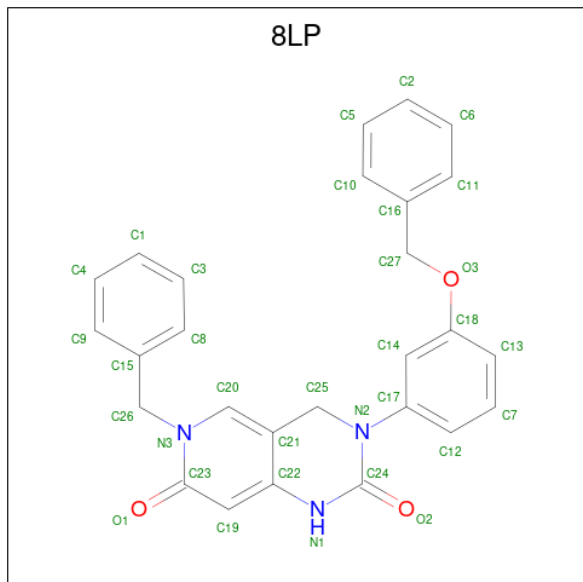
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLY	-	expression tag	UNP O75643
A	393	GLY	-	expression tag	UNP O75643
A	394	SER	-	expression tag	UNP O75643

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is 6-benzyl-3-[3-(benzyloxy)phenyl]-4,6-dihydropyrido[4,3-d]pyrimidine-2,7(1H,3H)-dione (CCD ID: 8LP) (formula: $C_{27}H_{23}N_3O_3$).

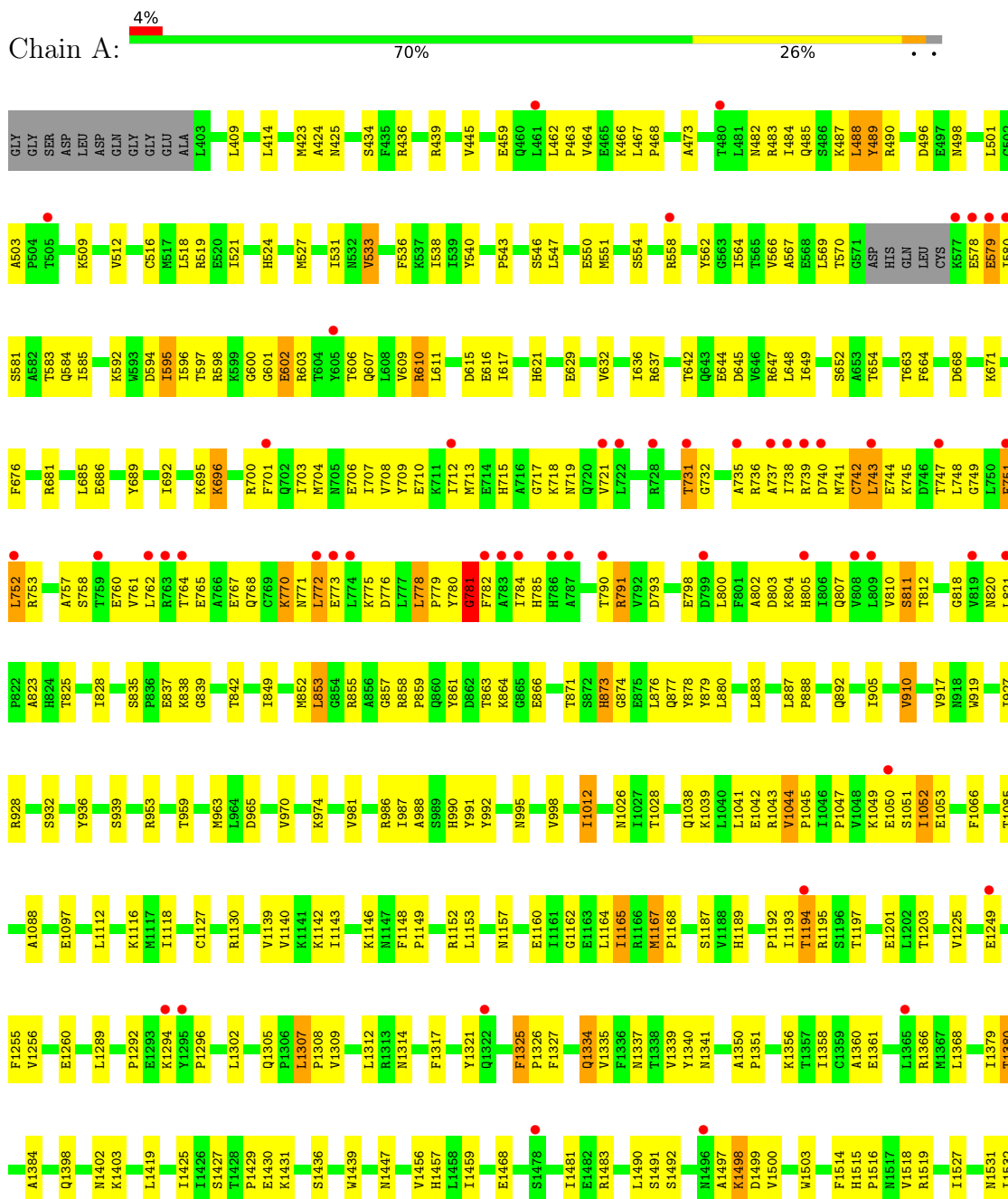


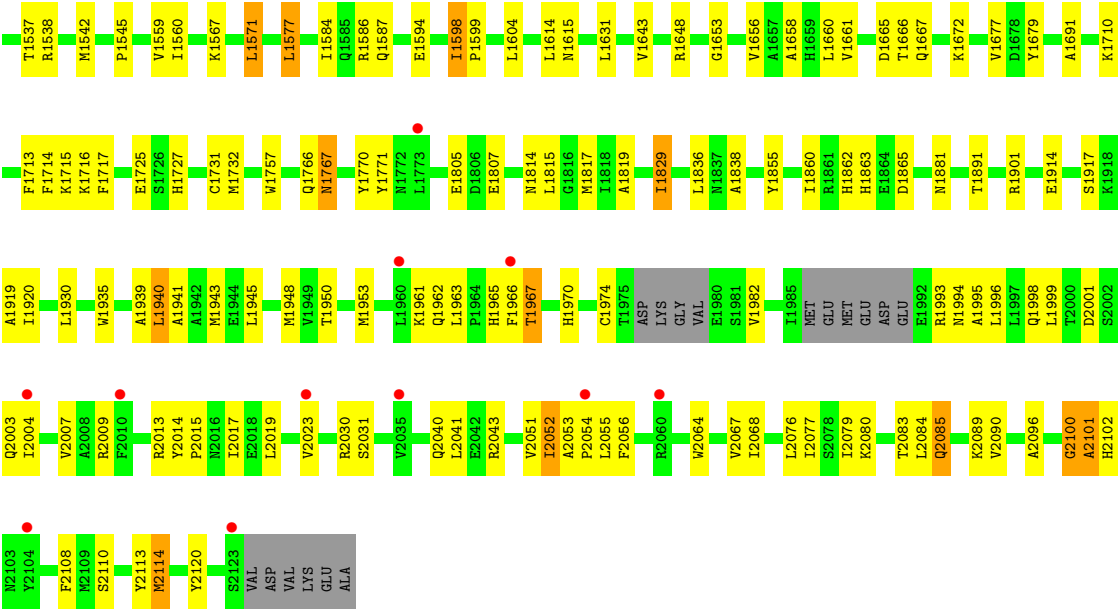
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	27	3	3	0	0

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: U5 small nuclear ribonucleoprotein 200 kDa helicase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.49Å 154.07Å 143.51Å 90.00° 120.74° 90.00°	Depositor
Resolution (Å)	48.67 – 2.95 48.67 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.67-2.95) 99.7 (48.67-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.9_1692, REFMAC	Depositor
R, R_{free}	0.233 , 0.277 0.238 , 0.283	Depositor DCC
R_{free} test set	2831 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13657	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: 8LP, GOL

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	0.49	1/13908 (0.0%)	1.00	46/18870 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1193	ILE	CA-CB	-5.11	1.50	1.55

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	752	LEU	N-CA-C	-12.00	99.04	112.72
1	A	717	GLY	N-CA-C	-11.01	95.90	111.20
1	A	1044	VAL	CA-C-N	8.44	128.05	118.85
1	A	1044	VAL	C-N-CA	8.44	128.05	118.85
1	A	2053	ALA	CA-C-N	7.57	128.25	119.47
1	A	2053	ALA	C-N-CA	7.57	128.25	119.47
1	A	873	HIS	N-CA-C	7.20	118.78	111.07
1	A	1998	GLN	N-CA-C	6.84	120.15	110.23
1	A	695	LYS	N-CA-C	-6.75	104.62	112.92
1	A	772	LEU	CB-CA-C	-6.69	106.98	116.34
1	A	2085	GLN	CB-CA-C	-6.67	108.15	117.23
1	A	741	MET	N-CA-C	-6.26	100.30	109.63
1	A	811	SER	N-CA-C	6.26	116.34	108.45
1	A	1167	MET	CA-C-N	6.22	126.13	119.28
1	A	1167	MET	C-N-CA	6.22	126.13	119.28
1	A	2083	THR	N-CA-C	-6.21	99.28	109.40
1	A	751	PHE	N-CA-C	6.17	118.14	110.91
1	A	1325	PHE	CA-C-N	6.11	125.51	118.85
1	A	1325	PHE	C-N-CA	6.11	125.51	118.85
1	A	1732	MET	N-CA-C	5.96	118.55	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	772	LEU	N-CA-C	5.83	116.64	108.00
1	A	1127	CYS	CA-C-N	5.68	126.06	119.47
1	A	1127	CYS	C-N-CA	5.68	126.06	119.47
1	A	781	GLY	N-CA-C	5.64	126.54	113.18
1	A	1307	LEU	CA-C-N	5.63	125.83	120.31
1	A	1307	LEU	C-N-CA	5.63	125.83	120.31
1	A	488	LEU	N-CA-C	5.61	120.12	113.28
1	A	1881	ASN	CA-C-N	5.58	126.02	119.99
1	A	1881	ASN	C-N-CA	5.58	126.02	119.99
1	A	803	ASP	N-CA-C	-5.49	106.35	113.16
1	A	1919	ALA	N-CA-C	5.46	117.66	111.11
1	A	1598	ILE	CB-CA-C	-5.34	108.62	113.70
1	A	778	LEU	CA-C-N	-5.30	113.45	119.28
1	A	778	LEU	C-N-CA	-5.30	113.45	119.28
1	A	1197	THR	N-CA-C	5.29	118.06	109.06
1	A	1012	ILE	CB-CA-C	-5.28	105.22	111.97
1	A	1767	ASN	CA-C-N	5.23	124.41	118.97
1	A	1767	ASN	C-N-CA	5.23	124.41	118.97
1	A	2023	VAL	N-CA-C	-5.21	99.60	107.73
1	A	798	GLU	N-CA-C	5.15	116.58	111.07
1	A	1052	ILE	CA-C-N	-5.11	113.33	122.32
1	A	1052	ILE	C-N-CA	-5.11	113.33	122.32
1	A	2096	ALA	CA-C-N	5.09	126.20	119.84
1	A	2096	ALA	C-N-CA	5.09	126.20	119.84
1	A	600	GLY	N-CA-C	-5.06	109.06	115.08
1	A	1643	VAL	N-CA-C	5.06	115.41	108.12

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	13618	0	13648	304	0
2	A	6	0	8	3	0
3	A	33	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13657	0	13656	305	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 11.

All (305) 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:742:CYS:O	1:A:744:GLU:N	2.07	0.88
1:A:820:ASN:OD1	1:A:855:ARG:NH1	2.11	0.83
1:A:1967:THR:O	1:A:1970:HIS:ND1	2.15	0.79
1:A:1255:PHE:HB2	3:A:2202:8LP:C27	2.12	0.79
1:A:780:TYR:O	1:A:782:PHE:N	2.18	0.77
1:A:768:GLN:O	1:A:775:LYS:NZ	2.18	0.76
1:A:732:GLY:O	1:A:736:ARG:HB2	1.85	0.76
1:A:2013:ARG:NH2	1:A:2113:TYR:OH	2.18	0.76
1:A:753:ARG:HG2	1:A:761:VAL:HG22	1.69	0.74
1:A:770:LYS:O	1:A:775:LYS:NZ	2.17	0.74
1:A:601:GLY:HA3	1:A:1537:THR:HG23	1.67	0.74
1:A:988:ALA:HB2	1:A:998:VAL:HG11	1.68	0.73
1:A:1814:ASN:HA	1:A:1817:MET:HE2	1.70	0.73
1:A:1157:ASN:HB3	1:A:1160:GLU:OE1	1.88	0.73
1:A:760:GLU:HG2	1:A:805:HIS:CE1	2.24	0.72
1:A:1337:ASN:OD1	1:A:1341:ASN:ND2	2.19	0.72
1:A:1727:HIS:HE2	1:A:1770:TYR:HH	1.37	0.72
1:A:488:LEU:HD11	1:A:501:LEU:HD13	1.71	0.71
1:A:2013:ARG:NH2	1:A:2052:ILE:H	1.89	0.71
1:A:610:ARG:NH2	1:A:645:ASP:O	2.24	0.69
1:A:2067:VAL:HG22	1:A:2079:ILE:HG13	1.74	0.69
1:A:715:HIS:HB3	1:A:719:ASN:HB3	1.77	0.66
1:A:736:ARG:NH1	1:A:773:GLU:OE2	2.27	0.66
1:A:1819:ALA:HB2	1:A:1829:ILE:HG12	1.77	0.65
1:A:423:MET:HG2	1:A:425:ASN:HB2	1.78	0.65
1:A:487:LYS:HE2	1:A:676:PHE:HE1	1.62	0.64
1:A:701:PHE:HA	1:A:704:MET:HE2	1.79	0.64
1:A:2054:PRO:HG2	1:A:2055:LEU:HD12	1.79	0.63
1:A:1514:PHE:HB3	1:A:1518:VAL:HG21	1.79	0.63
1:A:804:LYS:HE2	1:A:861:TYR:CE2	2.34	0.63
1:A:758:SER:HA	1:A:761:VAL:HB	1.79	0.62
1:A:463:PRO:HG2	1:A:466:LYS:HG3	1.80	0.62
1:A:986:ARG:O	1:A:990:HIS:ND1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ARG:HG3	1:A:1140:VAL:HG11	1.82	0.61
1:A:1148:PHE:CE2	1:A:1152:ARG:HD2	2.36	0.61
1:A:424:ALA:HB3	1:A:888:PRO:HG2	1.82	0.60
1:A:436:ARG:HG2	1:A:445:VAL:HG22	1.81	0.60
1:A:498:ASN:HD21	1:A:648:LEU:HD13	1.67	0.60
1:A:731:THR:HG23	1:A:810:VAL:HG13	1.84	0.60
1:A:742:CYS:HA	1:A:748:LEU:HD12	1.82	0.60
1:A:696:LYS:O	1:A:700:ARG:HG3	2.01	0.60
1:A:751:PHE:N	1:A:780:TYR:OH	2.35	0.60
1:A:566:VAL:HG22	1:A:585:ILE:HB	1.83	0.59
1:A:1195:ARG:NH1	1:A:1260:GLU:OE2	2.35	0.59
1:A:1962:GLN:NE2	1:A:2114:MET:O	2.33	0.59
1:A:745:LYS:O	1:A:748:LEU:HG	2.03	0.59
1:A:1049:LYS:HD3	1:A:1050:GLU:H	1.67	0.59
1:A:1358:ILE:HA	1:A:1361:GLU:HB2	1.83	0.59
1:A:712:ILE:HG23	1:A:721:VAL:HG21	1.85	0.59
1:A:876:LEU:HD22	1:A:879:TYR:HE2	1.67	0.59
1:A:1314:ASN:HB3	1:A:1317:PHE:HB2	1.84	0.59
1:A:1855:TYR:HB3	1:A:1891:THR:HG21	1.84	0.59
1:A:753:ARG:HD3	1:A:761:VAL:HG13	1.84	0.58
1:A:1939:ALA:C	1:A:1941:ALA:H	2.12	0.58
1:A:1667:GLN:NE2	1:A:1710:LYS:HE3	2.18	0.58
1:A:876:LEU:HD22	1:A:879:TYR:CE2	2.39	0.57
1:A:2076:LEU:HD21	1:A:2079:ILE:HB	1.85	0.57
1:A:617:ILE:HG22	1:A:652:SER:HB2	1.84	0.57
1:A:1341:ASN:O	1:A:1366:ARG:NH1	2.38	0.57
1:A:1666:THR:HG21	1:A:1714:PHE:CE2	2.40	0.56
1:A:738:ILE:HD11	1:A:782:PHE:CZ	2.40	0.56
1:A:1302:LEU:N	1:A:1334:GLN:OE1	2.30	0.56
1:A:1594:GLU:HG2	1:A:1614:LEU:HD22	1.86	0.56
1:A:1994:ASN:C	1:A:1996:LEU:H	2.13	0.56
1:A:703:ILE:O	1:A:707:ILE:HG12	2.05	0.56
1:A:1672:LYS:HG3	1:A:1860:ILE:HD13	1.89	0.55
1:A:731:THR:CG2	1:A:784:ILE:HB	2.37	0.55
1:A:838:LYS:HD2	1:A:842:THR:HG21	1.88	0.55
1:A:1560:ILE:HG13	1:A:1658:ALA:HB2	1.88	0.55
1:A:1350:ALA:HB3	1:A:1356:LYS:HD3	1.89	0.55
1:A:2068:ILE:O	1:A:2077:ILE:HG13	2.07	0.55
1:A:1368:LEU:HD22	1:A:1403:LYS:HE3	1.89	0.54
1:A:1567:LYS:O	1:A:1571:LEU:HD13	2.06	0.54
1:A:1577:LEU:HD11	1:A:1615:ASN:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1447:ASN:HA	1:A:1483:ARG:NH2	2.22	0.54
1:A:516:CYS:SG	1:A:649:ILE:HG12	2.48	0.54
1:A:1038:GLN:O	1:A:1042:GLU:HG2	2.07	0.54
1:A:668:ASP:HB3	1:A:671:LYS:HB2	1.90	0.54
1:A:876:LEU:C	1:A:878:TYR:N	2.66	0.54
1:A:1360:ALA:HB2	1:A:1490:LEU:HD11	1.90	0.54
1:A:503:ALA:HB3	1:A:509:LYS:HE3	1.89	0.53
1:A:1351:PRO:HG3	1:A:1516:PRO:HA	1.90	0.53
1:A:802:ALA:O	1:A:804:LYS:NZ	2.41	0.53
1:A:567:ALA:HB3	1:A:583:THR:HG21	1.89	0.53
1:A:1148:PHE:CZ	1:A:1152:ARG:HD2	2.43	0.53
1:A:597:THR:HA	1:A:602:GLU:HB2	1.91	0.53
1:A:708:VAL:O	1:A:712:ILE:HG13	2.08	0.53
1:A:540:TYR:OH	1:A:615:ASP:OD2	2.20	0.53
1:A:1335:VAL:O	1:A:1339:VAL:HG23	2.08	0.53
1:A:603:ARG:HH21	1:A:607:GLN:HG3	1.74	0.53
1:A:484:ILE:HD12	1:A:484:ILE:H	1.73	0.52
1:A:550:GLU:HB2	1:A:818:GLY:O	2.08	0.52
1:A:1146:LYS:HE3	1:A:1164:LEU:O	2.09	0.52
1:A:578:GLU:C	1:A:580:ILE:H	2.18	0.52
1:A:715:HIS:HB3	1:A:719:ASN:CB	2.39	0.52
1:A:790:THR:OG1	1:A:791:ARG:N	2.34	0.52
1:A:905:ILE:HG22	1:A:981:VAL:HG22	1.91	0.52
1:A:1112:LEU:HG	1:A:1116:LYS:HE3	1.90	0.52
1:A:974:LYS:H	1:A:974:LYS:HD2	1.75	0.52
1:A:2040:GLN:OE1	1:A:2089:LYS:HG2	2.10	0.51
1:A:459:GLU:OE2	1:A:483:ARG:NH2	2.43	0.51
1:A:1088:ALA:HB1	1:A:1118:ILE:HD13	1.93	0.51
1:A:1481:ILE:HG23	1:A:1483:ARG:H	1.75	0.51
1:A:1770:TYR:HE2	2:A:2201:GOL:H11	1.75	0.51
1:A:686:GLU:HB2	1:A:864:LYS:HE3	1.92	0.51
1:A:709:TYR:OH	1:A:748:LEU:HD22	2.11	0.51
1:A:743:LEU:HA	1:A:747:THR:HA	1.93	0.51
1:A:753:ARG:HE	1:A:780:TYR:HA	1.74	0.51
1:A:811:SER:OG	1:A:812:THR:N	2.44	0.51
1:A:1994:ASN:O	1:A:1996:LEU:N	2.43	0.51
1:A:713:MET:SD	1:A:749:GLY:HA3	2.51	0.50
1:A:781:GLY:O	1:A:807:GLN:N	2.43	0.50
1:A:538:ILE:HB	1:A:585:ILE:HG13	1.93	0.50
1:A:753:ARG:CG	1:A:761:VAL:HG22	2.39	0.50
1:A:1716:LYS:HD3	1:A:1717:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:HIS:HB3	1:A:1201:GLU:HB2	1.94	0.50
1:A:1499:ASP:OD2	1:A:1766:GLN:HG3	2.11	0.50
1:A:736:ARG:HH22	1:A:773:GLU:HB3	1.76	0.50
1:A:1457:HIS:CD2	1:A:1492:SER:H	2.30	0.50
1:A:621:HIS:O	1:A:892:GLN:NE2	2.29	0.50
1:A:965:ASP:HA	1:A:970:VAL:O	2.11	0.50
1:A:1666:THR:HG21	1:A:1714:PHE:CZ	2.47	0.50
1:A:1049:LYS:O	1:A:1051:SER:N	2.45	0.49
1:A:986:ARG:HG3	1:A:990:HIS:HE1	1.76	0.49
1:A:518:LEU:HD23	1:A:521:ILE:HD12	1.94	0.49
1:A:637:ARG:HH22	1:A:919:TRP:HB2	1.77	0.49
1:A:603:ARG:NH1	1:A:642:THR:HG21	2.28	0.49
1:A:1901:ARG:HG3	1:A:1961:LYS:NZ	2.28	0.49
1:A:1497:ALA:O	1:A:1500:VAL:HG12	2.13	0.49
1:A:423:MET:HE2	1:A:878:TYR:HB2	1.95	0.49
1:A:467:LEU:HB2	1:A:468:PRO:HD2	1.95	0.49
1:A:1661:VAL:HG23	1:A:1691:ALA:HB2	1.94	0.49
1:A:1836:LEU:HD22	1:A:1930:LEU:HD21	1.95	0.48
1:A:1456:VAL:HG12	1:A:1491:SER:HB2	1.95	0.48
1:A:1953:MET:CE	1:A:2114:MET:HG3	2.44	0.48
1:A:1966:PHE:HD2	1:A:1970:HIS:NE2	2.11	0.48
1:A:785:HIS:O	1:A:811:SER:HA	2.14	0.48
1:A:611:LEU:HD11	1:A:649:ILE:HD13	1.95	0.48
1:A:1456:VAL:CG1	1:A:1491:SER:HB2	2.44	0.48
1:A:2030:ARG:HG2	1:A:2100:GLY:H	1.78	0.48
1:A:487:LYS:HE2	1:A:676:PHE:CE1	2.46	0.48
1:A:632:VAL:O	1:A:636:ILE:HG12	2.13	0.48
1:A:762:LEU:HA	1:A:765:GLU:HG2	1.94	0.48
1:A:1559:VAL:HG22	1:A:1660:LEU:HB3	1.96	0.48
1:A:1963:LEU:HD22	1:A:2007:VAL:HG13	1.96	0.48
1:A:521:ILE:HG23	1:A:531:ILE:HD11	1.96	0.48
1:A:1531:ASN:O	1:A:1532:ILE:HG13	2.14	0.48
1:A:1419:LEU:HA	1:A:1425:ILE:HD13	1.96	0.47
1:A:1312:LEU:HD12	1:A:1340:TYR:CZ	2.49	0.47
1:A:579:GLU:C	1:A:581:SER:H	2.23	0.47
1:A:654:THR:HG21	1:A:676:PHE:O	2.15	0.47
1:A:1398:GLN:O	1:A:1402:ASN:HA	2.14	0.47
1:A:1945:LEU:HA	1:A:1948:MET:HG2	1.95	0.47
1:A:2043:ARG:NH2	1:A:2085:GLN:O	2.26	0.47
1:A:1012:ILE:HD12	1:A:1047:PRO:O	2.15	0.47
1:A:1994:ASN:OD1	1:A:1994:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:THR:O	1:A:810:VAL:HG11	2.14	0.47
1:A:986:ARG:HG3	1:A:990:HIS:CE1	2.50	0.47
1:A:1066:PHE:CG	1:A:1085:THR:HG21	2.50	0.47
1:A:757:ALA:O	1:A:761:VAL:HG21	2.14	0.47
1:A:823:ALA:O	1:A:857:GLY:N	2.45	0.47
1:A:2101:ALA:O	1:A:2102:HIS:ND1	2.48	0.47
1:A:547:LEU:HD11	1:A:551:MET:HE2	1.97	0.46
1:A:1044:VAL:HA	1:A:1045:PRO:HD3	1.73	0.46
1:A:1321:TYR:HD2	1:A:1325:PHE:CZ	2.33	0.46
1:A:2064:TRP:CZ3	1:A:2110:SER:HB2	2.49	0.46
1:A:1187:SER:HB3	1:A:1203:THR:HB	1.96	0.46
1:A:1770:TYR:CE2	2:A:2201:GOL:H11	2.50	0.46
1:A:1940:LEU:HD23	1:A:1943:MET:SD	2.56	0.46
1:A:594:ASP:O	1:A:598:ARG:HG3	2.16	0.46
1:A:790:THR:O	1:A:791:ARG:HB2	2.14	0.46
1:A:1309:VAL:HG23	1:A:1326:PRO:O	2.16	0.46
1:A:498:ASN:ND2	1:A:648:LEU:HD13	2.29	0.46
1:A:1542:MET:C	1:A:1545:PRO:HD2	2.41	0.46
1:A:1953:MET:HE3	1:A:2114:MET:HG3	1.98	0.46
1:A:2041:LEU:HD11	1:A:2108:PHE:CE1	2.50	0.46
1:A:1970:HIS:HD2	1:A:1974:CYS:SG	2.38	0.46
1:A:595:ILE:HG22	1:A:596:ILE:HD12	1.98	0.46
1:A:1194:THR:HG22	1:A:1195:ARG:H	1.80	0.46
1:A:1292:PRO:HG3	1:A:1767:ASN:OD1	2.15	0.46
1:A:704:MET:O	1:A:708:VAL:HG23	2.16	0.46
1:A:1012:ILE:HD11	1:A:1047:PRO:HD2	1.98	0.46
1:A:1337:ASN:O	1:A:1341:ASN:HB2	2.16	0.46
1:A:1815:LEU:H	1:A:1815:LEU:HD12	1.81	0.46
1:A:768:GLN:CD	1:A:779:PRO:HD3	2.41	0.46
1:A:1308:PRO:HA	1:A:1327:PHE:HD1	1.81	0.46
1:A:1515:HIS:O	1:A:1518:VAL:HG22	2.15	0.46
1:A:519:ARG:HD3	1:A:647:ARG:NH1	2.31	0.46
1:A:876:LEU:C	1:A:878:TYR:H	2.24	0.46
1:A:1148:PHE:HE1	1:A:1153:LEU:HD12	1.80	0.46
1:A:1195:ARG:HD2	1:A:1294:LYS:HB2	1.97	0.46
1:A:2009:ARG:HH11	1:A:2052:ILE:HD12	1.80	0.46
1:A:873:HIS:CG	1:A:874:GLY:N	2.85	0.45
1:A:1604:LEU:HD21	1:A:1631:LEU:HD23	1.97	0.45
1:A:1398:GLN:HA	1:A:1403:LYS:O	2.16	0.45
1:A:409:LEU:HD13	1:A:414:LEU:HD11	1.99	0.45
1:A:439:ARG:HA	1:A:439:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:THR:HB	1:A:793:ASP:HB2	1.99	0.45
1:A:642:THR:C	1:A:644:GLU:H	2.25	0.45
1:A:554:SER:O	1:A:558:ARG:HG3	2.17	0.45
1:A:1527:ILE:HD13	1:A:1715:LYS:HG2	1.98	0.45
1:A:1713:PHE:HB2	3:A:2202:8LP:C27	2.47	0.45
1:A:1966:PHE:HD2	1:A:1970:HIS:CE1	2.35	0.45
1:A:2014:TYR:HA	1:A:2015:PRO:HD3	1.77	0.45
1:A:2019:LEU:HD22	1:A:2120:TYR:CE2	2.51	0.45
1:A:737:ALA:HA	1:A:740:ASP:HB3	1.99	0.45
2:A:2201:GOL:H2	3:A:2202:8LP:C8	2.47	0.45
1:A:804:LYS:HE2	1:A:861:TYR:CD2	2.52	0.45
1:A:760:GLU:HG2	1:A:805:HIS:ND1	2.32	0.45
1:A:1384:ALA:HB1	1:A:1653:GLY:HA2	1.98	0.45
1:A:1296:PRO:HG3	1:A:1498:LYS:HE3	2.00	0.44
1:A:853:LEU:HD23	1:A:853:LEU:HA	1.70	0.44
1:A:1865:ASP:OD1	1:A:1865:ASP:N	2.50	0.44
1:A:837:GLU:O	1:A:1026:ASN:HB2	2.18	0.44
1:A:482:ASN:HB3	1:A:485:GLN:CD	2.42	0.44
1:A:629:GLU:HA	1:A:664:PHE:HZ	1.83	0.44
1:A:689:TYR:HE2	1:A:883:LEU:HD12	1.83	0.44
1:A:1950:THR:HA	1:A:2056:PHE:CD2	2.53	0.44
1:A:917:VAL:HG13	1:A:953:ARG:HB3	1.99	0.44
1:A:1142:LYS:HD2	1:A:1167:MET:HE3	2.00	0.44
1:A:701:PHE:HA	1:A:704:MET:CE	2.47	0.44
1:A:473:ALA:O	1:A:562:TYR:OH	2.30	0.44
1:A:484:ILE:HG23	1:A:676:PHE:CE2	2.53	0.44
1:A:991:TYR:CE2	1:A:1097:GLU:HG3	2.53	0.44
1:A:473:ALA:HB3	1:A:562:TYR:CZ	2.53	0.43
1:A:2051:VAL:HG13	1:A:2113:TYR:OH	2.18	0.43
1:A:928:ARG:HB3	1:A:936:TYR:CE1	2.53	0.43
1:A:464:VAL:O	1:A:467:LEU:HG	2.18	0.43
1:A:496:ASP:CG	1:A:519:ARG:HH11	2.27	0.43
1:A:606:THR:HA	1:A:609:VAL:HG23	2.00	0.43
1:A:771:ASN:OD1	1:A:772:LEU:N	2.44	0.43
1:A:1225:VAL:HG11	1:A:1256:VAL:HG11	2.01	0.43
1:A:1041:LEU:HA	1:A:1044:VAL:HG22	2.01	0.43
1:A:1162:GLY:HA3	1:A:1168:PRO:HA	2.00	0.43
1:A:764:THR:HB	1:A:778:LEU:O	2.18	0.43
1:A:767:GLU:HG3	1:A:800:LEU:HD11	2.01	0.43
1:A:2084:LEU:O	1:A:2085:GLN:HB2	2.19	0.43
1:A:611:LEU:HD12	1:A:647:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLU:O	1:A:710:GLU:HG2	2.18	0.43
1:A:825:THR:HA	1:A:866:GLU:O	2.19	0.43
1:A:959:THR:HG22	1:A:963:MET:HE3	2.00	0.43
1:A:1379:ILE:HA	1:A:1427:SER:O	2.19	0.43
1:A:1380:THR:O	1:A:1429:PRO:HD3	2.19	0.43
1:A:663:THR:HB	1:A:927:ILE:HD13	2.00	0.43
1:A:1165:ILE:HG23	1:A:1167:MET:HB3	2.00	0.42
1:A:1192:PRO:HG3	1:A:1289:LEU:HD11	2.01	0.42
1:A:1950:THR:HA	1:A:2056:PHE:HD2	1.84	0.42
1:A:1648:ARG:HD2	1:A:1679:TYR:CE1	2.55	0.42
1:A:1939:ALA:C	1:A:1941:ALA:N	2.76	0.42
1:A:692:ILE:HG12	1:A:871:THR:O	2.20	0.42
1:A:569:LEU:O	1:A:592:LYS:HE2	2.19	0.42
1:A:681:ARG:NH1	1:A:685:LEU:HD22	2.34	0.42
1:A:887:LEU:HA	1:A:888:PRO:HD3	1.79	0.42
1:A:995:ASN:O	1:A:998:VAL:HG22	2.19	0.42
1:A:1725:GLU:HB3	1:A:1771:TYR:OH	2.20	0.42
1:A:543:PRO:HG3	1:A:616:GLU:HB2	2.02	0.42
1:A:718:LYS:HE3	1:A:718:LYS:HB3	1.88	0.42
1:A:1914:GLU:O	1:A:1917:SER:HB3	2.19	0.42
1:A:2080:LYS:HE3	1:A:2080:LYS:HB2	1.81	0.42
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.63	0.42
1:A:1012:ILE:CD1	1:A:1047:PRO:HD2	2.50	0.42
1:A:1598:ILE:HB	1:A:1599:PRO:HD3	2.01	0.42
1:A:2068:ILE:CG2	1:A:2077:ILE:HD11	2.50	0.42
1:A:739:ARG:NH2	1:A:776:ASP:OD1	2.53	0.42
1:A:1838:ALA:HB2	1:A:1935:TRP:NE1	2.35	0.42
1:A:753:ARG:HH21	1:A:780:TYR:HB2	1.85	0.42
1:A:828:ILE:HD13	1:A:852:MET:HE3	2.02	0.42
1:A:987:ILE:HG23	1:A:991:TYR:CD2	2.55	0.42
1:A:1515:HIS:CG	1:A:1516:PRO:HD2	2.55	0.42
1:A:2019:LEU:HD12	1:A:2041:LEU:HD21	2.01	0.42
1:A:518:LEU:HD23	1:A:518:LEU:HA	1.93	0.41
1:A:1503:TRP:NE1	1:A:1757:TRP:O	2.54	0.41
1:A:1920:ILE:HD13	1:A:1920:ILE:HA	1.90	0.41
1:A:1538:ARG:HG2	1:A:1542:MET:HE3	2.02	0.41
1:A:1863:HIS:O	1:A:1863:HIS:ND1	2.54	0.41
1:A:1966:PHE:HD2	1:A:1970:HIS:CD2	2.39	0.41
1:A:1965:HIS:HB3	1:A:2003:GLN:HE21	1.85	0.41
1:A:595:ILE:HG13	1:A:992:TYR:CD1	2.56	0.41
1:A:905:ILE:HG12	1:A:910:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:SER:O	1:A:839:GLY:N	2.54	0.41
1:A:928:ARG:NH2	1:A:932:SER:OG	2.51	0.41
1:A:1139:VAL:O	1:A:1143:ILE:HG13	2.20	0.41
1:A:489:TYR:HE1	1:A:490:ARG:NH1	2.18	0.41
1:A:524:HIS:CD2	1:A:536:PHE:CD1	3.09	0.41
1:A:533:VAL:HG13	1:A:584:GLN:CD	2.44	0.41
1:A:2013:ARG:NH1	1:A:2052:ILE:HB	2.36	0.41
1:A:2040:GLN:HE22	1:A:2089:LYS:HD2	1.86	0.41
1:A:462:LEU:HD13	1:A:489:TYR:CE1	2.55	0.41
1:A:1459:ILE:HD11	1:A:1468:GLU:HB2	2.03	0.41
1:A:1519:ARG:NH2	1:A:1691:ALA:O	2.37	0.41
1:A:1586:ARG:O	1:A:1587:GLN:HB2	2.20	0.41
1:A:564:ILE:HD12	1:A:584:GLN:HG2	2.03	0.41
1:A:2089:LYS:HB3	1:A:2089:LYS:HE2	1.84	0.40
1:A:735:ALA:HB2	1:A:810:VAL:CG1	2.50	0.40
1:A:488:LEU:HD13	1:A:512:VAL:HG11	2.04	0.40
1:A:858:ARG:HA	1:A:859:PRO:HD3	1.88	0.40
1:A:877:GLN:O	1:A:880:LEU:HB2	2.20	0.40
1:A:1039:LYS:O	1:A:1043:ARG:HG3	2.21	0.40
1:A:1430:GLU:HG2	1:A:1431:LYS:N	2.35	0.40
1:A:1436:SER:O	1:A:1439:TRP:HB3	2.21	0.40
1:A:2051:VAL:HG13	1:A:2113:TYR:CZ	2.57	0.40
1:A:1948:MET:HB2	1:A:1953:MET:O	2.20	0.40
1:A:462:LEU:HA	1:A:463:PRO:HD2	1.89	0.40
1:A:1149:PRO:HG2	1:A:1152:ARG:HB2	2.04	0.40
1:A:1447:ASN:HA	1:A:1483:ARG:HH22	1.85	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	1698/1738 (98%)	1609 (95%)	72 (4%)	17 (1%)	12	32

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	MET
1	A	743	LEU
1	A	781	GLY
1	A	791	ARG
1	A	1995	ALA
1	A	2031	SER
1	A	2100	GLY
1	A	770	LYS
1	A	1665	ASP
1	A	1993	ARG
1	A	2101	ALA
1	A	579	GLU
1	A	696	LYS
1	A	742	CYS
1	A	1940	LEU
1	A	1052	ILE
1	A	1584	ILE

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	1503/1551 (97%)	1459 (97%)	44 (3%)	37	61

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	SER
1	A	489	TYR
1	A	533	VAL
1	A	546	SER

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Mol	Chain	Res	Type
1	A	570	THR
1	A	595	ILE
1	A	602	GLU
1	A	610	ARG
1	A	731	THR
1	A	752	LEU
1	A	821	LEU
1	A	849	ILE
1	A	853	LEU
1	A	863	THR
1	A	910	VAL
1	A	939	SER
1	A	1028	THR
1	A	1053	GLU
1	A	1165	ILE
1	A	1194	THR
1	A	1249	GLU
1	A	1305	GLN
1	A	1307	LEU
1	A	1334	GLN
1	A	1380	THR
1	A	1498	LYS
1	A	1571	LEU
1	A	1577	LEU
1	A	1656	VAL
1	A	1677	VAL
1	A	1731	CYS
1	A	1805	GLU
1	A	1807	GLU
1	A	1829	ILE
1	A	1862	HIS
1	A	1967	THR
1	A	1982	VAL
1	A	1999	LEU
1	A	2001	ASP
1	A	2004	ILE
1	A	2017	ILE
1	A	2052	ILE
1	A	2090	VAL
1	A	2114	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	526	ASN
1	A	702	GLN
1	A	824	HIS
1	A	832	GLN
1	A	884	ASN
1	A	902	ASN
1	A	911	GLN
1	A	978	ASN
1	A	1101	ASN
1	A	1175	HIS
1	A	1402	ASN
1	A	1778	HIS
1	A	1857	ASN
1	A	2058	GLN
1	A	2086	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](#)

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
3	8LP	A	2202	-	37,37,37	0.92	1 (2%)	46,51,51	1.34	7 (15%)
2	GOL	A	2201	-	5,5,5	0.41	0	5,5,5	0.27	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
3	8LP	A	2202	-	-	0/13/25/25	0/5/5/5
2	GOL	A	2201	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2202	8LP	C23-N3	-2.48	1.36	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2202	8LP	C27-O3-C18	-3.97	108.17	117.62
3	A	2202	8LP	C22-N1-C24	2.94	126.54	122.77
3	A	2202	8LP	O1-C23-N3	2.86	122.24	119.51
3	A	2202	8LP	C12-C17-N2	-2.86	116.06	120.18
3	A	2202	8LP	O2-C24-N2	-2.39	120.26	122.03
3	A	2202	8LP	C15-C26-N3	-2.26	109.34	112.84
3	A	2202	8LP	C21-C20-N3	-2.18	120.78	123.56

There are no chirality outliers.

There are no torsion outliers.

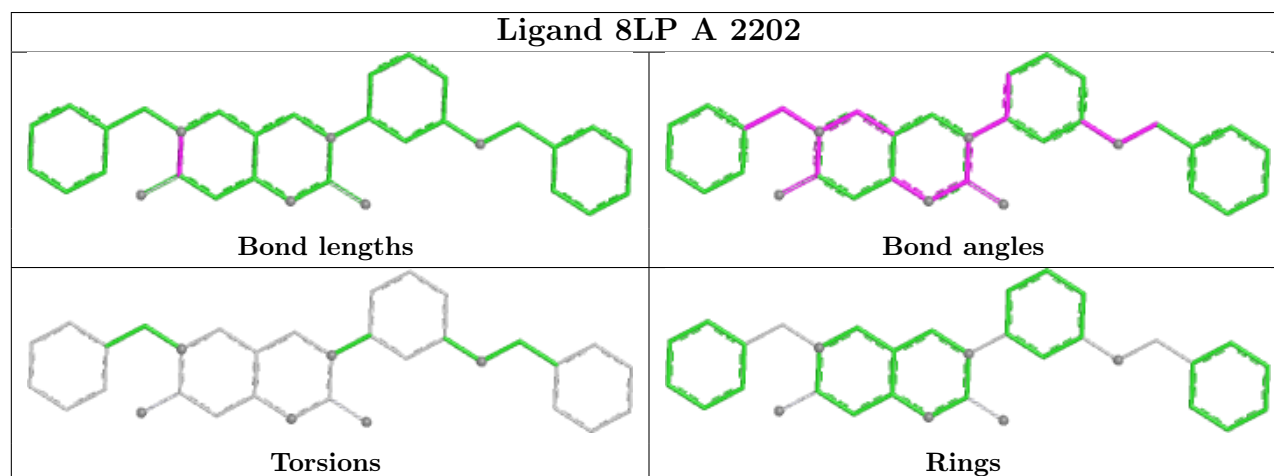
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2202	8LP	3	0
2	A	2201	GOL	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1706/1738 (98%)	0.38	63 (3%) 45 37	57, 102, 157, 200	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	722	LEU	6.1
1	A	752	LEU	4.5
1	A	735	ALA	4.3
1	A	580	ILE	4.1
1	A	721	VAL	4.1
1	A	787	ALA	4.0
1	A	743	LEU	3.9
1	A	790	THR	3.5
1	A	783	ALA	3.5
1	A	737	ALA	3.4
1	A	821	LEU	3.3
1	A	1249	GLU	3.3
1	A	809	LEU	3.3
1	A	1295	TYR	3.1
1	A	1496	ASN	3.1
1	A	2035	VAL	2.9
1	A	1365	LEU	2.9
1	A	578	GLU	2.7
1	A	739	ARG	2.7
1	A	762	LEU	2.7
1	A	747	THR	2.6
1	A	740	ASP	2.6
1	A	579	GLU	2.6
1	A	2023	VAL	2.6
1	A	461	LEU	2.5
1	A	772	LEU	2.5
1	A	505	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	786	HIS	2.5
1	A	1050	GLU	2.5
1	A	764	THR	2.5
1	A	808	VAL	2.4
1	A	1478	SER	2.4
1	A	2123	SER	2.4
1	A	577	LYS	2.4
1	A	774	LEU	2.4
1	A	819	VAL	2.3
1	A	701	PHE	2.3
1	A	1960	LEU	2.3
1	A	782	PHE	2.3
1	A	805	HIS	2.3
1	A	2104	TYR	2.3
1	A	799	ASP	2.2
1	A	759	THR	2.2
1	A	1966	PHE	2.2
1	A	712	ILE	2.2
1	A	2060	ARG	2.2
1	A	728	ARG	2.2
1	A	784	ILE	2.2
1	A	2054	PRO	2.1
1	A	1773	LEU	2.1
1	A	1322	GLN	2.1
1	A	1194	THR	2.1
1	A	751	PHE	2.1
1	A	2010	PHE	2.1
1	A	480	THR	2.1
1	A	731	THR	2.1
1	A	763	ARG	2.1
1	A	2004	ILE	2.1
1	A	773	GLU	2.1
1	A	558	ARG	2.0
1	A	738	ILE	2.0
1	A	605	TYR	2.0
1	A	1294	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

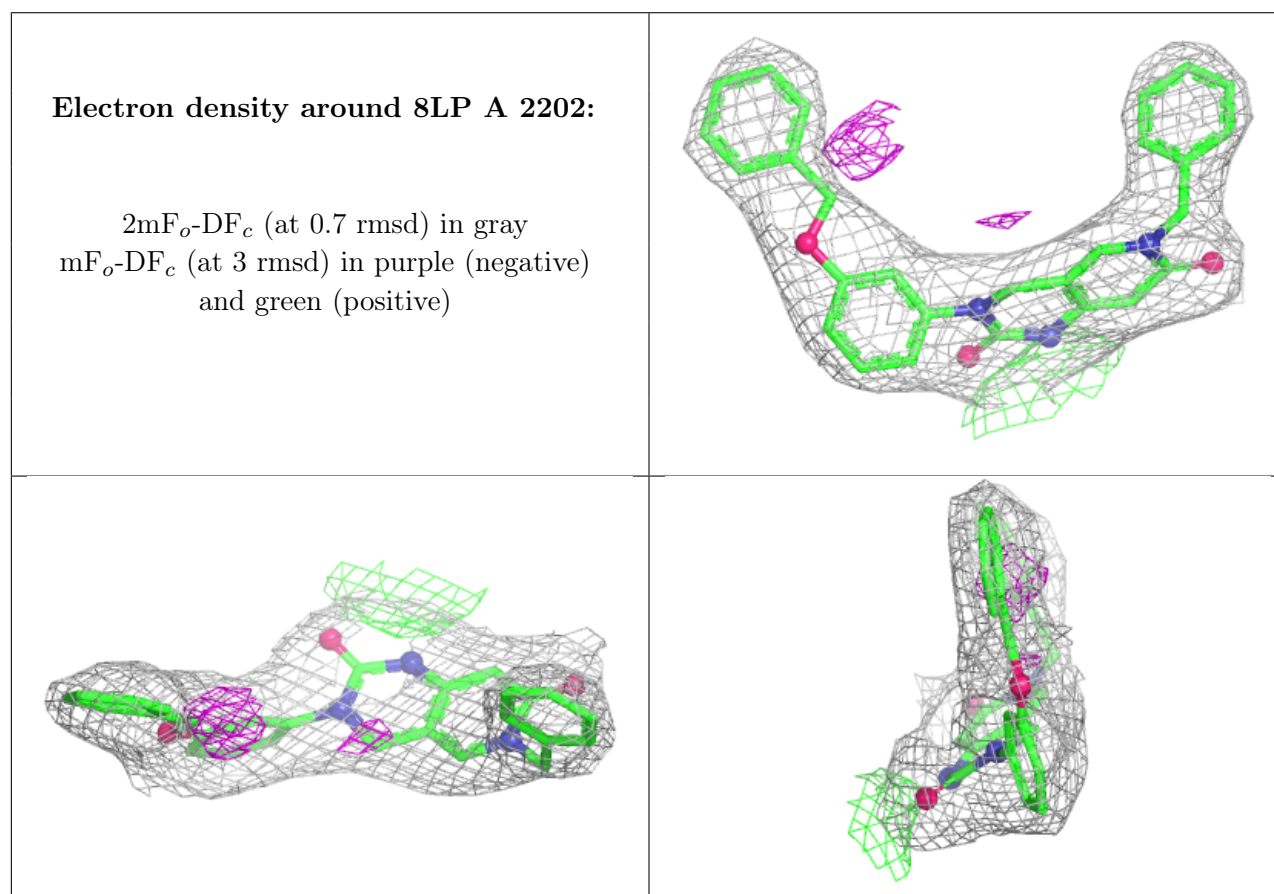
There are no oligosaccharides in this entry.

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	GOL	A	2201	6/6	0.88	0.13	71,71,76,81	0
3	8LP	A	2202	33/33	0.93	0.11	63,71,78,83	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.