



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:41 AM UTC

PDB ID : 8BCB / pdb_00008bcb
Title : Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and compound 34
Authors : Vester, K.; Loll, B.; Wahl, M.C.
Deposited on : 2022-10-15
Resolution : 2.38 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)
Xtrriage (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

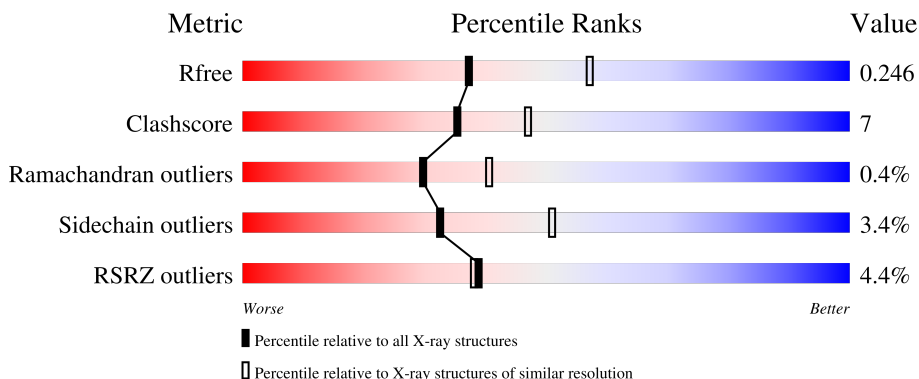
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	B	1747	 4% 78% 20% ..
2	J	263	 5% 82% 16% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16261 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	B	1721	13838	8845	2368	2553	72	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLY	-	expression tag	UNP O75643
B	391	ALA	-	expression tag	UNP O75643
B	392	GLU	-	expression tag	UNP O75643
B	393	PHE	-	expression tag	UNP O75643

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	263	2123	1358	365	388	12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2058	GLY	-	expression tag	UNP Q6P2Q9
J	2059	PRO	-	expression tag	UNP Q6P2Q9
J	2060	LEU	-	expression tag	UNP Q6P2Q9
J	2061	GLY	-	expression tag	UNP Q6P2Q9
J	2062	SER	-	expression tag	UNP Q6P2Q9
J	2063	MET	-	expression tag	UNP Q6P2Q9

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



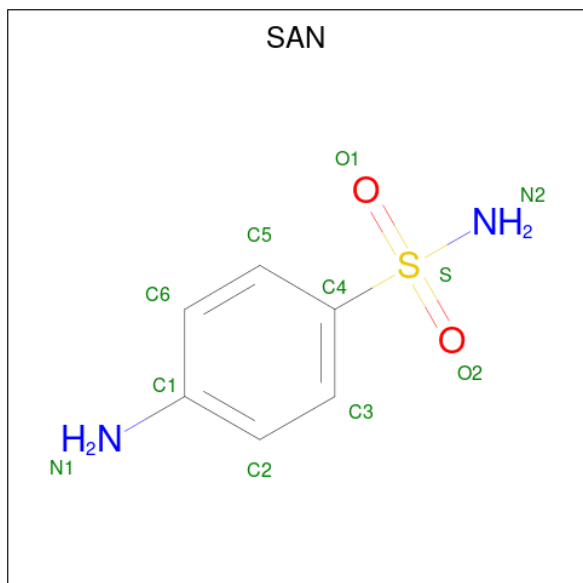
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFANILAMIDE (CCD ID: SAN) (formula: C₆H₈N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O S 11 6 2 2 1	0	0
4	B	1	Total C N O S 11 6 2 2 1	0	0

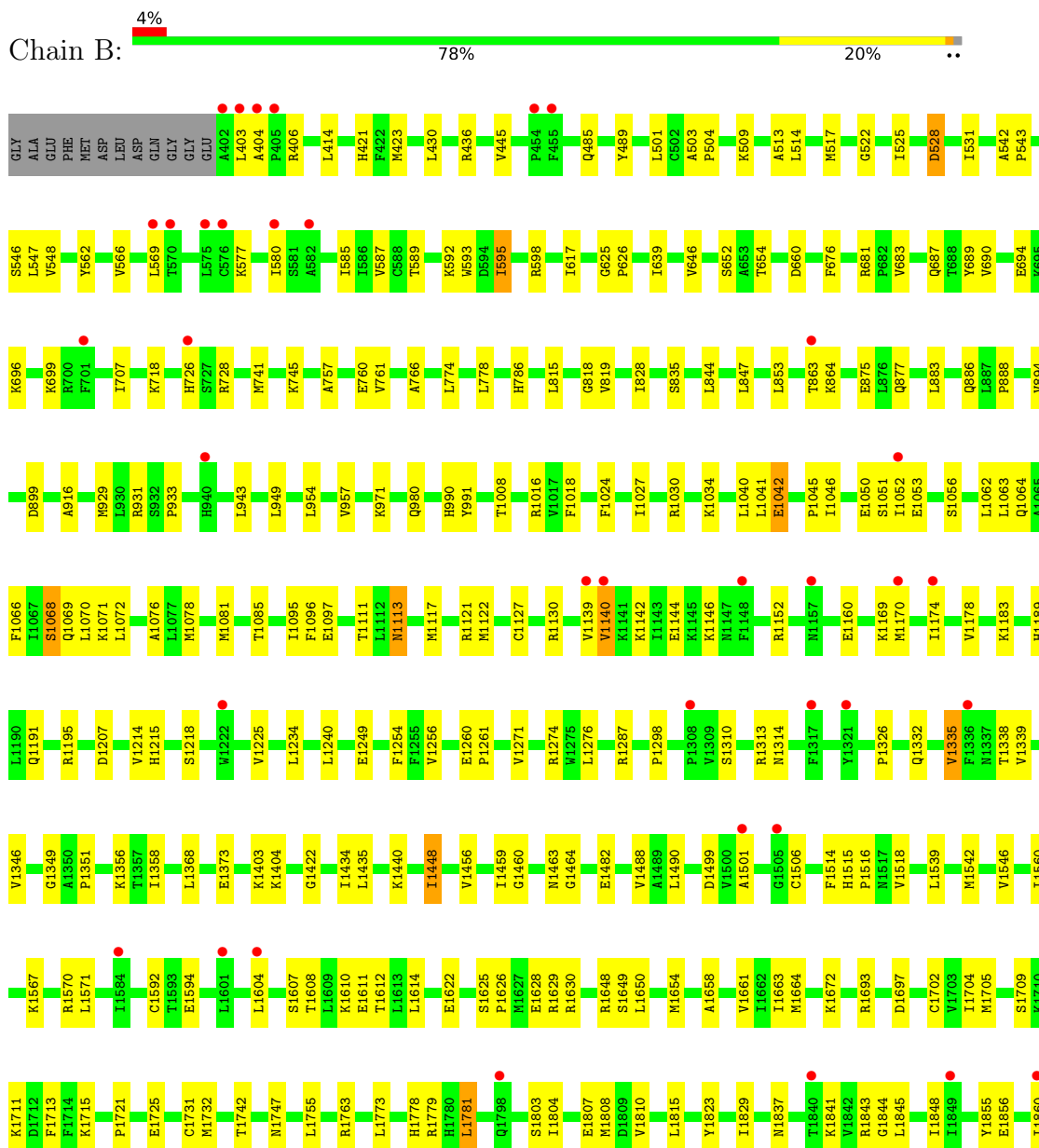
- Molecule 5 is water.

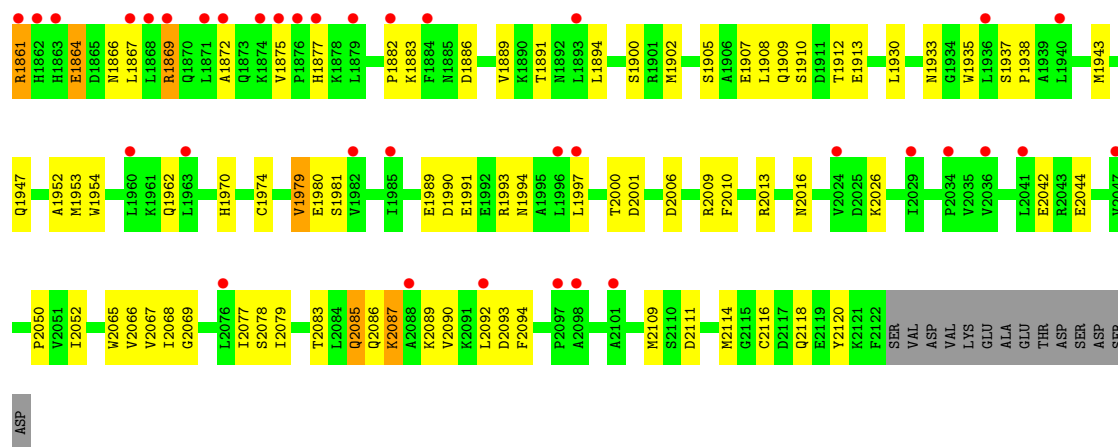
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	190	Total O 190 190	0	0
5	J	24	Total O 24 24	0	0

3 Residue-property plots [i](#)

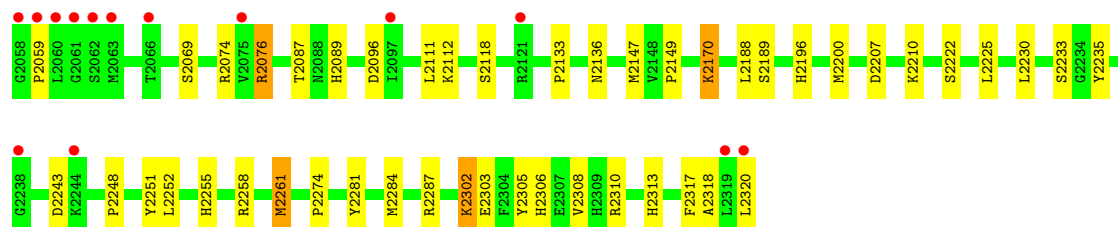
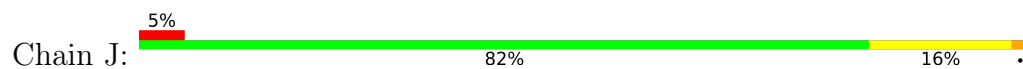
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 2: Pre-mRNA-processing-splicing factor 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.20Å 119.23Å 186.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.38 48.39 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.39-2.38) 98.9 (48.39-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.37Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.205 , 0.258 (Not available) , 0.246	Depositor DCC
R_{free} test set	2100 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16261	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: SAN, EDO

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	B	0.44	0/14132	0.60	0/19148
2	J	0.46	0/2190	0.62	0/2981
All	All	0.44	0/16322	0.61	0/22129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	13838	0	13983	211	1
2	J	2123	0	2063	31	0
3	B	60	0	90	5	0
3	J	4	0	6	2	0
4	B	22	0	16	3	0
5	B	190	0	0	1	0
5	J	24	0	0	1	0
All	All	16261	0	16158	238	1

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 7.

All (238) 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:J:2284:MET:HB3	2:J:2287:ARG:HD3	1.57	0.83
1:B:1872:ALA:HA	1:B:1875:VAL:HB	1.63	0.78
1:B:598:ARG:HH22	3:B:2202:EDO:H11	1.50	0.76
1:B:1943:MET:HE3	1:B:2065:TRP:HB2	1.67	0.75
1:B:1024:PHE:HB3	1:B:1027:ILE:HD12	1.70	0.74
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.70	0.74
1:B:1672:LYS:HB2	1:B:1860:ILE:HG21	1.68	0.74
1:B:406:ARG:HD3	1:B:954:LEU:HG	1.71	0.73
1:B:2068:ILE:HD13	1:B:2078:SER:HB2	1.70	0.72
1:B:2042:GLU:HG3	1:B:2087:LYS:HD2	1.72	0.71
1:B:1515:HIS:CE1	1:B:1721:PRO:HG3	2.26	0.71
1:B:1943:MET:HE2	1:B:2109:MET:HB2	1.72	0.70
1:B:1693:ARG:HD3	1:B:1697:ASP:OD2	1.90	0.70
1:B:1907:GLU:HB3	3:B:2214:EDO:H12	1.73	0.69
1:B:991:TYR:OH	1:B:1097:GLU:OE1	2.09	0.69
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.28	0.68
1:B:1604:LEU:HD23	1:B:1628:GLU:HG2	1.77	0.67
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.77	0.67
1:B:1607:SER:HA	1:B:1610:LYS:HE3	1.78	0.65
1:B:1626:PRO:O	1:B:1630:ARG:HG2	1.97	0.65
1:B:436:ARG:HG2	1:B:445:VAL:HG22	1.79	0.64
1:B:1732:MET:HE1	1:B:1755:LEU:HD21	1.80	0.64
1:B:1189:HIS:CE1	1:B:1191:GLN:HE21	2.16	0.64
1:B:2068:ILE:HD11	1:B:2092:LEU:HD13	1.79	0.64
2:J:2225:LEU:HD13	2:J:2261:MET:HE1	1.78	0.64
1:B:741:MET:HE3	1:B:745:LYS:HE3	1.81	0.63
1:B:1943:MET:HG2	1:B:2065:TRP:CE3	2.33	0.63
1:B:654:THR:HG21	1:B:676:PHE:O	2.00	0.62
1:B:1041:LEU:HD22	1:B:1052:ILE:HG23	1.82	0.62
1:B:1747:ASN:HB2	1:B:1808:MET:HE3	1.82	0.62
1:B:1287:ARG:HH21	3:B:2208:EDO:H11	1.65	0.61
1:B:1713:PHE:HB2	3:B:2203:EDO:H12	1.81	0.61
1:B:1499:ASP:OD2	1:B:1763:ARG:NH1	2.32	0.60
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.15	0.60
1:B:1993:ARG:O	1:B:1997:LEU:HG	2.02	0.60
1:B:1539:LEU:HD22	1:B:1664:MET:HE3	1.84	0.59
1:B:1127:CYS:HB2	1:B:1144:GLU:HG2	1.84	0.59
1:B:514:LEU:HA	1:B:517:MET:HE2	1.85	0.59
1:B:595:ILE:HD11	1:B:990:HIS:O	2.03	0.58
1:B:1016:ARG:HD2	1:B:1050:GLU:OE2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1607:SER:O	1:B:1611:GLU:HG2	2.04	0.58
1:B:1953:MET:HE1	1:B:1962:GLN:HG3	1.86	0.57
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.86	0.57
1:B:899:ASP:HB3	3:B:2202:EDO:H12	1.87	0.56
1:B:1042:GLU:HG3	2:J:2069:SER:O	2.05	0.56
1:B:1249:GLU:OE1	5:B:2301:HOH:O	2.17	0.56
1:B:1900:SER:HG	1:B:1954:TRP:CD1	2.23	0.56
1:B:577:LYS:HA	1:B:580:ILE:HB	1.88	0.56
1:B:726:HIS:CE1	1:B:844:LEU:HD11	2.41	0.56
1:B:2013:ARG:HD2	1:B:2052:ILE:HG12	1.88	0.55
1:B:528:ASP:OD1	1:B:528:ASP:N	2.38	0.55
1:B:1864:GLU:HG2	1:B:1867:LEU:HD12	1.87	0.55
1:B:1404:LYS:HB3	1:B:1422:GLY:HA2	1.87	0.55
1:B:1066:PHE:O	1:B:1121:ARG:NH1	2.38	0.55
1:B:1062:LEU:HD22	1:B:1081:MET:HB2	1.88	0.54
1:B:1886:ASP:O	1:B:1889:VAL:HG22	2.08	0.54
2:J:2087:THR:HB	2:J:2112:LYS:HD3	1.88	0.54
1:B:1140:VAL:O	1:B:1144:GLU:HG3	2.07	0.54
1:B:1974:CYS:HB3	1:B:1979:VAL:HG22	1.88	0.54
1:B:728:ARG:HG2	1:B:786:HIS:ND1	2.22	0.54
2:J:2147:MET:O	2:J:2274:PRO:HD3	2.08	0.54
1:B:1910:SER:HA	1:B:1913:GLU:OE1	2.09	0.54
1:B:1886:ASP:HB3	1:B:1889:VAL:HG13	1.91	0.53
1:B:1943:MET:HE3	1:B:2065:TRP:CB	2.38	0.53
2:J:2313:HIS:HA	3:J:2401:EDO:H11	1.91	0.53
1:B:1608:THR:O	1:B:1612:THR:HG23	2.09	0.53
1:B:404:ALA:O	1:B:406:ARG:N	2.42	0.53
1:B:1346:VAL:HB	1:B:1488:VAL:HG22	1.91	0.53
1:B:1908:LEU:O	1:B:1912:THR:HG23	2.09	0.53
1:B:566:VAL:HG13	1:B:585:ILE:HB	1.90	0.52
1:B:1844:GLY:O	1:B:1848:ILE:HG12	2.09	0.52
1:B:639:ILE:HD11	1:B:646:VAL:HB	1.91	0.52
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.91	0.51
1:B:2118:GLN:HB3	1:B:2120:TYR:HE1	1.75	0.51
2:J:2074:ARG:NH2	3:J:2401:EDO:O2	2.43	0.51
2:J:2076:ARG:HB3	2:J:2305:TYR:OH	2.11	0.51
1:B:1456:VAL:HG12	1:B:1490:LEU:O	2.11	0.51
1:B:1648:ARG:HG3	1:B:1649:SER:N	2.26	0.51
1:B:1040:LEU:HD11	1:B:1072:LEU:HD21	1.92	0.51
1:B:689:TYR:HE2	1:B:883:LEU:HD12	1.75	0.51
1:B:1546:VAL:HG22	1:B:1705:MET:HE1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2196:HIS:HD2	2:J:2200:MET:HE2	1.76	0.51
2:J:2096:ASP:HB2	2:J:2258:ARG:HB2	1.92	0.50
1:B:1045:PRO:HD3	2:J:2317:PHE:CD2	2.46	0.50
1:B:1732:MET:HE1	1:B:1755:LEU:CD2	2.41	0.50
1:B:531:ILE:HD13	1:B:562:TYR:O	2.12	0.50
1:B:757:ALA:O	1:B:761:VAL:HG23	2.12	0.50
1:B:1440:LYS:NZ	1:B:1742:THR:O	2.41	0.50
1:B:513:ALA:O	1:B:517:MET:HG3	2.11	0.50
1:B:2077:ILE:HG23	1:B:2094:PHE:CD1	2.46	0.50
1:B:1567:LYS:O	1:B:1571:LEU:HG	2.12	0.49
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.94	0.49
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.93	0.49
1:B:2066:VAL:O	1:B:2079:ILE:HA	2.12	0.49
1:B:1622:GLU:CD	1:B:1622:GLU:H	2.20	0.49
1:B:1629:ARG:NH1	1:B:1650:LEU:HD22	2.27	0.49
1:B:1773:LEU:HD21	1:B:1781:LEU:HD12	1.94	0.49
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.95	0.49
1:B:1113:ASN:O	1:B:1117:MET:HG3	2.13	0.49
1:B:1195:ARG:HD3	1:B:1260:GLU:OE2	2.12	0.49
2:J:2111:LEU:HD21	2:J:2225:LEU:HD11	1.95	0.49
2:J:2200:MET:HE3	2:J:2235:TYR:HD1	1.78	0.49
1:B:1142:LYS:O	1:B:1146:LYS:HG2	2.13	0.48
1:B:1894:LEU:HB3	1:B:1912:THR:HG22	1.95	0.48
1:B:694:GLU:HG2	1:B:699:LYS:HB3	1.95	0.48
2:J:2303:GLU:OE1	2:J:2303:GLU:N	2.40	0.48
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.33	0.48
1:B:1218:SER:HB2	1:B:1240:LEU:HD11	1.95	0.48
1:B:1943:MET:CE	1:B:2065:TRP:HB2	2.42	0.48
1:B:1174:ILE:O	1:B:1178:VAL:HG23	2.13	0.48
2:J:2243:ASP:OD2	2:J:2248:PRO:HA	2.14	0.48
2:J:2306:HIS:ND1	2:J:2308:VAL:HG22	2.29	0.47
1:B:1069:GLN:HA	1:B:1121:ARG:NH1	2.28	0.47
1:B:774:LEU:O	1:B:778:LEU:HB2	2.14	0.47
1:B:2078:SER:OG	1:B:2093:ASP:O	2.25	0.47
1:B:828:ILE:HD11	1:B:853:LEU:HG	1.96	0.47
1:B:2013:ARG:HD3	1:B:2050:PRO:O	2.14	0.47
1:B:593:TRP:HZ2	4:B:2217:SAN:HN21	1.61	0.47
1:B:1979:VAL:O	1:B:1981:SER:N	2.47	0.47
2:J:2170:LYS:HA	2:J:2170:LYS:HD3	1.69	0.47
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.95	0.47
1:B:1864:GLU:HG2	1:B:1867:LEU:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1654:MET:HE3	1:B:1654:MET:HB2	1.67	0.47
1:B:1869:ARG:NH1	1:B:1883:LYS:O	2.48	0.47
1:B:2067:VAL:HG12	1:B:2069:GLY:H	1.80	0.47
1:B:1459:ILE:O	1:B:1464:GLY:HA3	2.15	0.46
1:B:2000:THR:HG22	1:B:2001:ASP:N	2.30	0.46
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.96	0.46
1:B:1841:LYS:O	1:B:1845:LEU:HG	2.15	0.46
1:B:886:GLN:O	1:B:888:PRO:HD3	2.14	0.46
1:B:403:LEU:H	1:B:954:LEU:HD21	1.79	0.46
1:B:766:ALA:HB2	1:B:778:LEU:HB3	1.97	0.46
1:B:1658:ALA:C	1:B:1693:ARG:HD2	2.40	0.46
1:B:1990:ASP:O	1:B:1994:ASN:ND2	2.49	0.46
1:B:2016:ASN:ND2	1:B:2044:GLU:OE1	2.48	0.46
1:B:1460:GLY:HA2	1:B:1725:GLU:O	2.16	0.46
1:B:593:TRP:HZ2	4:B:2217:SAN:N2	2.14	0.46
1:B:1815:LEU:HD22	1:B:1829:ILE:HG22	1.98	0.46
1:B:1368:LEU:HD22	1:B:1403:LYS:HE3	1.98	0.46
1:B:1930:LEU:HD22	1:B:1938:PRO:HB2	1.96	0.46
1:B:403:LEU:O	1:B:406:ARG:NH1	2.49	0.45
1:B:916:ALA:HB3	1:B:957:VAL:HG11	1.97	0.45
1:B:1448:ILE:HD13	1:B:1448:ILE:HA	1.74	0.45
2:J:2149:PRO:HB3	2:J:2281:TYR:CE1	2.51	0.45
2:J:2207:ASP:HB3	2:J:2210:LYS:HB2	1.98	0.45
1:B:1068:SER:HB3	2:J:2318:ALA:HA	1.97	0.45
1:B:1869:ARG:O	1:B:1872:ALA:HB3	2.16	0.45
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.15	0.45
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.16	0.45
1:B:1070:LEU:HD13	2:J:2320:LEU:HD22	1.98	0.45
1:B:1130:ARG:HD2	1:B:1144:GLU:OE2	2.17	0.45
2:J:2133:PRO:HG2	2:J:2136:ASN:HB3	1.98	0.45
2:J:2302:LYS:N	2:J:2302:LYS:HD2	2.30	0.45
1:B:681:ARG:NH1	1:B:683:VAL:O	2.39	0.45
1:B:1900:SER:HG	1:B:1954:TRP:NE1	2.14	0.45
1:B:1804:ILE:HG22	1:B:1807:GLU:HA	1.99	0.44
1:B:1900:SER:OG	1:B:1954:TRP:NE1	2.50	0.44
1:B:1214:VAL:HG12	1:B:1215:HIS:CD2	2.51	0.44
2:J:2188:LEU:O	2:J:2251:TYR:OH	2.36	0.44
1:B:1183:LYS:NZ	1:B:1207:ASP:OD2	2.46	0.44
1:B:1225:VAL:HG21	1:B:1254:PHE:CE1	2.51	0.44
2:J:2200:MET:HE2	2:J:2230:LEU:HD22	1.99	0.44
1:B:1661:VAL:O	1:B:1702:CYS:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1435:LEU:HA	1:B:1435:LEU:HD23	1.64	0.44
1:B:1843:ARG:HG3	1:B:1844:GLY:N	2.32	0.44
2:J:2149:PRO:HD3	2:J:2274:PRO:HG3	1.99	0.44
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.52	0.44
1:B:1542:MET:O	1:B:1546:VAL:HG23	2.18	0.44
2:J:2089:HIS:O	2:J:2222:SER:HB2	2.18	0.44
1:B:1225:VAL:HG11	1:B:1256:VAL:HG11	1.99	0.44
1:B:542:ALA:O	1:B:589:THR:HA	2.18	0.43
1:B:2009:ARG:HG3	1:B:2010:PHE:N	2.33	0.43
1:B:1349:GLY:O	1:B:1514:PHE:HB2	2.18	0.43
1:B:1947:GLN:HB3	1:B:2114:MET:HG2	2.00	0.43
1:B:2000:THR:HG22	1:B:2001:ASP:H	1.84	0.43
1:B:414:LEU:HB2	1:B:894:VAL:HG11	2.00	0.43
2:J:2200:MET:HE3	2:J:2235:TYR:CD1	2.53	0.43
1:B:592:LYS:O	1:B:595:ILE:HG22	2.18	0.43
1:B:1030:ARG:HH21	1:B:1076:ALA:HB1	1.83	0.43
1:B:1069:GLN:HA	1:B:1121:ARG:HH12	1.84	0.43
1:B:1803:SER:O	1:B:1810:VAL:HA	2.18	0.43
1:B:1225:VAL:O	1:B:1234:LEU:N	2.52	0.43
1:B:1594:GLU:HG3	1:B:1614:LEU:HD22	1.99	0.43
1:B:1709:SER:H	4:B:2216:SAN:HN22	1.67	0.43
1:B:1953:MET:HE1	1:B:1962:GLN:CG	2.49	0.43
1:B:543:PRO:HD2	1:B:547:LEU:HD23	2.00	0.43
1:B:1298:PRO:HB3	1:B:1515:HIS:CD2	2.53	0.43
1:B:815:LEU:HD12	1:B:819:VAL:HB	2.01	0.43
1:B:1096:PHE:HB2	1:B:1111:THR:HG22	2.01	0.43
1:B:1953:MET:HE3	1:B:1953:MET:HB2	1.55	0.43
1:B:1018:PHE:CE2	1:B:1063:LEU:HD22	2.54	0.42
1:B:2026:LYS:HE2	1:B:2026:LYS:HB3	1.81	0.42
1:B:1122:MET:HE2	1:B:1276:LEU:HD23	2.00	0.42
1:B:2068:ILE:HG22	1:B:2068:ILE:O	2.19	0.42
1:B:1900:SER:CB	1:B:1902:MET:HE3	2.49	0.42
1:B:2085:GLN:HB3	1:B:2086:GLN:H	1.61	0.42
1:B:929:MET:HE3	1:B:949:LEU:HD13	2.01	0.42
1:B:1260:GLU:HA	1:B:1261:PRO:C	2.43	0.42
1:B:1930:LEU:HD13	1:B:1938:PRO:C	2.44	0.42
1:B:1160:GLU:H	1:B:1160:GLU:HG3	1.69	0.42
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	2.01	0.42
1:B:1843:ARG:HB3	1:B:1877:HIS:HB3	2.01	0.42
1:B:546:SER:HB2	1:B:818:GLY:HA3	2.02	0.42
1:B:2109:MET:HE3	1:B:2109:MET:HB3	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2310:ARG:HD2	2:J:2313:HIS:ND1	2.35	0.42
1:B:1046:ILE:HB	1:B:1064:GLN:NE2	2.35	0.42
1:B:1711:LYS:O	1:B:1715:LYS:HG3	2.20	0.42
1:B:1933:ASN:HB3	1:B:1935:TRP:CE2	2.55	0.42
1:B:2006:ASP:HA	1:B:2009:ARG:HG2	2.02	0.41
1:B:1732:MET:HE2	1:B:1732:MET:HB3	1.88	0.41
1:B:501:LEU:HD23	1:B:509:LYS:HG2	2.01	0.41
1:B:1332:GLN:NE2	1:B:1358:ILE:HD12	2.35	0.41
2:J:2118:SER:HB2	5:J:2501:HOH:O	2.19	0.41
1:B:514:LEU:HD12	1:B:517:MET:CE	2.51	0.41
1:B:430:LEU:HD23	1:B:430:LEU:HA	1.75	0.41
1:B:501:LEU:CD2	1:B:509:LYS:HG2	2.51	0.41
1:B:625:GLY:N	1:B:626:PRO:CD	2.83	0.41
1:B:718:LYS:HB3	1:B:718:LYS:HE2	1.81	0.41
1:B:1779:ARG:CZ	1:B:1779:ARG:HB3	2.49	0.41
1:B:423:MET:SD	1:B:877:GLN:HG2	2.61	0.41
1:B:1169:LYS:HB3	1:B:1170:MET:HE2	2.02	0.41
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	2.03	0.41
1:B:1937:SER:HB3	1:B:1938:PRO:HD3	2.03	0.41
1:B:1943:MET:HE1	1:B:2067:VAL:CG2	2.51	0.41
1:B:1991:GLU:HA	1:B:1994:ASN:HD22	1.85	0.41
1:B:1034:LYS:NZ	1:B:1053:GLU:HG2	2.36	0.40
1:B:1843:ARG:HB3	1:B:1877:HIS:ND1	2.36	0.40
2:J:2252:LEU:HB2	2:J:2255:HIS:CE1	2.56	0.40
1:B:503:ALA:HB1	1:B:504:PRO:HD2	2.03	0.40
1:B:1356:LYS:HB2	1:B:1356:LYS:HE2	1.82	0.40
1:B:1614:LEU:HD23	1:B:1614:LEU:HA	1.90	0.40
1:B:548:VAL:HG22	1:B:587:VAL:HG12	2.04	0.40
1:B:1040:LEU:HD11	1:B:1072:LEU:CD2	2.52	0.40
1:B:2065:TRP:CZ3	1:B:2111:ASP:HB3	2.57	0.40
1:B:595:ILE:HD12	1:B:595:ILE:HA	1.87	0.40
1:B:660:ASP:OD1	1:B:931:ARG:HG3	2.21	0.40
1:B:1570:ARG:HD2	1:B:1608:THR:HG21	2.03	0.40
1:B:2068:ILE:HD12	1:B:2068:ILE:N	2.36	0.40

All (1) 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:B:522:GLY:O	1:B:1313:ARG:NH2[3_544]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1719/1747 (98%)	1652 (96%)	61 (4%)	6 (0%)	36	48
2	J	261/263 (99%)	251 (96%)	9 (3%)	1 (0%)	30	40
All	All	1980/2010 (98%)	1903 (96%)	70 (4%)	7 (0%)	30	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1980	GLU
1	B	1861	ARG
2	J	2059	PRO
1	B	1314	ASN
1	B	1882	PRO
1	B	1952	ALA
1	B	1326	PRO

5.3.2 Protein sidechains [i](#)

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	B	1539/1560 (99%)	1484 (96%)	55 (4%)	31	49
2	J	236/236 (100%)	230 (98%)	6 (2%)	42	61
All	All	1775/1796 (99%)	1714 (97%)	61 (3%)	32	51

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	485	GLN
1	B	489	TYR
1	B	525	ILE
1	B	528	ASP
1	B	569	LEU
1	B	595	ILE
1	B	696	LYS
1	B	760	GLU
1	B	835	SER
1	B	847	LEU
1	B	863	THR
1	B	864	LYS
1	B	1008	THR
1	B	1042	GLU
1	B	1051	SER
1	B	1056	SER
1	B	1068	SER
1	B	1071	LYS
1	B	1078	MET
1	B	1095	ILE
1	B	1113	ASN
1	B	1139	VAL
1	B	1140	VAL
1	B	1152	ARG
1	B	1271	VAL
1	B	1274	ARG
1	B	1310	SER
1	B	1335	VAL
1	B	1338	THR
1	B	1373	GLU
1	B	1448	ILE
1	B	1463	ASN
1	B	1482	GLU
1	B	1592	CYS
1	B	1625	SER
1	B	1731	CYS
1	B	1778	HIS
1	B	1781	LEU
1	B	1837	ASN
1	B	1856	GLU
1	B	1861	ARG
1	B	1864	GLU
1	B	1866	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1869	ARG
1	B	1905	SER
1	B	1909	GLN
1	B	1970	HIS
1	B	1979	VAL
1	B	1989	GLU
1	B	2083	THR
1	B	2085	GLN
1	B	2087	LYS
1	B	2089	LYS
1	B	2090	VAL
1	B	2116	CYS
2	J	2076	ARG
2	J	2170	LYS
2	J	2189	SER
2	J	2233	SER
2	J	2261	MET
2	J	2302	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	532	ASN
1	B	951	GLN
1	B	978	ASN
1	B	1101	ASN
1	B	1191	GLN
1	B	1322	GLN
1	B	1337	ASN
1	B	1341	ASN
1	B	1513	ASN
1	B	1553	HIS
1	B	1655	ASN
1	B	1667	GLN
1	B	1837	ASN
1	B	1863	HIS
1	B	1965	HIS
1	B	1994	ASN
2	J	2089	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	EDO	B	2208	-	3,3,3	0.47	0	2,2,2	0.58	0
3	EDO	B	2209	-	3,3,3	0.46	0	2,2,2	0.33	0
4	SAN	B	2217	-	11,11,11	2.25	4 (36%)	16,16,16	3.57	4 (25%)
3	EDO	B	2202	-	3,3,3	0.54	0	2,2,2	1.10	0
3	EDO	B	2207	-	3,3,3	0.62	0	2,2,2	0.39	0
3	EDO	B	2213	-	3,3,3	0.56	0	2,2,2	0.36	0
3	EDO	J	2401	-	3,3,3	0.27	0	2,2,2	1.03	0
3	EDO	B	2205	-	3,3,3	0.57	0	2,2,2	0.52	0
4	SAN	B	2216	-	11,11,11	2.03	2 (18%)	16,16,16	3.93	6 (37%)
3	EDO	B	2203	-	3,3,3	0.32	0	2,2,2	1.50	0
3	EDO	B	2201	-	3,3,3	0.21	0	2,2,2	1.22	0
3	EDO	B	2210	-	3,3,3	0.40	0	2,2,2	0.28	0
3	EDO	B	2211	-	3,3,3	0.35	0	2,2,2	0.48	0
3	EDO	B	2212	-	3,3,3	0.48	0	2,2,2	0.42	0
3	EDO	B	2214	-	3,3,3	0.48	0	2,2,2	0.08	0
3	EDO	B	2215	-	3,3,3	0.35	0	2,2,2	0.69	0
3	EDO	B	2204	-	3,3,3	0.52	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	2206	-	3,3,3	0.86	0	2,2,2	0.41	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	EDO	B	2208	-	-	1/1/1/1	-
3	EDO	B	2209	-	-	0/1/1/1	-
4	SAN	B	2217	-	-	2/6/6/6	0/1/1/1
3	EDO	B	2202	-	-	1/1/1/1	-
3	EDO	B	2207	-	-	1/1/1/1	-
3	EDO	B	2213	-	-	0/1/1/1	-
3	EDO	J	2401	-	-	1/1/1/1	-
3	EDO	B	2205	-	-	1/1/1/1	-
4	SAN	B	2216	-	-	4/6/6/6	0/1/1/1
3	EDO	B	2203	-	-	1/1/1/1	-
3	EDO	B	2201	-	-	1/1/1/1	-
3	EDO	B	2210	-	-	0/1/1/1	-
3	EDO	B	2211	-	-	0/1/1/1	-
3	EDO	B	2212	-	-	0/1/1/1	-
3	EDO	B	2214	-	-	0/1/1/1	-
3	EDO	B	2215	-	-	1/1/1/1	-
3	EDO	B	2204	-	-	0/1/1/1	-
3	EDO	B	2206	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2217	SAN	S-N2	5.48	1.71	1.60
4	B	2216	SAN	S-N2	4.50	1.69	1.60
4	B	2217	SAN	C4-S	3.62	1.82	1.77
4	B	2216	SAN	C4-S	3.27	1.82	1.77
4	B	2217	SAN	O1-S	2.24	1.47	1.43
4	B	2217	SAN	C1-N1	2.14	1.45	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2216	SAN	O2-S-O1	-12.87	99.00	118.80
4	B	2217	SAN	O2-S-O1	-12.13	100.14	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2216	SAN	O1-S-N2	5.34	115.05	107.35
4	B	2216	SAN	O2-S-C4	5.23	113.26	107.35
4	B	2217	SAN	O1-S-N2	4.95	114.49	107.35
4	B	2217	SAN	C4-S-N2	4.13	114.16	108.40
4	B	2216	SAN	O1-S-C4	2.64	110.33	107.35
4	B	2216	SAN	O2-S-N2	2.57	111.05	107.35
4	B	2217	SAN	O2-S-C4	2.52	110.19	107.35
4	B	2216	SAN	C6-C1-C2	2.22	121.50	118.16

There are no chirality outliers.

All (15) torsion outliers are listed below:

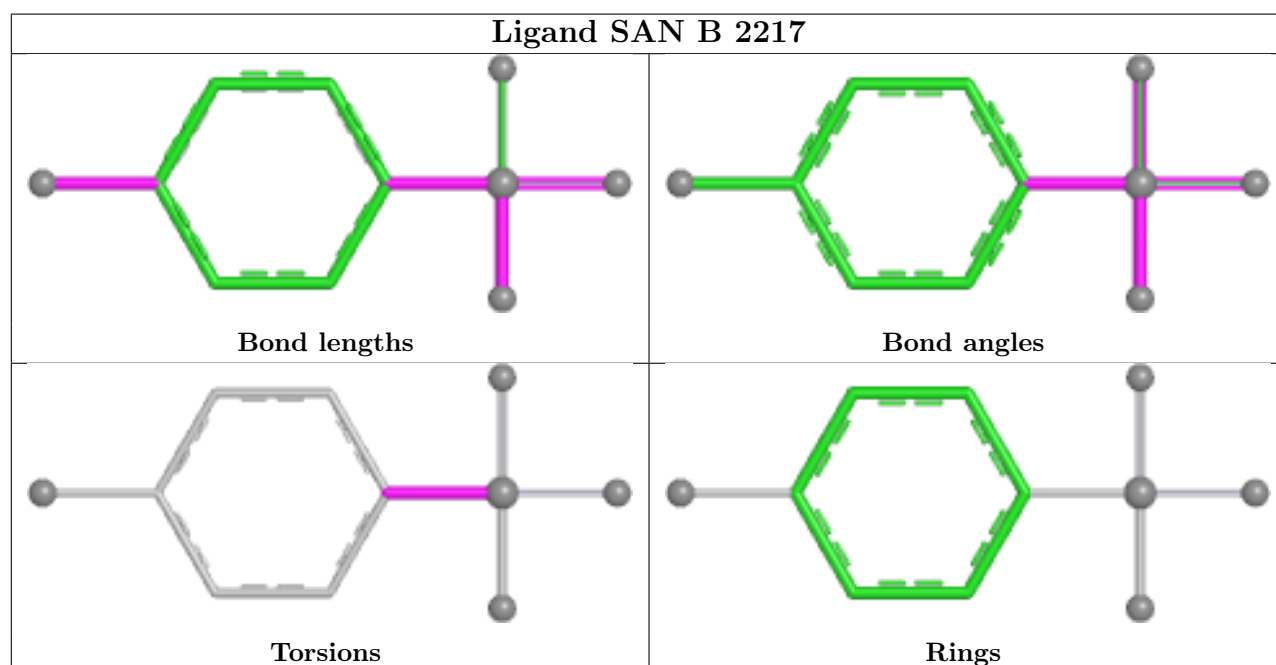
Mol	Chain	Res	Type	Atoms
3	B	2205	EDO	O1-C1-C2-O2
3	B	2206	EDO	O1-C1-C2-O2
4	B	2216	SAN	C5-C4-S-N2
4	B	2216	SAN	C3-C4-S-N2
4	B	2216	SAN	C3-C4-S-O2
4	B	2216	SAN	C5-C4-S-O2
3	B	2203	EDO	O1-C1-C2-O2
4	B	2217	SAN	C5-C4-S-O1
4	B	2217	SAN	C3-C4-S-O1
3	B	2202	EDO	O1-C1-C2-O2
3	B	2201	EDO	O1-C1-C2-O2
3	B	2207	EDO	O1-C1-C2-O2
3	B	2215	EDO	O1-C1-C2-O2
3	B	2208	EDO	O1-C1-C2-O2
3	J	2401	EDO	O1-C1-C2-O2

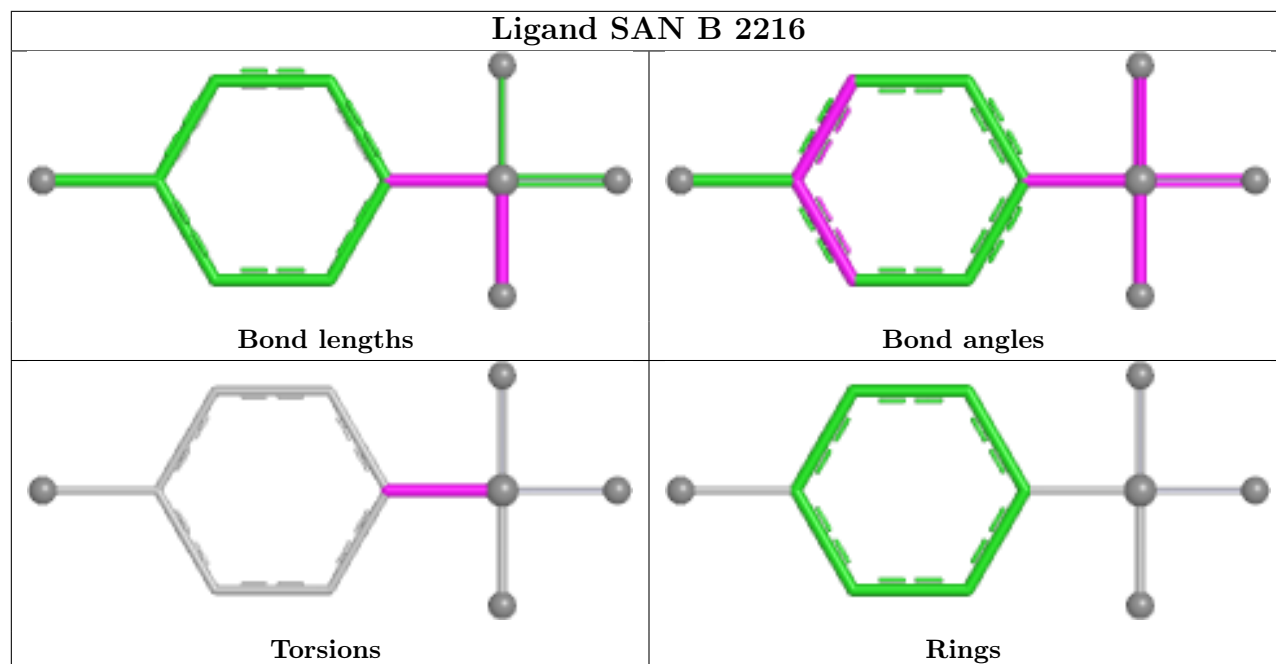
There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2208	EDO	1	0
4	B	2217	SAN	2	0
3	B	2202	EDO	2	0
3	J	2401	EDO	2	0
4	B	2216	SAN	1	0
3	B	2203	EDO	1	0
3	B	2214	EDO	1	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	B	1721/1747 (98%)	0.39	73 (4%) 40 40	35, 64, 129, 230	0
2	J	263/263 (100%)	0.25	14 (5%) 32 31	37, 60, 129, 191	0
All	All	1984/2010 (98%)	0.37	87 (4%) 39 38	35, 63, 129, 230	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1601	LEU	5.3
1	B	402	ALA	5.0
2	J	2060	LEU	4.7
2	J	2058	GLY	4.6
1	B	1996	LEU	4.5
1	B	403	LEU	4.2
1	B	404	ALA	3.9
1	B	1936	LEU	3.9
2	J	2320	LEU	3.7
1	B	1876	PRO	3.7
1	B	1863	HIS	3.7
1	B	1875	VAL	3.5
1	B	455	PHE	3.4
1	B	1862	HIS	3.4
2	J	2319	LEU	3.3
1	B	1501	ALA	3.2
1	B	1963	LEU	3.2
1	B	1861	ARG	3.2
1	B	582	ALA	3.2
1	B	454	PRO	3.1
2	J	2097	ILE	3.1
1	B	940	HIS	3.1
1	B	2047	VAL	3.1
1	B	1148	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2029	ILE	3.0
1	B	1869	ARG	3.0
2	J	2244	LYS	3.0
1	B	1877	HIS	3.0
1	B	726	HIS	3.0
1	B	1174	ILE	2.9
1	B	1982	VAL	2.9
1	B	1584	ILE	2.9
1	B	570	THR	2.9
1	B	1882	PRO	2.9
1	B	1317	PHE	2.9
1	B	1868	LEU	2.9
2	J	2063	MET	2.8
1	B	1940	LEU	2.8
1	B	1336	PHE	2.8
1	B	1860	ILE	2.7
1	B	2101	ALA	2.7
1	B	1867	LEU	2.7
1	B	1884	PHE	2.7
1	B	1139	VAL	2.7
1	B	1879	LEU	2.7
1	B	1997	LEU	2.7
1	B	405	PRO	2.6
1	B	2036	VAL	2.6
2	J	2062	SER	2.5
1	B	575	LEU	2.5
2	J	2059	PRO	2.5
1	B	2041	LEU	2.4
1	B	1170	MET	2.4
1	B	580	ILE	2.4
2	J	2075	VAL	2.4
1	B	1871	LEU	2.4
1	B	2097	PRO	2.4
1	B	1872	ALA	2.4
1	B	1874	LYS	2.4
1	B	569	LEU	2.4
1	B	2076	LEU	2.4
2	J	2066	THR	2.3
1	B	1505	GLY	2.3
1	B	1140	VAL	2.3
1	B	701	PHE	2.3
2	J	2238	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	863	THR	2.3
1	B	1798	GLN	2.3
1	B	1985	ILE	2.3
1	B	576	CYS	2.2
2	J	2121	ARG	2.2
1	B	1222	TRP	2.2
1	B	1893	LEU	2.2
1	B	1960	LEU	2.2
1	B	1308	PRO	2.2
2	J	2061	GLY	2.2
1	B	1840	THR	2.2
1	B	1052	ILE	2.2
1	B	1849	ILE	2.2
1	B	1321	TYR	2.1
1	B	2024	VAL	2.1
1	B	2098	ALA	2.1
1	B	2092	LEU	2.1
1	B	2034	PRO	2.1
1	B	1157	ASN	2.0
1	B	2088	ALA	2.0
1	B	1604	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(\AA^2)	Q<0.9
3	EDO	B	2206	4/4	0.75	0.17	53,53,58,58	0
3	EDO	B	2211	4/4	0.75	0.20	87,88,90,95	0

Continued on next page...

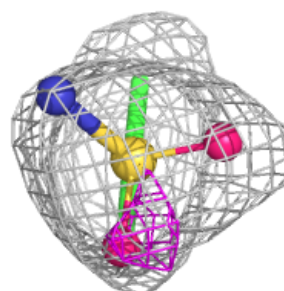
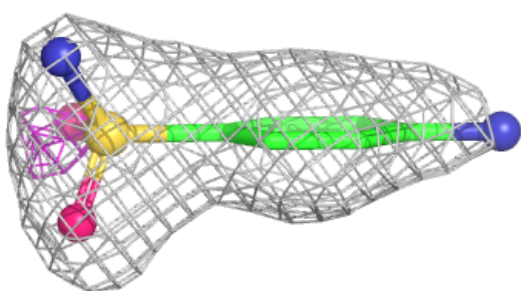
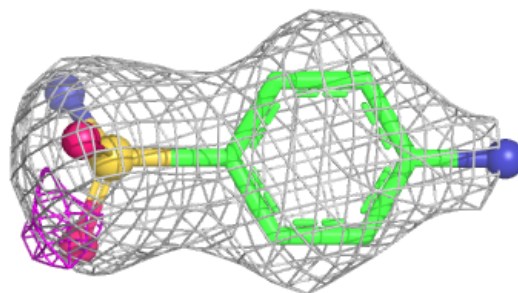
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	2210	4/4	0.83	0.19	87,90,91,92	0
3	EDO	B	2214	4/4	0.83	0.17	87,99,106,114	0
3	EDO	B	2212	4/4	0.84	0.12	74,78,79,85	0
3	EDO	B	2215	4/4	0.84	0.20	73,76,83,86	0
3	EDO	J	2401	4/4	0.86	0.17	72,75,77,84	0
3	EDO	B	2209	4/4	0.87	0.15	65,67,68,71	0
3	EDO	B	2207	4/4	0.88	0.11	54,59,60,67	0
3	EDO	B	2204	4/4	0.88	0.12	55,58,58,62	0
3	EDO	B	2205	4/4	0.88	0.12	40,43,49,51	0
3	EDO	B	2202	4/4	0.88	0.10	39,42,43,45	0
3	EDO	B	2213	4/4	0.89	0.12	53,56,59,61	0
3	EDO	B	2208	4/4	0.89	0.12	59,61,61,63	0
3	EDO	B	2203	4/4	0.93	0.13	51,52,52,54	0
4	SAN	B	2217	11/11	0.93	0.11	54,57,64,65	0
4	SAN	B	2216	11/11	0.95	0.08	46,50,53,55	0
3	EDO	B	2201	4/4	0.96	0.08	49,50,52,56	0

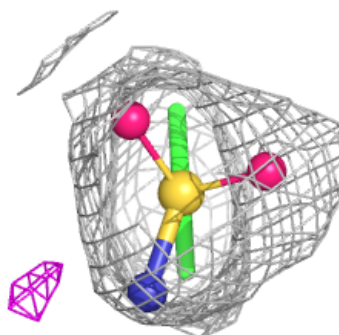
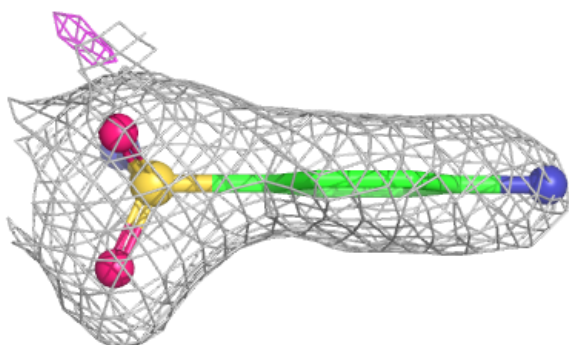
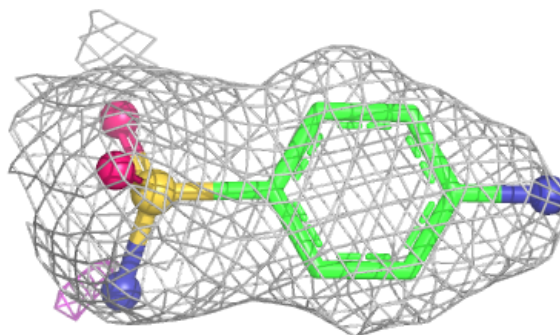
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAN B 2217:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SAN B 2216:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.