Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2023 – 12:20 pm GMT

PDB ID	:	8BCG
Title	:	Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and compound 86
Authors	:	Vester, K.; Loll, B.; Wahl, M.C.
Deposited on	:	2022-10-15
Resolution	:	2.39 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:

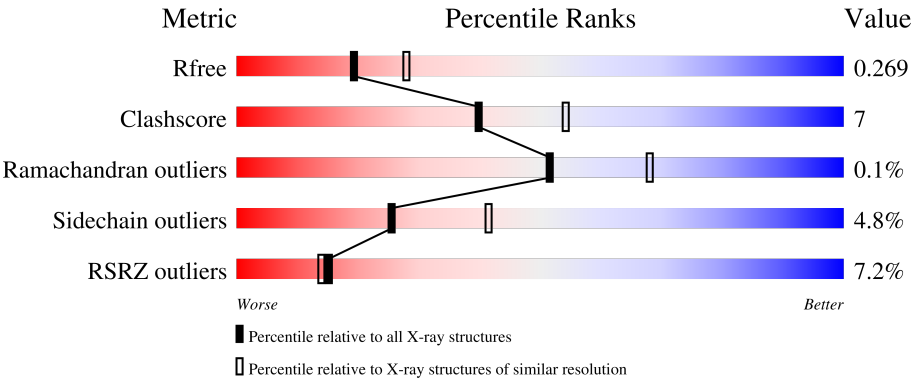
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	7% 77% 21%
2	J	263	5% 84% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16360 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
1	B	1725	Total	C	N	O	S	0	0	0
			13870	8865	2373	2560	72			

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

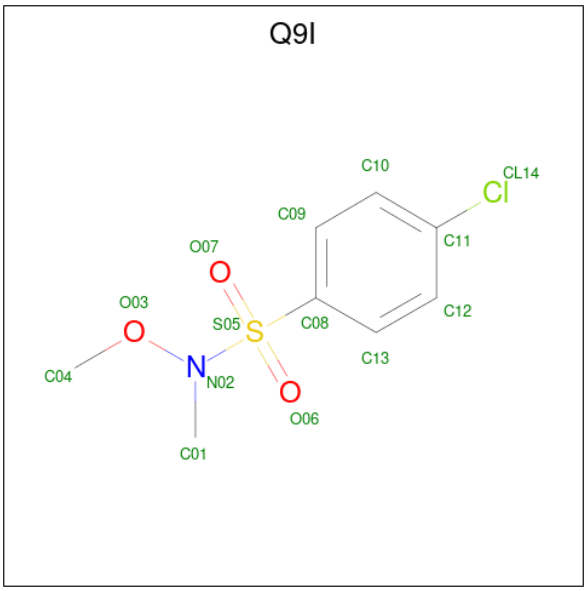
- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	260	Total	C	N	O	S	0	0	0
			2104	1345	362	385	12			

There are 6 discrepancies between the modelled and reference sequences:

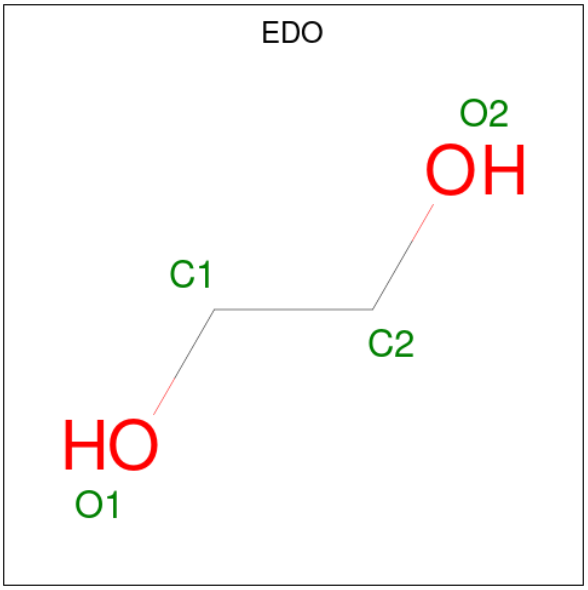
Chain	Residue	Modelled	Actual	Comment	Reference
J	2058	GLY	-	expression tag	UNP Q6P2Q9
J	2059	PRO	-	expression tag	UNP Q6P2Q9
J	2060	LEU	-	expression tag	UNP Q6P2Q9
J	2061	GLY	-	expression tag	UNP Q6P2Q9
J	2062	SER	-	expression tag	UNP Q6P2Q9
J	2063	MET	-	expression tag	UNP Q6P2Q9

- Molecule 3 is 4-chloranyl- {N}-methoxy- {N}-methyl-benzenesulfonamide (three-letter code: Q9I) (formula: $C_8H_{10}ClNO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	S	0	0
			14	8	1	1	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 5 is water.

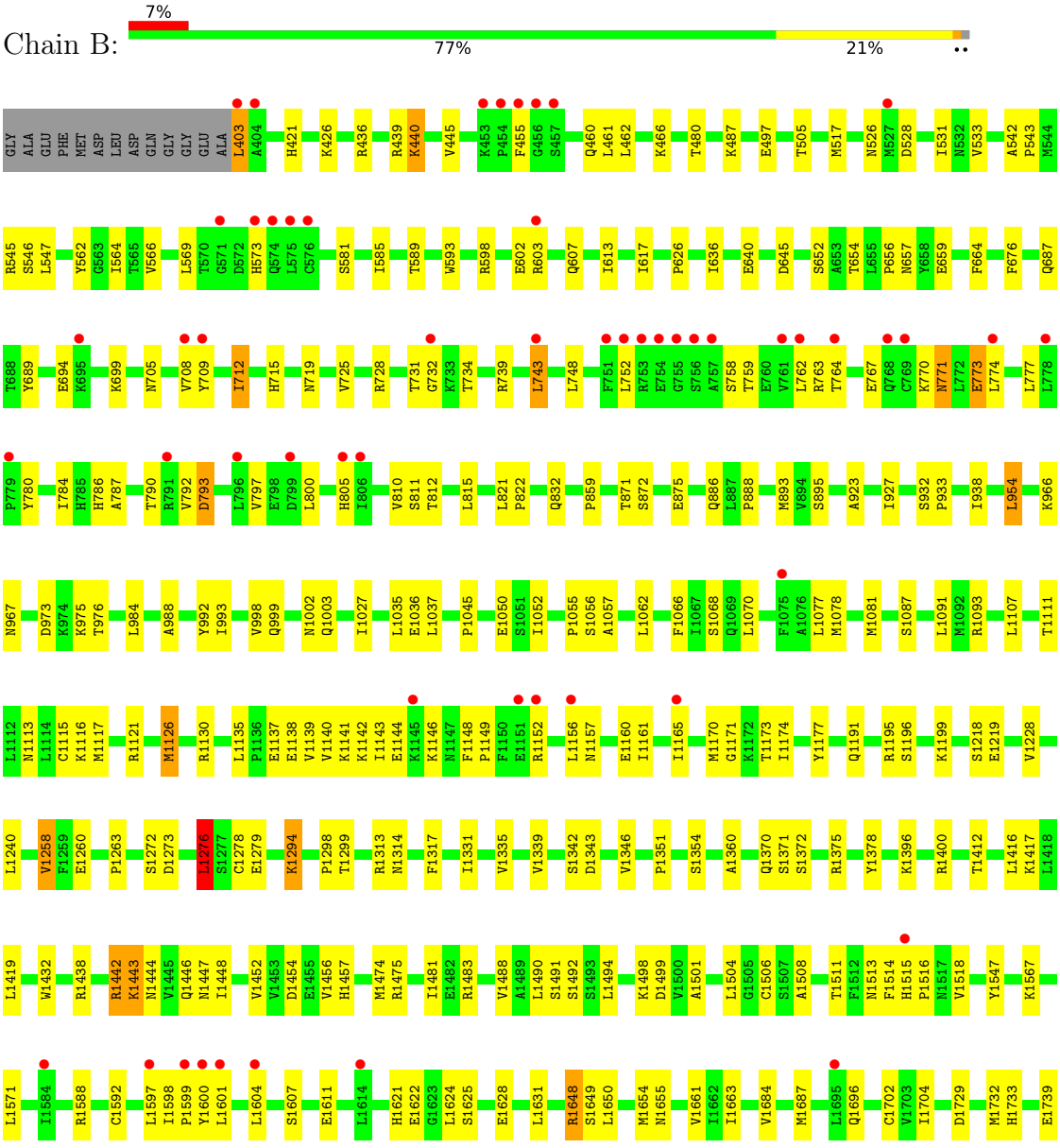
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	287	Total O 287 287	0	0
5	J	49	Total O 49 49	0	0

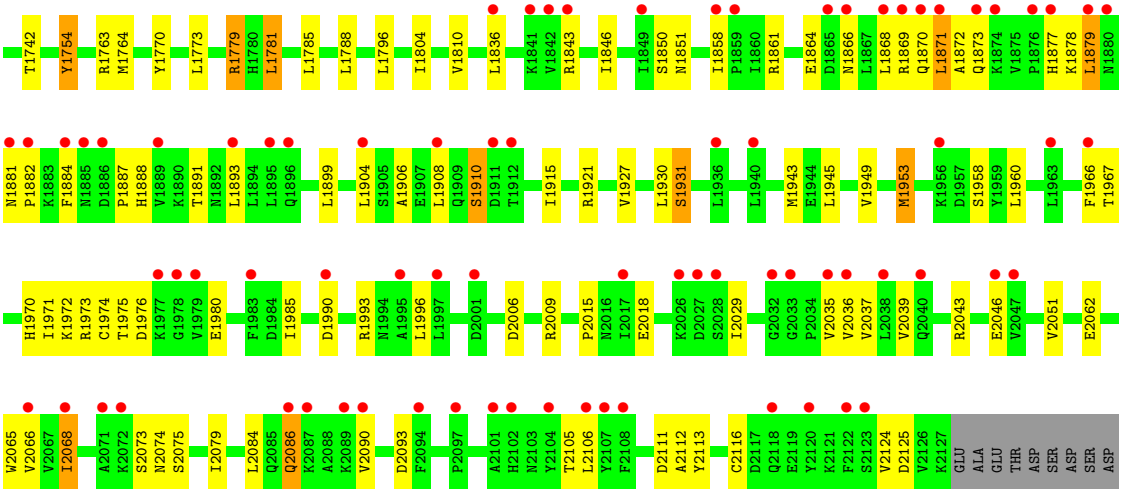
3 Residue-property plots (i)

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

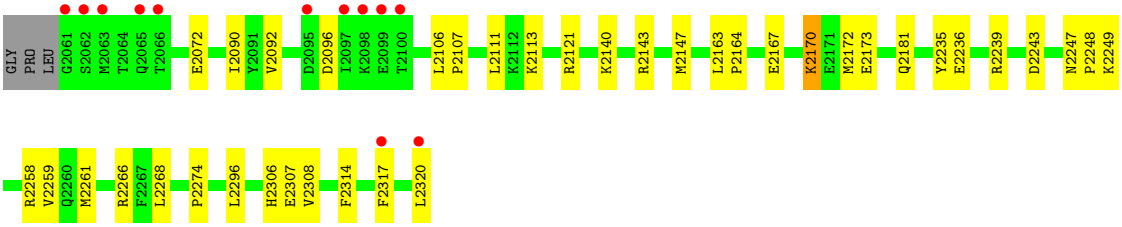
Chain B:





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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.92Å 118.92Å 188.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.06 – 2.39 46.06 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.06-2.39) 99.7 (46.06-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.214 , 0.269 0.213 , 0.269	Depositor DCC
R_{free} test set	2101 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16360	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, Q9I

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	0.39	0/14164	0.59	1/19191 (0.0%)
2	J	0.41	0/2170	0.58	0/2953
All	All	0.40	0/16334	0.59	1/22144 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1276	LEU	CA-CB-CG	5.26	127.40	115.30

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	13870	0	14018	218	0
2	J	2104	0	2042	18	0
3	B	14	0	0	1	0
4	B	36	0	54	1	0
5	B	287	0	0	8	0
5	J	49	0	0	1	0
All	All	16360	0	16114	235	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 7.

All (235) 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:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.51	0.90
1:B:1879:LEU:HD11	1:B:1882:PRO:HB3	1.58	0.85
1:B:440:LYS:H	1:B:440:LYS:HD3	1.45	0.82
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.16	0.74
1:B:2006:ASP:HA	1:B:2009:ARG:HH11	1.53	0.73
1:B:1836:LEU:HD22	1:B:1930:LEU:HD21	1.71	0.72
1:B:728:ARG:HE	1:B:787:ALA:HB3	1.54	0.72
1:B:762:LEU:HD21	1:B:805:HIS:HB3	1.71	0.71
1:B:1475:ARG:HD2	1:B:1504:LEU:HA	1.72	0.70
1:B:2043:ARG:NH2	1:B:2084:LEU:O	2.26	0.69
1:B:763:ARG:NH2	1:B:764:THR:OG1	2.26	0.68
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.77	0.66
1:B:984:LEU:HD21	1:B:1002:ASN:HB2	1.77	0.64
1:B:1696:GLN:OE1	5:B:2301:HOH:O	2.14	0.63
1:B:790:THR:HG22	1:B:792:VAL:H	1.64	0.62
1:B:1604:LEU:HD23	1:B:1628:GLU:HG2	1.82	0.62
1:B:1684:VAL:HA	1:B:1687:MET:HE2	1.81	0.61
1:B:1754:TYR:OH	5:B:2302:HOH:O	2.16	0.61
1:B:1456:VAL:HG12	1:B:1491:SER:HB2	1.83	0.60
1:B:436:ARG:HG3	1:B:445:VAL:HG22	1.83	0.60
2:J:2235:TYR:O	2:J:2239:ARG:HG2	2.01	0.60
1:B:1906:ALA:O	1:B:1910:SER:OG	2.20	0.60
1:B:1764:MET:HE3	1:B:1773:LEU:HD11	1.82	0.59
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.84	0.59
1:B:2006:ASP:OD1	1:B:2009:ARG:NH1	2.34	0.59
1:B:497:GLU:HG3	5:B:2330:HOH:O	2.01	0.59
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.84	0.59
1:B:793:ASP:OD1	1:B:793:ASP:N	2.36	0.59
1:B:1499:ASP:OD2	1:B:1763:ARG:NH1	2.32	0.59
1:B:1299:THR:HG22	5:B:2583:HOH:O	2.03	0.58
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.38	0.58
1:B:1452:VAL:HG22	1:B:1488:VAL:HB	1.85	0.58
1:B:1729:ASP:HA	1:B:1732:MET:HE2	1.86	0.57
1:B:975:LYS:HG3	1:B:976:THR:HG23	1.87	0.57
1:B:1138:GLU:H	1:B:1138:GLU:CD	2.07	0.56
1:B:1442:ARG:HE	1:B:1442:ARG:HA	1.70	0.56
1:B:1142:LYS:O	1:B:1146:LYS:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.87	0.56
1:B:1066:PHE:CZ	1:B:1121:ARG:HD3	2.39	0.56
1:B:1515:HIS:HB3	1:B:1516:PRO:HD2	1.88	0.56
1:B:598:ARG:HH22	4:B:2206:EDO:H11	1.69	0.56
1:B:1592:CYS:SG	1:B:1597:LEU:HD13	2.47	0.55
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.87	0.55
1:B:1444:ASN:HA	1:B:1447:ASN:ND2	2.21	0.55
1:B:1967:THR:HG22	1:B:1970:HIS:ND1	2.22	0.55
1:B:1598:ILE:HA	1:B:1601:LEU:HB2	1.88	0.55
1:B:1191:GLN:OE1	1:B:1199:LYS:HE3	2.08	0.54
1:B:1346:VAL:HG13	1:B:1488:VAL:HG13	1.90	0.54
1:B:1739:GLU:HA	1:B:1742:THR:HG22	1.89	0.54
1:B:1648:ARG:HG3	1:B:1649:SER:N	2.22	0.54
1:B:1843:ARG:HD3	1:B:1877:HIS:ND1	2.22	0.54
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.90	0.53
1:B:664:PHE:HB2	1:B:927:ILE:HD13	1.91	0.53
1:B:1161:ILE:HD11	1:B:1171:GLY:HA2	1.90	0.53
1:B:1858:ILE:HB	1:B:1887:PRO:HB3	1.90	0.53
1:B:1864:GLU:HB3	1:B:1868:LEU:HD23	1.90	0.53
2:J:2236:GLU:OE2	2:J:2239:ARG:NH1	2.42	0.53
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.91	0.53
1:B:1416:LEU:HD22	1:B:1442:ARG:HD3	1.90	0.52
1:B:2015:PRO:HG2	1:B:2116:CYS:SG	2.49	0.52
1:B:2037:VAL:HG11	1:B:2068:ILE:HD12	1.90	0.52
1:B:593:TRP:HE1	3:B:2201:Q9I:C01	2.22	0.52
1:B:1107:LEU:O	1:B:1111:THR:HG23	2.09	0.52
1:B:1866:ASN:HA	1:B:1869:ARG:HB2	1.92	0.52
1:B:725:VAL:HG21	1:B:731:THR:HA	1.92	0.52
1:B:1037:LEU:HB3	1:B:1052:ILE:HD11	1.92	0.52
1:B:2074:ASN:ND2	1:B:2074:ASN:O	2.43	0.52
1:B:1732:MET:HE3	1:B:1788:LEU:HG	1.92	0.52
1:B:1343:ASP:OD1	1:B:1370:GLN:NE2	2.42	0.52
1:B:1973:ARG:HG2	1:B:1996:LEU:HD11	1.92	0.52
1:B:2066:VAL:O	1:B:2079:ILE:HA	2.10	0.52
1:B:815:LEU:HD21	1:B:821:LEU:HD22	1.92	0.51
1:B:1851:ASN:HA	1:B:1888:HIS:ND1	2.26	0.51
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.46	0.51
1:B:1156:LEU:HD12	1:B:1161:ILE:HG22	1.92	0.50
1:B:694:GLU:HG2	1:B:699:LYS:HG3	1.94	0.50
1:B:1149:PRO:O	1:B:1152:ARG:HG2	2.11	0.50
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:THR:HG21	1:B:676:PHE:O	2.12	0.50
1:B:2073:SER:HB2	1:B:2075:SER:HB3	1.93	0.50
1:B:2051:VAL:HG11	1:B:2112:ALA:HB1	1.93	0.49
1:B:439:ARG:HH21	1:B:440:LYS:HZ3	1.60	0.49
1:B:933:PRO:HB2	1:B:938:ILE:HB	1.94	0.49
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.95	0.49
1:B:1195:ARG:NH1	1:B:1260:GLU:OE2	2.46	0.49
1:B:709:TYR:O	1:B:712:ILE:HG22	2.13	0.49
1:B:1943:MET:HG2	1:B:2065:TRP:CE3	2.48	0.49
1:B:2046:GLU:HG2	1:B:2086:GLN:HB2	1.95	0.49
1:B:1170:MET:HB2	1:B:1173:THR:HB	1.95	0.49
1:B:1219:GLU:HG3	5:B:2319:HOH:O	2.12	0.48
2:J:2181:GLN:NE2	5:J:2402:HOH:O	2.46	0.48
1:B:1135:LEU:HD13	1:B:1177:TYR:CD2	2.49	0.48
1:B:1879:LEU:HD22	1:B:1893:LEU:HD21	1.94	0.48
1:B:1140:VAL:O	1:B:1144:GLU:HG2	2.14	0.48
1:B:1621:HIS:CE1	1:B:1624:LEU:HG	2.48	0.48
1:B:1481:ILE:O	1:B:1483:ARG:HG2	2.14	0.48
1:B:822:PRO:HG3	1:B:859:PRO:HD3	1.96	0.48
1:B:531:ILE:HD13	1:B:562:TYR:O	2.13	0.48
1:B:566:VAL:HG22	1:B:585:ILE:HB	1.95	0.48
1:B:1066:PHE:CE2	1:B:1121:ARG:HD3	2.49	0.47
1:B:1165:ILE:HD13	1:B:1174:ILE:HD13	1.95	0.47
1:B:705:ASN:HA	1:B:708:VAL:HG12	1.96	0.47
1:B:1062:LEU:HD21	1:B:1077:LEU:HD22	1.96	0.47
1:B:1137:GLU:HG2	1:B:1141:LYS:HD3	1.95	0.47
1:B:1904:LEU:HD13	1:B:1908:LEU:HD13	1.95	0.47
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.95	0.47
1:B:1126:MET:HB3	1:B:1130:ARG:HD2	1.96	0.47
1:B:505:THR:HG22	5:B:2388:HOH:O	2.14	0.47
1:B:1035:LEU:HD23	1:B:1036:GLU:H	1.80	0.47
1:B:487:LYS:HD2	1:B:676:PHE:HE1	1.80	0.47
1:B:1156:LEU:HB3	1:B:1160:GLU:HB2	1.97	0.47
1:B:1882:PRO:HB2	1:B:1884:PHE:CZ	2.50	0.47
1:B:2065:TRP:CZ3	1:B:2111:ASP:HB3	2.50	0.47
1:B:743:LEU:HD22	1:B:748:LEU:HD13	1.97	0.47
1:B:1196:SER:HA	1:B:1258:VAL:HG12	1.97	0.47
1:B:871:THR:OG1	1:B:872:SER:N	2.47	0.46
1:B:728:ARG:O	1:B:731:THR:HG22	2.16	0.46
1:B:1156:LEU:HB2	1:B:1161:ILE:HG23	1.97	0.46
1:B:421:HIS:ND1	5:B:2306:HOH:O	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:GLU:O	1:B:770:LYS:HE3	2.14	0.46
1:B:800:LEU:O	1:B:805:HIS:HB2	2.14	0.46
1:B:1457:HIS:HB3	1:B:1494:LEU:HD21	1.97	0.46
1:B:752:LEU:HD13	1:B:759:THR:HG23	1.98	0.46
1:B:771:ASN:HB2	1:B:774:LEU:HB3	1.98	0.46
1:B:758:SER:O	1:B:762:LEU:HG	2.16	0.46
1:B:1396:LYS:O	1:B:1400:ARG:HB2	2.15	0.46
1:B:1870:GLN:O	1:B:1873:GLN:HB3	2.16	0.46
2:J:2140:LYS:NZ	2:J:2173:GLU:OE2	2.34	0.46
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.98	0.46
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.12	0.45
2:J:2243:ASP:OD2	2:J:2248:PRO:HA	2.16	0.45
1:B:1868:LEU:HD13	1:B:1871:LEU:HD12	1.98	0.45
1:B:1975:THR:HG22	1:B:1980:GLU:OE1	2.17	0.45
1:B:886:GLN:O	1:B:888:PRO:HD3	2.16	0.45
1:B:1218:SER:HB2	1:B:1240:LEU:HD11	1.99	0.45
1:B:1779:ARG:HB3	1:B:1779:ARG:NH1	2.31	0.45
1:B:2036:VAL:HG22	1:B:2093:ASP:HB3	1.99	0.45
1:B:1045:PRO:HD3	2:J:2317:PHE:CD2	2.51	0.45
1:B:1148:PHE:HD2	1:B:1152:ARG:HD3	1.81	0.45
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.16	0.45
1:B:1378:TYR:OH	1:B:1454:ASP:OD2	2.23	0.45
1:B:636:ILE:O	1:B:640:GLU:HG2	2.17	0.44
1:B:542:ALA:HB1	1:B:547:LEU:HD23	1.99	0.44
1:B:1113:ASN:O	1:B:1117:MET:HG3	2.18	0.44
1:B:1622:GLU:OE1	1:B:1622:GLU:N	2.41	0.44
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	1.98	0.44
1:B:1513:ASN:ND2	5:B:2303:HOH:O	2.28	0.44
1:B:2039:VAL:HG21	1:B:2106:LEU:HD11	1.99	0.44
1:B:999:GLN:OE1	1:B:1003:GLN:NE2	2.30	0.44
1:B:1442:ARG:HH12	1:B:1444:ASN:ND2	2.15	0.44
1:B:1607:SER:O	1:B:1611:GLU:HG3	2.18	0.44
1:B:2029:ILE:HG13	1:B:2124:VAL:CG1	2.48	0.44
1:B:1068:SER:HB2	1:B:1070:LEU:HD13	1.99	0.44
1:B:1650:LEU:O	1:B:1654:MET:HE3	2.17	0.44
1:B:2051:VAL:HG22	1:B:2062:GLU:HG2	2.00	0.44
1:B:1126:MET:HG2	1:B:1130:ARG:NH1	2.33	0.44
1:B:1878:LYS:HA	1:B:1878:LYS:HD3	1.53	0.44
1:B:1985:ILE:HG22	1:B:1993:ARG:HH21	1.82	0.44
2:J:2163:LEU:HD23	2:J:2163:LEU:HA	1.80	0.44
1:B:1272:SER:HB2	1:B:1278:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1442:ARG:HA	1:B:1442:ARG:NE	2.33	0.43
1:B:1116:LYS:HB2	1:B:1276:LEU:HD13	2.00	0.43
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.99	0.43
1:B:517:MET:HE3	1:B:613:ILE:HD12	2.00	0.43
1:B:1062:LEU:HD22	1:B:1081:MET:HB2	2.00	0.43
1:B:1157:ASN:ND2	1:B:1160:GLU:OE2	2.49	0.43
1:B:1442:ARG:HH21	1:B:1443:LYS:HE2	1.82	0.43
2:J:2167:GLU:HA	2:J:2170:LYS:HE3	2.00	0.43
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.57	0.43
2:J:2096:ASP:OD1	2:J:2096:ASP:N	2.52	0.43
1:B:739:ARG:HH11	1:B:780:TYR:HE2	1.66	0.43
1:B:1142:LYS:HE2	1:B:1142:LYS:HB2	1.92	0.43
2:J:2320:LEU:HD23	2:J:2320:LEU:HA	1.80	0.43
1:B:562:TYR:HB2	1:B:564:ILE:HD12	2.00	0.43
1:B:1567:LYS:O	1:B:1571:LEU:HG	2.19	0.43
1:B:1598:ILE:N	1:B:1599:PRO:HD2	2.33	0.43
1:B:771:ASN:HB2	1:B:774:LEU:CB	2.49	0.43
2:J:2113:LYS:HE2	2:J:2113:LYS:HB2	1.86	0.43
1:B:602:GLU:HG3	1:B:603:ARG:H	1.84	0.43
1:B:1846:ILE:O	1:B:1850:SER:OG	2.32	0.43
1:B:975:LYS:HG3	1:B:976:THR:N	2.34	0.43
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.19	0.43
1:B:1419:LEU:HG	1:B:1444:ASN:HB3	2.00	0.43
1:B:531:ILE:O	1:B:533:VAL:HG13	2.19	0.42
1:B:1191:GLN:HB3	1:B:1770:TYR:CD1	2.54	0.42
1:B:1872:ALA:HB1	1:B:1879:LEU:HD21	2.00	0.42
1:B:967:ASN:HB3	1:B:999:GLN:HB2	2.01	0.42
1:B:973:ASP:OD1	1:B:975:LYS:HG2	2.20	0.42
1:B:1139:VAL:O	1:B:1143:ILE:HD12	2.19	0.42
1:B:1228:VAL:CG2	1:B:1263:PRO:HB2	2.49	0.42
1:B:1066:PHE:HA	1:B:1081:MET:HE3	2.01	0.42
1:B:1375:ARG:HB3	1:B:1448:ILE:HD12	2.02	0.42
1:B:1661:VAL:O	1:B:1702:CYS:HA	2.19	0.42
1:B:793:ASP:O	1:B:797:VAL:HG23	2.20	0.42
1:B:923:ALA:O	1:B:927:ILE:HD12	2.20	0.42
1:B:1891:THR:HG22	1:B:1915:ILE:HD11	2.01	0.42
1:B:626:PRO:HG3	1:B:893:MET:HA	2.01	0.42
1:B:731:THR:HG23	1:B:732:GLY:N	2.35	0.42
1:B:988:ALA:HB2	1:B:998:VAL:HG11	2.02	0.42
1:B:1195:ARG:HD2	1:B:1294:LYS:HG3	2.00	0.42
1:B:1498:LYS:HD2	1:B:1498:LYS:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2037:VAL:HG11	1:B:2068:ILE:CD1	2.49	0.42
1:B:439:ARG:HE	1:B:440:LYS:NZ	2.18	0.41
1:B:462:LEU:HD11	1:B:466:LYS:HB2	2.02	0.41
1:B:1148:PHE:CD2	1:B:1152:ARG:HD3	2.55	0.41
2:J:2307:GLU:HG3	2:J:2314:PHE:CE1	2.55	0.41
1:B:569:LEU:HB3	1:B:573:HIS:NE2	2.35	0.41
2:J:2164:PRO:HB3	2:J:2296:LEU:HD11	2.02	0.41
1:B:1967:THR:HG22	1:B:1970:HIS:CE1	2.55	0.41
1:B:2029:ILE:HD12	1:B:2035:VAL:HG22	2.03	0.41
1:B:1050:GLU:HB2	1:B:1057:ALA:HB2	2.03	0.41
1:B:1438:ARG:O	1:B:1442:ARG:HB2	2.20	0.41
1:B:1858:ILE:HG13	1:B:1891:THR:CG2	2.50	0.41
1:B:715:HIS:HB3	1:B:719:ASN:HB2	2.01	0.41
1:B:784:ILE:HA	1:B:810:VAL:O	2.20	0.41
1:B:1417:LYS:HA	1:B:1417:LYS:HD3	1.77	0.41
1:B:1600:TYR:HD1	1:B:1631:LEU:HD22	1.86	0.41
2:J:2147:MET:O	2:J:2274:PRO:HD3	2.20	0.41
1:B:542:ALA:O	1:B:589:THR:HA	2.21	0.41
1:B:811:SER:OG	1:B:812:THR:N	2.54	0.41
1:B:1547:TYR:OH	1:B:1588:ARG:NH2	2.54	0.41
1:B:1899:LEU:HD22	1:B:1953:MET:O	2.21	0.41
1:B:1927:VAL:O	1:B:1931:SER:HB2	2.21	0.41
1:B:1945:LEU:O	1:B:1949:VAL:HG23	2.21	0.41
1:B:1093:ARG:NH2	1:B:1273:ASP:OD1	2.54	0.40
1:B:1432:TRP:HE1	1:B:1474:MET:HE3	1.86	0.40
1:B:439:ARG:HE	1:B:440:LYS:HZ3	1.70	0.40
2:J:2306:HIS:ND1	2:J:2308:VAL:HG22	2.37	0.40
1:B:773:GLU:O	1:B:777:LEU:HD12	2.21	0.40
1:B:1733:HIS:HB3	1:B:1796:LEU:HD21	2.04	0.40
1:B:403:LEU:HB2	1:B:954:LEU:HD23	2.02	0.40
1:B:1375:ARG:HB3	1:B:1448:ILE:CD1	2.51	0.40
1:B:656:PRO:O	1:B:657:ASN:HB2	2.22	0.40
1:B:1498:LYS:HE2	1:B:1508:ALA:HA	2.04	0.40
1:B:1781:LEU:O	1:B:1785:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

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	1723/1747 (99%)	1648 (96%)	73 (4%)	2 (0%)	51 68
2	J	258/263 (98%)	245 (95%)	13 (5%)	0	100 100
All	All	1981/2010 (99%)	1893 (96%)	86 (4%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2086	GLN
1	B	1881	ASN

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	1544/1560 (99%)	1470 (95%)	74 (5%)	25 41
2	J	234/236 (99%)	223 (95%)	11 (5%)	26 42
All	All	1778/1796 (99%)	1693 (95%)	85 (5%)	25 41

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

Mol	Chain	Res	Type
1	B	403	LEU
1	B	426	LYS
1	B	440	LYS
1	B	455	PHE

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Mol	Chain	Res	Type
1	B	460	GLN
1	B	461	LEU
1	B	480	THR
1	B	526	ASN
1	B	528	ASP
1	B	545	ARG
1	B	546	SER
1	B	581	SER
1	B	607	GLN
1	B	645	ASP
1	B	659	GLU
1	B	712	ILE
1	B	734	THR
1	B	743	LEU
1	B	771	ASN
1	B	773	GLU
1	B	786	HIS
1	B	793	ASP
1	B	832	GLN
1	B	895	SER
1	B	932	SER
1	B	954	LEU
1	B	966	LYS
1	B	992	TYR
1	B	1027	ILE
1	B	1055	PRO
1	B	1056	SER
1	B	1078	MET
1	B	1087	SER
1	B	1126	MET
1	B	1258	VAL
1	B	1276	LEU
1	B	1279	GLU
1	B	1294	LYS
1	B	1313	ARG
1	B	1342	SER
1	B	1371	SER
1	B	1372	SER
1	B	1412	THR
1	B	1442	ARG
1	B	1443	LYS
1	B	1446	GLN

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Mol	Chain	Res	Type
1	B	1492	SER
1	B	1511	THR
1	B	1625	SER
1	B	1648	ARG
1	B	1655	ASN
1	B	1754	TYR
1	B	1779	ARG
1	B	1781	LEU
1	B	1861	ARG
1	B	1871	LEU
1	B	1879	LEU
1	B	1910	SER
1	B	1921	ARG
1	B	1931	SER
1	B	1953	MET
1	B	1958	SER
1	B	1960	LEU
1	B	1966	PHE
1	B	1971	ILE
1	B	1972	LYS
1	B	1974	CYS
1	B	1976	ASP
1	B	1990	ASP
1	B	2018	GLU
1	B	2068	ILE
1	B	2090	VAL
1	B	2105	THR
1	B	2125	ASP
2	J	2072	GLU
2	J	2121	ARG
2	J	2143	ARG
2	J	2170	LYS
2	J	2172	MET
2	J	2247	ASN
2	J	2249	LYS
2	J	2258	ARG
2	J	2259	VAL
2	J	2266	ARG
2	J	2268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

10 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	$\#\|Z\| > 2$
4	EDO	B	2210	-	3,3,3	0.53	0	2,2,2	0.46	0
4	EDO	B	2208	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	B	2207	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	B	2209	-	3,3,3	0.42	0	2,2,2	0.73	0
4	EDO	B	2204	-	3,3,3	0.53	0	2,2,2	0.31	0
3	Q9I	B	2201	-	13,14,14	2.58	6 (46%)	19,20,20	3.23	4 (21%)
4	EDO	B	2202	-	3,3,3	0.65	0	2,2,2	0.34	0
4	EDO	B	2205	-	3,3,3	0.46	0	2,2,2	1.03	0
4	EDO	B	2206	-	3,3,3	0.47	0	2,2,2	0.63	0
4	EDO	B	2203	-	3,3,3	0.58	0	2,2,2	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	2210	-	-	0/1/1/1	-
4	EDO	B	2208	-	-	1/1/1/1	-
4	EDO	B	2207	-	-	1/1/1/1	-
4	EDO	B	2209	-	-	1/1/1/1	-
4	EDO	B	2204	-	-	1/1/1/1	-
3	Q9I	B	2201	-	-	7/12/14/14	0/1/1/1
4	EDO	B	2202	-	-	0/1/1/1	-
4	EDO	B	2205	-	-	1/1/1/1	-
4	EDO	B	2206	-	-	1/1/1/1	-
4	EDO	B	2203	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2201	Q9I	O07-S05	5.88	1.50	1.43
3	B	2201	Q9I	O06-S05	4.42	1.48	1.43
3	B	2201	Q9I	C08-S05	3.02	1.80	1.76
3	B	2201	Q9I	C13-C08	-2.32	1.35	1.38
3	B	2201	Q9I	C11-CL14	2.12	1.79	1.74
3	B	2201	Q9I	O03-C04	-2.06	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2201	Q9I	O07-S05-O06	-12.18	99.78	119.52
3	B	2201	Q9I	O06-S05-C08	4.53	113.77	108.05
3	B	2201	Q9I	O03-N02-C01	2.65	118.90	114.28
3	B	2201	Q9I	C09-C08-S05	-2.44	117.19	119.76

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2201	Q9I	C13-C08-S05-N02
3	B	2201	Q9I	C09-C08-S05-N02
3	B	2201	Q9I	C01-N02-O03-C04
4	B	2204	EDO	O1-C1-C2-O2
3	B	2201	Q9I	C09-C08-S05-O06
3	B	2201	Q9I	C01-N02-S05-C08
3	B	2201	Q9I	C01-N02-S05-O07
3	B	2201	Q9I	C13-C08-S05-O06
4	B	2206	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	2208	EDO	O1-C1-C2-O2
4	B	2209	EDO	O1-C1-C2-O2
4	B	2207	EDO	O1-C1-C2-O2
4	B	2203	EDO	O1-C1-C2-O2
4	B	2205	EDO	O1-C1-C2-O2

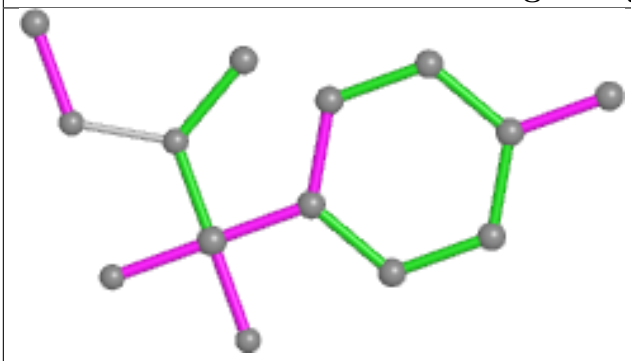
There are no ring outliers.

2 monomers are involved in 2 short contacts:

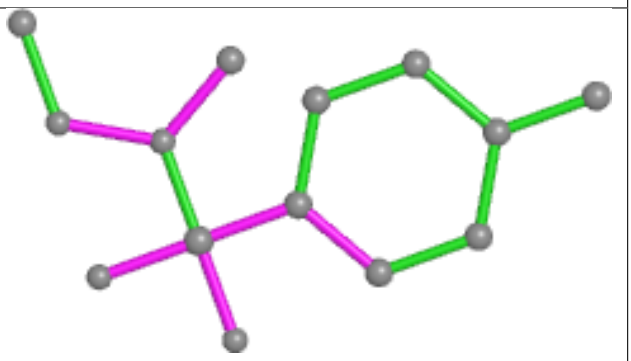
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2201	Q9I	1	0
4	B	2206	EDO	1	0

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 then 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.

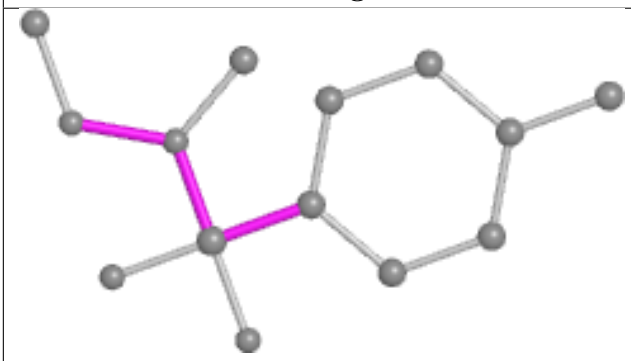
Ligand Q9I B 2201



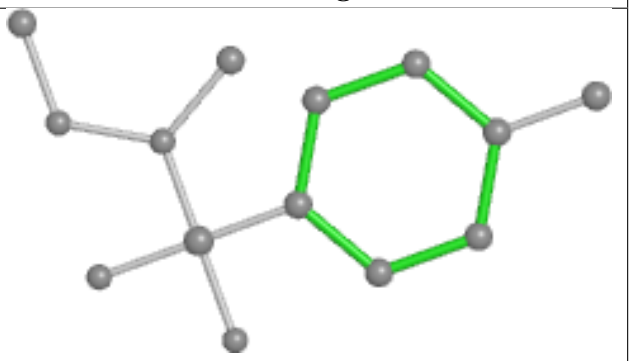
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	1725/1747 (98%)	0.24	131 (7%)	13	12	31, 61, 125, 178	0
2	J	260/263 (98%)	-0.00	12 (4%)	32	31	37, 56, 107, 164	0
All	All	1985/2010 (98%)	0.20	143 (7%)	15	14	31, 60, 124, 178	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2027	ASP	8.8
1	B	2122	PHE	6.7
1	B	1584	ILE	6.1
1	B	1895	LEU	5.8
1	B	754	GLU	5.6
1	B	2038	LEU	5.5
1	B	2101	ALA	5.4
2	J	2097	ILE	5.3
2	J	2061	GLY	5.2
1	B	1881	ASN	5.1
1	B	456	GLY	4.8
1	B	753	ARG	4.6
1	B	2033	GLY	4.6
1	B	1882	PRO	4.5
2	J	2098	LYS	4.5
1	B	2106	LEU	4.5
1	B	769	CYS	4.4
1	B	1868	LEU	4.4
1	B	1977	LYS	4.4
1	B	2089	LYS	4.3
1	B	1940	LEU	4.2
1	B	1880	ASN	4.2
1	B	1836	LEU	4.1
1	B	2035	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	2120	TYR	4.0
1	B	1841	LYS	4.0
1	B	404	ALA	4.0
1	B	1908	LEU	3.9
1	B	574	GLN	3.9
1	B	1889	VAL	3.9
1	B	779	PRO	3.8
1	B	805	HIS	3.8
1	B	1842	VAL	3.8
1	B	575	LEU	3.7
1	B	1597	LEU	3.7
1	B	455	PHE	3.7
1	B	1893	LEU	3.7
1	B	2046	GLU	3.6
1	B	1866	ASN	3.6
1	B	2108	PHE	3.5
1	B	1849	ILE	3.5
1	B	573	HIS	3.5
1	B	1978	GLY	3.4
1	B	2066	VAL	3.4
2	J	2062	SER	3.4
1	B	1979	VAL	3.3
1	B	762	LEU	3.3
1	B	2036	VAL	3.3
1	B	756	SER	3.2
1	B	2047	VAL	3.2
1	B	2072	LYS	3.2
2	J	2100	THR	3.2
1	B	761	VAL	3.2
2	J	2099	GLU	3.1
2	J	2320	LEU	3.1
1	B	2017	ILE	3.1
1	B	2028	SER	3.1
1	B	778	LEU	3.1
1	B	1873	GLN	3.1
1	B	1879	LEU	3.1
1	B	1600	TYR	3.1
1	B	1886	ASP	3.1
1	B	1885	ASN	3.0
1	B	1145	LYS	3.0
1	B	1983	PHE	3.0
2	J	2063	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	2086	GLN	3.0
1	B	2087	LYS	3.0
1	B	1936	LEU	2.9
1	B	1871	LEU	2.9
1	B	1874	LYS	2.9
1	B	571	GLY	2.9
1	B	2123	SER	2.9
1	B	799	ASP	2.9
1	B	1843	ARG	2.9
1	B	1896	GLN	2.8
1	B	2026	LYS	2.8
1	B	603	ARG	2.8
1	B	1912	THR	2.7
1	B	743	LEU	2.7
1	B	2040	GLN	2.7
1	B	1997	LEU	2.7
1	B	1604	LEU	2.6
1	B	576	CYS	2.6
1	B	2102	HIS	2.6
1	B	2090	VAL	2.6
1	B	806	ILE	2.6
1	B	1911	ASP	2.6
1	B	774	LEU	2.6
1	B	2032	GLY	2.6
1	B	1695	LEU	2.6
1	B	2094	PHE	2.6
1	B	791	ARG	2.6
1	B	768	GLN	2.5
1	B	2071	ALA	2.5
1	B	1884	PHE	2.5
1	B	1876	PRO	2.5
1	B	457	SER	2.5
1	B	1877	HIS	2.5
2	J	2317	PHE	2.5
1	B	1601	LEU	2.5
2	J	2065	GLN	2.5
1	B	764	THR	2.4
1	B	1966	PHE	2.4
1	B	2068	ILE	2.4
1	B	1156	LEU	2.4
1	B	1859	PRO	2.4
1	B	2107	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	454	PRO	2.4
1	B	453	LYS	2.3
1	B	1865	ASP	2.3
1	B	1870	GLN	2.3
2	J	2066	THR	2.3
1	B	709	TYR	2.3
1	B	1990	ASP	2.2
1	B	1152	ARG	2.2
1	B	1995	ALA	2.2
1	B	755	GLY	2.2
1	B	2097	PRO	2.2
1	B	1869	ARG	2.2
1	B	403	LEU	2.2
1	B	1614	LEU	2.2
1	B	527	MET	2.2
1	B	695	LYS	2.1
2	J	2095	ASP	2.1
1	B	2001	ASP	2.1
1	B	1858	ILE	2.1
1	B	1599	PRO	2.1
1	B	708	VAL	2.1
1	B	2104	TYR	2.1
1	B	796	LEU	2.1
1	B	1904	LEU	2.1
1	B	1963	LEU	2.1
1	B	1515	HIS	2.1
1	B	751	PHE	2.1
1	B	1151	GLU	2.1
1	B	757	ALA	2.1
1	B	1075	PHE	2.1
1	B	1956	LYS	2.0
1	B	752	LEU	2.0
1	B	1165	ILE	2.0
1	B	732	GLY	2.0
1	B	2118	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

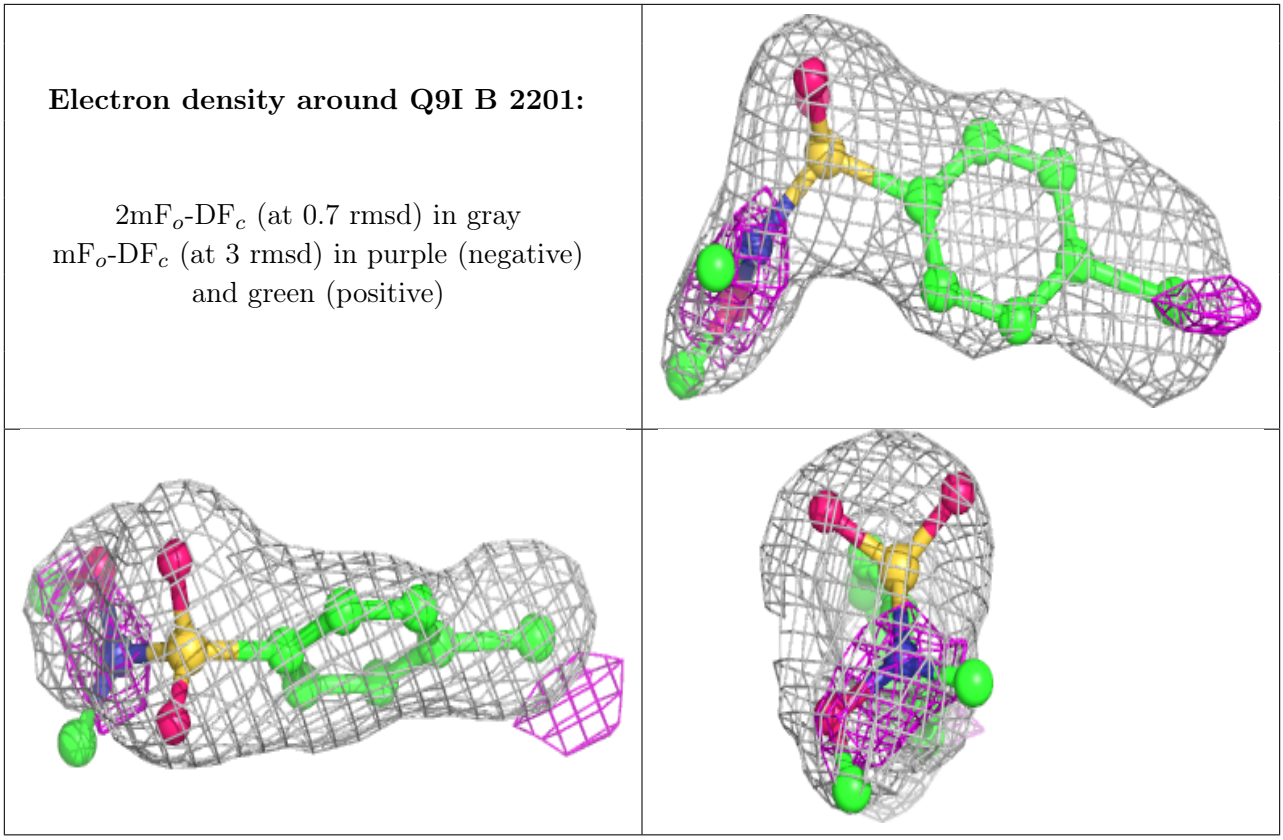
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	2202	4/4	0.77	0.29	52,54,54,59	0
4	EDO	B	2208	4/4	0.78	0.19	46,50,56,57	0
4	EDO	B	2209	4/4	0.85	0.14	58,59,61,65	0
4	EDO	B	2204	4/4	0.86	0.15	51,54,57,63	0
4	EDO	B	2210	4/4	0.90	0.12	48,51,52,61	0
4	EDO	B	2207	4/4	0.92	0.14	65,67,68,69	0
4	EDO	B	2203	4/4	0.93	0.16	53,54,54,60	0
4	EDO	B	2206	4/4	0.93	0.16	37,38,43,47	0
4	EDO	B	2205	4/4	0.94	0.16	45,48,49,56	0
3	Q9I	B	2201	14/14	0.94	0.20	47,55,59,64	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 Q9I B 2201:

$2mF_o$-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.