



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:40 AM UTC

PDB ID : 2HFE / pdb_00002hfe
Title : Rb⁺ complex of a K channel with an amide to ester substitution in the selectivity filter
Authors : Valiyaveetil, F.I.; MacKinnon, R.; Muir, T.W.
Deposited on : 2006-06-23
Resolution : 2.25 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

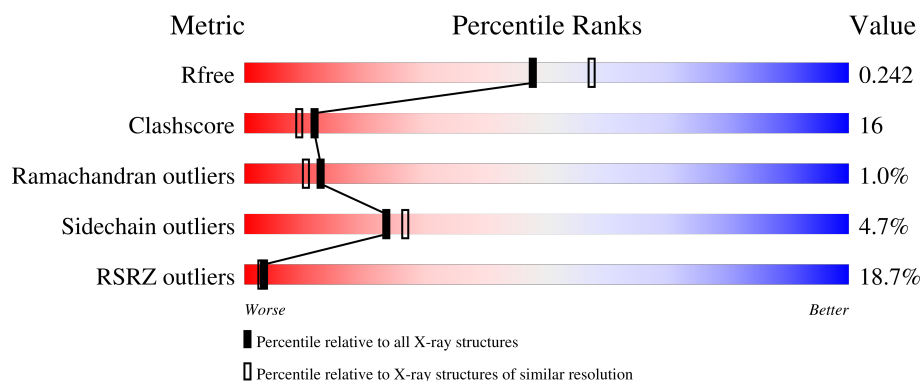
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	219	24% 65% 30% .
2	B	211	18% 64% 32% .
3	C	101	9% 78% 21% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4172 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 FAB Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1648	1042	275	325	6			

- Molecule 2 is a protein called FAB Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1641	1019	281	336	5			

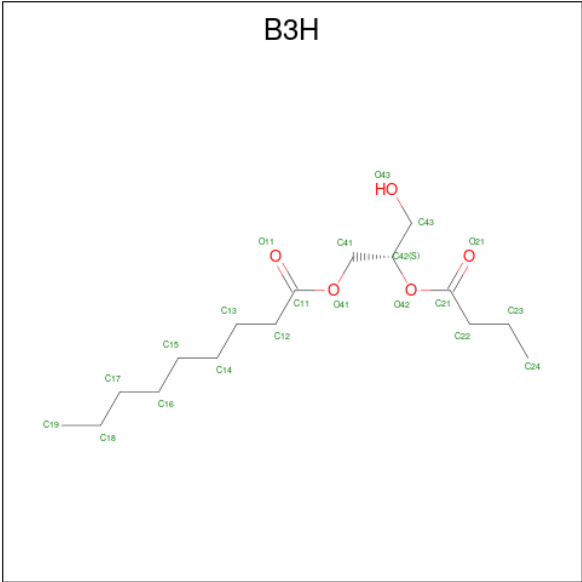
- Molecule 3 is a protein called KcsA channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	101	Total	C	N	O	S	0	0	0
			757	497	127	131	2			

- Molecule 4 is RUBIDIUM ION (CCD ID: RB) (formula: Rb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	5	Total	Rb	0	0
			5	5		

- Molecule 5 is (2S)-2-(BUTYRYLOXY)-3-HYDROXYPROPYL NONANOATE (CCD ID: B3H) (formula: C₁₆H₃₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			21	16	5		

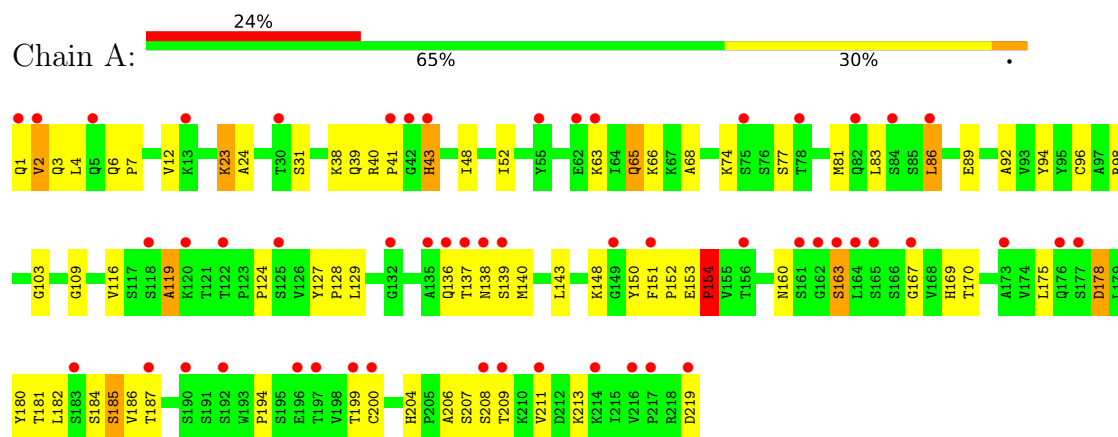
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	52	Total	O	0	0
			52	52		
6	C	18	Total	O	0	0
			18	18		

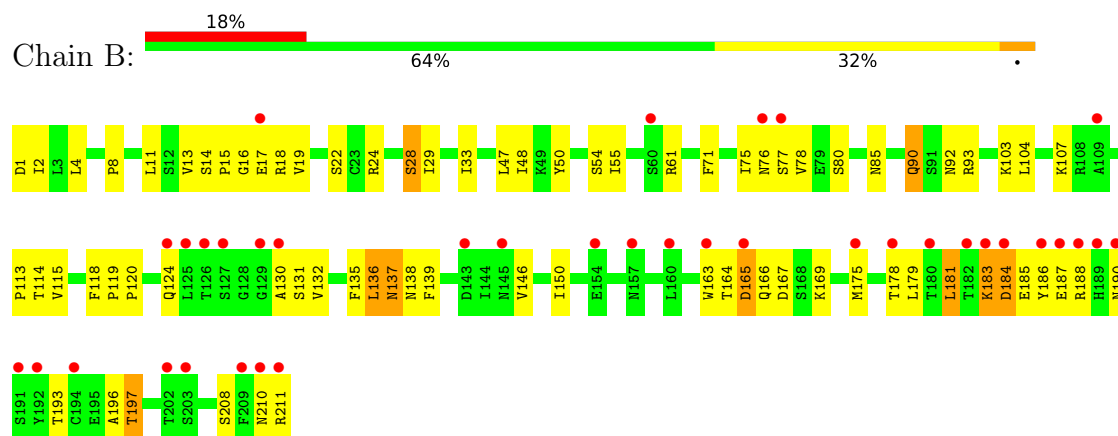
3 Residue-property plots [i](#)

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.

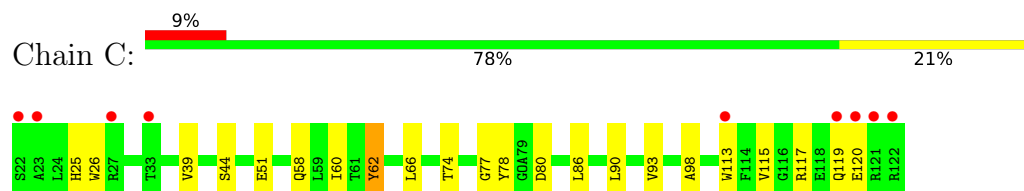
• Molecule 1: FAB Heavy Chain



• Molecule 2: FAB Light Chain



• Molecule 3: KcsA channel



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	156.14Å 156.14Å 75.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.78 – 2.25 26.78 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.9 (26.78-2.25) 98.9 (26.78-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.251 0.226 , 0.242	Depositor DCC
R_{free} test set	2155 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4172	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: RB, GOA, B3H

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	0.75	0/1692	1.08	9/2312 (0.4%)
2	B	0.76	0/1678	1.06	5/2276 (0.2%)
3	C	1.15	3/771 (0.4%)	1.17	4/1058 (0.4%)
All	All	0.84	3/4141 (0.1%)	1.09	18/5646 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	98	ALA	CA-CB	6.75	1.63	1.53
3	C	39	VAL	CA-CB	5.97	1.61	1.54
3	C	74	THR	CA-C	5.61	1.60	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	60	ILE	N-CA-C	10.74	123.52	113.10
1	A	103	GLY	N-CA-C	10.16	128.87	115.36
2	B	2	ILE	N-CA-C	7.73	119.36	108.93
1	A	96	CYS	N-CA-C	-6.80	99.60	110.14
2	B	137	ASN	N-CA-C	6.29	119.66	109.40
3	C	51	GLU	N-CA-C	6.25	120.10	112.23
1	A	66	LYS	N-CA-C	6.15	119.56	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	HIS	N-CA-C	6.12	119.35	109.79
1	A	204	HIS	CA-C-N	6.01	127.35	119.84
1	A	204	HIS	C-N-CA	6.01	127.35	119.84
3	C	74	THR	N-CA-C	-5.97	105.76	113.16
1	A	68	ALA	N-CA-C	5.87	119.29	109.95
1	A	86	LEU	N-CA-C	5.80	118.18	110.53
3	C	62	TYR	N-CA-C	5.60	122.19	109.81
2	B	80	SER	N-CA-C	5.57	118.07	111.33
1	A	143	LEU	N-CA-C	-5.32	101.63	109.18
2	B	136	LEU	N-CA-C	-5.19	98.81	107.99
2	B	28	SER	N-CA-C	5.04	117.53	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	TYR	Sidechain

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	1648	0	1616	52	0
2	B	1641	0	1570	67	0
3	C	757	0	767	18	0
4	C	5	0	0	0	0
5	C	21	0	30	7	0
6	A	30	0	0	5	0
6	B	52	0	0	16	0
6	C	18	0	0	1	0
All	All	4172	0	3983	129	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 16.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ILE:N	6:B:301:HOH:O	1.82	1.12
2:B:1:ASP:HB2	6:B:346:HOH:O	1.66	0.96
3:C:25:HIS:ND1	6:C:301:HOH:O	2.00	0.94
2:B:169:LYS:HG3	6:B:344:HOH:O	1.68	0.93
1:A:98:ARG:HD2	6:A:320:HOH:O	1.67	0.92
3:C:90:LEU:HD23	5:C:206:B3H:H172	1.52	0.91
2:B:61:ARG:HG3	2:B:76:ASN:O	1.84	0.78
3:C:90:LEU:CD2	5:C:206:B3H:H172	2.12	0.78
2:B:28:SER:HA	6:B:301:HOH:O	1.83	0.77
2:B:29:ILE:HG12	6:B:301:HOH:O	1.85	0.77
3:C:115:VAL:O	3:C:119:GLN:HG2	1.84	0.77
1:A:65:GLN:NE2	1:A:65:GLN:H	1.83	0.75
1:A:160:ASN:O	1:A:163:SER:HB3	1.89	0.72
2:B:78:VAL:HG21	2:B:104:LEU:HD21	1.72	0.72
1:A:1:GLN:OE1	1:A:1:GLN:N	2.23	0.72
2:B:28:SER:C	6:B:301:HOH:O	2.27	0.71
2:B:13:VAL:CG2	2:B:17:GLU:HB3	2.21	0.71
1:A:153:GLU:OE1	1:A:154:PRO:HA	1.89	0.71
2:B:16:GLY:O	2:B:77:SER:HA	1.91	0.70
1:A:169:HIS:HE1	2:B:138:ASN:HD21	1.38	0.70
2:B:183:LYS:O	2:B:187:GLU:HG2	1.91	0.70
1:A:6:GLN:HE21	1:A:109:GLY:HA3	1.55	0.70
3:C:86:LEU:CD1	5:C:206:B3H:H132	2.22	0.69
2:B:90:GLN:HE22	2:B:93:ARG:H	1.41	0.68
2:B:178:THR:HG23	6:B:307:HOH:O	1.94	0.67
2:B:92:ASN:HD21	3:C:58:GLN:HE21	1.41	0.67
3:C:86:LEU:HD12	5:C:206:B3H:H132	1.75	0.67
2:B:197:THR:OG1	6:B:302:HOH:O	2.12	0.66
2:B:28:SER:CA	6:B:301:HOH:O	2.41	0.66
1:A:169:HIS:HE1	2:B:138:ASN:ND2	1.95	0.64
3:C:93:VAL:HG21	5:C:206:B3H:H192	1.80	0.64
2:B:136:LEU:HD11	2:B:196:ALA:HB2	1.79	0.63
1:A:148:LYS:HB3	1:A:181:THR:HG23	1.81	0.63
3:C:90:LEU:HD23	5:C:206:B3H:C17	2.26	0.62
2:B:19:VAL:HG12	2:B:75:ILE:HB	1.81	0.61
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.83	0.61
1:A:207:SER:O	1:A:209:THR:HG23	2.00	0.61
2:B:115:VAL:HG22	2:B:136:LEU:HD13	1.82	0.60
2:B:90:GLN:NE2	2:B:92:ASN:H	2.00	0.60
1:A:39:GLN:O	1:A:92:ALA:HB1	2.02	0.60
2:B:132:VAL:N	6:B:307:HOH:O	2.34	0.59
2:B:190:ASN:O	2:B:210:ASN:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:C	1:A:182:LEU:HD12	2.29	0.58
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.85	0.57
2:B:1:ASP:HB3	6:B:335:HOH:O	2.05	0.56
2:B:164:THR:OG1	6:B:303:HOH:O	2.18	0.56
2:B:132:VAL:C	6:B:307:HOH:O	2.46	0.56
1:A:169:HIS:CE1	2:B:138:ASN:HD21	2.21	0.56
2:B:137:ASN:HB3	2:B:138:ASN:HD22	1.72	0.55
2:B:211:ARG:O	2:B:211:ARG:HG3	2.06	0.55
1:A:219:ASP:OXT	1:A:219:ASP:OD1	2.25	0.54
1:A:185:SER:HB2	2:B:135:PHE:CE2	2.42	0.54
1:A:12:VAL:O	1:A:116:VAL:HA	2.06	0.54
3:C:77:GLY:O	3:C:78:TYR:C	2.50	0.54
2:B:184:ASP:O	2:B:187:GLU:N	2.35	0.53
1:A:65:GLN:H	1:A:65:GLN:CD	2.12	0.53
1:A:38:LYS:HB2	1:A:48:ILE:HD11	1.89	0.52
1:A:1:GLN:N	1:A:1:GLN:CD	2.68	0.52
1:A:63:LYS:HG3	6:A:330:HOH:O	2.08	0.52
1:A:74:LYS:HG3	6:A:321:HOH:O	2.08	0.52
2:B:13:VAL:HG22	2:B:14:SER:N	2.24	0.51
2:B:8:PRO:HG2	2:B:11:LEU:HD13	1.93	0.51
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.92	0.51
3:C:113:TRP:HE1	3:C:117:ARG:NH1	2.08	0.51
1:A:1:GLN:CD	1:A:1:GLN:H1	2.17	0.50
2:B:90:GLN:NE2	2:B:92:ASN:N	2.60	0.50
2:B:115:VAL:HG22	2:B:136:LEU:CD1	2.42	0.50
3:C:86:LEU:HD13	5:C:206:B3H:H132	1.93	0.50
1:A:43:HIS:CD2	1:A:43:HIS:N	2.78	0.49
1:A:167:GLY:O	1:A:186:VAL:HA	2.12	0.49
1:A:140:MET:HE2	1:A:187:THR:HG22	1.95	0.49
1:A:40:ARG:HB3	1:A:41:PRO:HD2	1.93	0.49
2:B:28:SER:OG	6:B:304:HOH:O	2.20	0.49
1:A:1:GLN:O	1:A:2:VAL:C	2.56	0.49
1:A:83:LEU:HB3	1:A:86:LEU:HD21	1.95	0.49
3:C:44:SER:OG	3:C:66:LEU:HA	2.12	0.48
2:B:15:PRO:HD3	2:B:107:LYS:O	2.13	0.48
2:B:114:THR:HG22	6:B:329:HOH:O	2.13	0.48
1:A:140:MET:CE	1:A:187:THR:HG22	2.44	0.47
2:B:146:VAL:HG13	2:B:146:VAL:O	2.15	0.47
1:A:152:PRO:HD2	1:A:206:ALA:CB	2.45	0.47
2:B:163:TRP:CD1	2:B:175:MET:HG3	2.50	0.47
1:A:170:THR:HA	1:A:184:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASN:O	2:B:77:SER:HB3	2.14	0.46
1:A:52:ILE:O	1:A:52:ILE:HG23	2.15	0.46
2:B:47:LEU:C	2:B:48:ILE:HG12	2.40	0.46
1:A:31:SER:HB2	3:C:62:TYR:CE1	2.52	0.45
1:A:119:ALA:HB3	1:A:151:PHE:CE2	2.51	0.45
1:A:178:ASP:OD2	1:A:178:ASP:N	2.49	0.45
1:A:152:PRO:HD2	1:A:206:ALA:HB1	1.99	0.45
2:B:187:GLU:HA	2:B:211:ARG:NH2	2.31	0.45
1:A:23:LYS:HZ1	1:A:77:SER:HB2	1.82	0.45
2:B:187:GLU:HA	2:B:211:ARG:CZ	2.47	0.45
2:B:16:GLY:C	2:B:77:SER:HA	2.42	0.44
2:B:187:GLU:O	2:B:211:ARG:NH2	2.40	0.44
1:A:7:PRO:HD3	6:A:306:HOH:O	2.16	0.44
1:A:65:GLN:H	1:A:65:GLN:HE21	1.63	0.44
2:B:92:ASN:ND2	3:C:58:GLN:HE21	2.12	0.44
1:A:127:TYR:CE2	2:B:124:GLN:HG3	2.53	0.44
1:A:23:LYS:HE3	1:A:23:LYS:C	2.42	0.44
2:B:13:VAL:CG2	2:B:14:SER:N	2.81	0.44
2:B:167:ASP:OD2	2:B:169:LYS:HB2	2.18	0.44
1:A:23:LYS:HE3	1:A:24:ALA:N	2.32	0.44
3:C:80:ASP:OD1	3:C:80:ASP:N	2.50	0.44
2:B:181:LEU:HD12	2:B:186:TYR:HB2	1.99	0.44
2:B:54:SER:O	2:B:55:ILE:HD13	2.17	0.43
2:B:150:ILE:HD11	2:B:179:LEU:HD21	2.00	0.43
2:B:169:LYS:CG	6:B:344:HOH:O	2.46	0.43
1:A:81:MET:HE1	1:A:94:TYR:CD1	2.54	0.43
2:B:124:GLN:HE22	2:B:131:SER:CB	2.32	0.42
2:B:90:GLN:HE21	2:B:92:ASN:H	1.64	0.42
1:A:199:THR:HG23	1:A:213:LYS:C	2.43	0.42
1:A:98:ARG:CD	6:A:320:HOH:O	2.46	0.42
1:A:175:LEU:HB2	1:A:180:TYR:CE2	2.55	0.42
1:A:128:PRO:O	1:A:129:LEU:HD23	2.20	0.42
1:A:138:ASN:CG	1:A:139:SER:H	2.28	0.41
2:B:17:GLU:HG2	2:B:18:ARG:H	1.85	0.41
2:B:85:ASN:HD22	2:B:103:LYS:HA	1.84	0.41
2:B:184:ASP:O	2:B:185:GLU:C	2.62	0.41
1:A:136:GLN:O	1:A:136:GLN:HG2	2.21	0.41
2:B:13:VAL:HG23	2:B:17:GLU:CD	2.45	0.41
2:B:165:ASP:O	2:B:166:GLN:C	2.61	0.41
1:A:40:ARG:HB3	1:A:41:PRO:CD	2.51	0.41
2:B:33:ILE:HG21	2:B:71:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:TRP:CE3	3:C:26:TRP:HA	2.54	0.41
2:B:193:THR:HG23	2:B:208:SER:OG	2.22	0.40
1:A:40:ARG:NH2	1:A:89:GLU:O	2.54	0.40
3:C:117:ARG:O	3:C:120:GLU:HB3	2.22	0.40
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.87	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	A	217/219 (99%)	206 (95%)	8 (4%)	3 (1%)	9	5
2	B	209/211 (99%)	195 (93%)	12 (6%)	2 (1%)	12	10
3	C	97/101 (96%)	96 (99%)	1 (1%)	0	100	100
All	All	523/531 (98%)	497 (95%)	21 (4%)	5 (1%)	12	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA
2	B	184	ASP
2	B	188	ARG
1	A	2	VAL
1	A	154	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	A	185/185 (100%)	172 (93%)	13 (7%)	14	13
2	B	189/189 (100%)	181 (96%)	8 (4%)	26	31
3	C	72/73 (99%)	72 (100%)	0	100	100
All	All	446/447 (100%)	425 (95%)	21 (5%)	23	26

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	LEU
1	A	23	LYS
1	A	65	GLN
1	A	137	THR
1	A	154	PRO
1	A	163	SER
1	A	178	ASP
1	A	185	SER
1	A	194	PRO
1	A	200	CYS
1	A	208	SER
1	A	211	VAL
2	B	4	LEU
2	B	22	SER
2	B	24	ARG
2	B	90	GLN
2	B	165	ASP
2	B	181	LEU
2	B	183	LYS
2	B	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	6	GLN
1	A	43	HIS
1	A	65	GLN
1	A	82	GLN

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Mol	Chain	Res	Type
1	A	169	HIS
1	A	176	GLN
2	B	85	ASN
2	B	90	GLN
2	B	92	ASN
2	B	124	GLN
2	B	138	ASN

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](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	B3H	C	206	-	20,20,20	1.40	3 (15%)	22,22,22	1.22	2 (9%)

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
5	B3H	C	206	-	-	7/22/22/22	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	206	B3H	O41-C11	3.84	1.44	1.33
5	C	206	B3H	O42-C21	3.55	1.44	1.34
5	C	206	B3H	O41-C41	-2.40	1.39	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	206	B3H	O42-C21-C22	3.70	119.48	111.48
5	C	206	B3H	O41-C11-C12	2.02	117.99	111.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	206	B3H	O21-C21-O42-C42
5	C	206	B3H	C22-C21-O42-C42
5	C	206	B3H	C21-C22-C23-C24
5	C	206	B3H	O41-C11-C12-C13
5	C	206	B3H	O41-C41-C42-O42
5	C	206	B3H	O11-C11-C12-C13
5	C	206	B3H	O42-C21-C22-C23

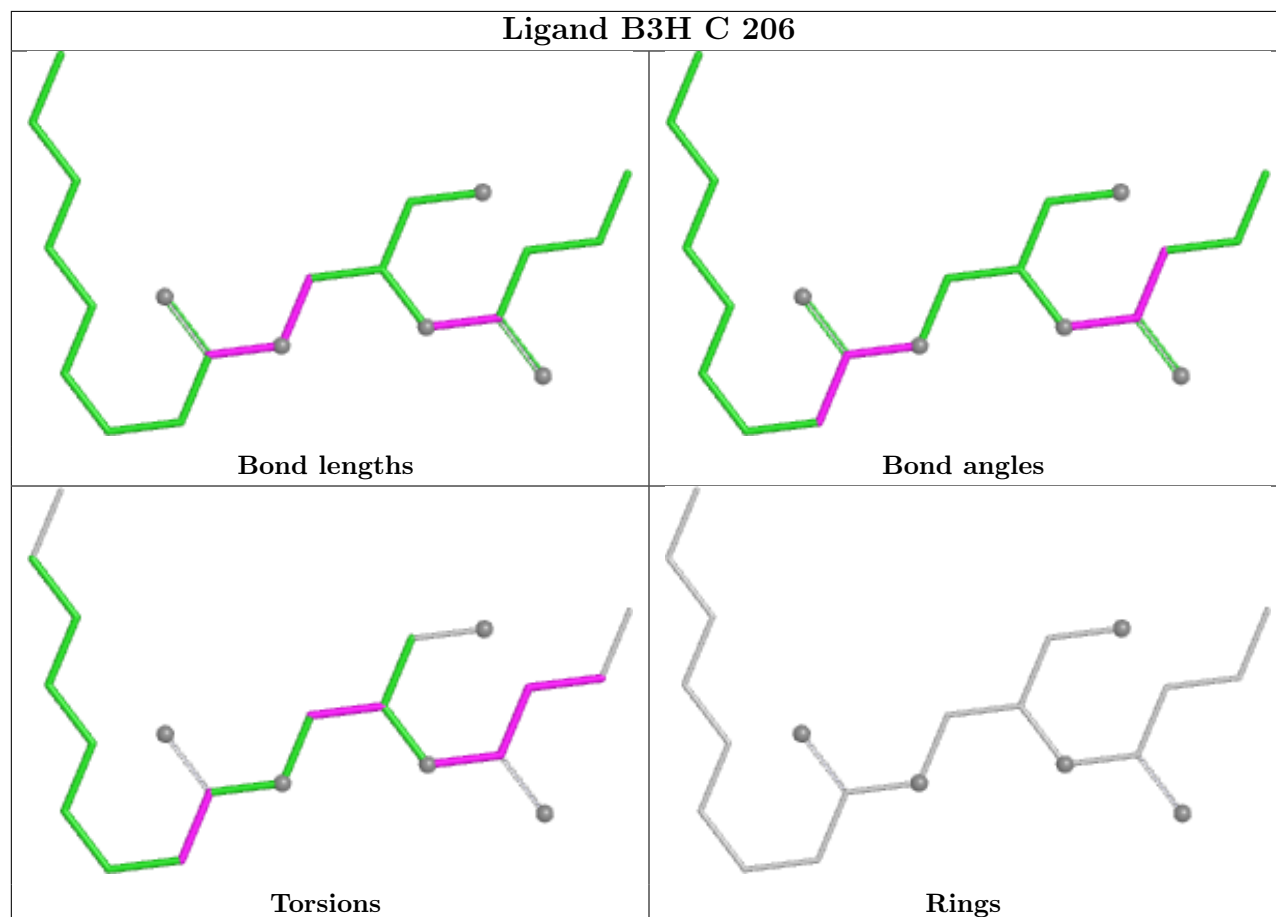
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	206	B3H	7	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	219/219 (100%)	1.30	53 (24%) 2 1	28, 58, 74, 86	0
2	B	211/211 (100%)	0.99	37 (17%) 4 3	23, 55, 80, 88	0
3	C	100/101 (99%)	0.45	9 (9%) 15 14	21, 31, 69, 78	0
All	All	530/531 (99%)	1.02	99 (18%) 3 3	21, 54, 77, 88	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	THR	5.3
3	C	23	ALA	4.8
1	A	136	GLN	4.6
1	A	137	THR	4.6
2	B	190	ASN	4.5
1	A	211	VAL	3.9
3	C	119	GLN	3.9
3	C	120	GLU	3.6
1	A	177	SER	3.6
1	A	164	LEU	3.5
1	A	139	SER	3.5
2	B	180	THR	3.4
1	A	120	LYS	3.4
2	B	209	PHE	3.3
2	B	210	ASN	3.2
1	A	217	PRO	3.2
1	A	2	VAL	3.2
2	B	194	CYS	3.1
2	B	202	THR	3.1
1	A	42	GLY	3.1
1	A	149	GLY	3.1
1	A	219	ASP	3.1
2	B	126	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	125	LEU	3.1
1	A	208	SER	3.1
2	B	186	TYR	3.0
2	B	211	ARG	3.0
2	B	157	ASN	3.0
2	B	127	SER	3.0
1	A	199	THR	3.0
1	A	216	VAL	2.9
1	A	1	GLN	2.9
2	B	109	ALA	2.9
1	A	122	THR	2.9
1	A	197	THR	2.9
2	B	182	THR	2.9
2	B	183	LYS	2.9
1	A	138	ASN	2.8
1	A	151	PHE	2.8
2	B	189	HIS	2.7
1	A	167	GLY	2.7
1	A	162	GLY	2.6
2	B	188	ARG	2.6
1	A	75	SER	2.6
2	B	77	SER	2.6
2	B	145	ASN	2.6
3	C	27	ARG	2.5
1	A	30	THR	2.5
1	A	43	HIS	2.5
1	A	165	SER	2.5
1	A	196	GLU	2.5
1	A	84	SER	2.5
3	C	22	SER	2.5
2	B	17	GLU	2.4
2	B	184	ASP	2.4
3	C	122	ARG	2.4
1	A	82	GLN	2.4
2	B	124	GLN	2.4
1	A	78	THR	2.3
1	A	118	SER	2.3
2	B	163	TRP	2.3
2	B	60	SER	2.3
2	B	154	GLU	2.3
1	A	200	CYS	2.3
1	A	41	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	33	THR	2.3
3	C	121	ARG	2.3
1	A	187	THR	2.2
1	A	13	LYS	2.2
1	A	5	GLN	2.2
2	B	178	THR	2.2
2	B	203	SER	2.2
1	A	62	GLU	2.2
2	B	191	SER	2.2
2	B	192	TYR	2.1
1	A	63	LYS	2.1
1	A	183	SER	2.1
1	A	55	TYR	2.1
2	B	175	MET	2.1
3	C	113	TRP	2.1
1	A	132	GLY	2.1
2	B	129	GLY	2.1
1	A	173	ALA	2.1
1	A	214	LYS	2.1
2	B	165	ASP	2.1
1	A	125	SER	2.1
1	A	156	THR	2.1
1	A	161	SER	2.1
1	A	192	SER	2.1
1	A	135	ALA	2.1
2	B	160	LEU	2.1
2	B	76	ASN	2.1
1	A	190	SER	2.0
1	A	86	LEU	2.0
1	A	163	SER	2.0
2	B	187	GLU	2.0
2	B	130	ALA	2.0
1	A	176	GLN	2.0
2	B	143	ASP	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](#)

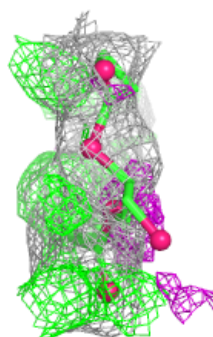
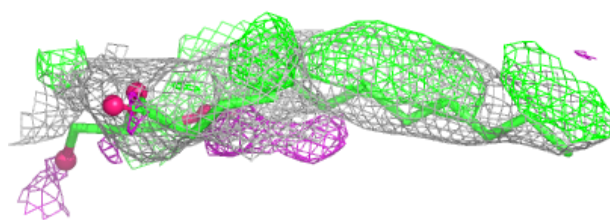
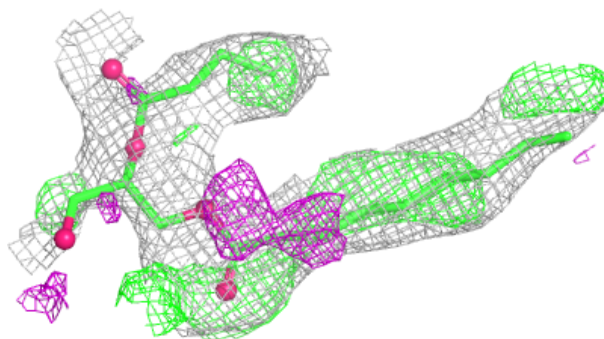
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	B3H	C	206	21/21	0.65	0.31	71,81,91,92	0
4	RB	C	201	1/1	0.93	0.13	55,55,55,55	1
4	RB	C	203	1/1	0.99	0.05	29,29,29,29	1
4	RB	C	204	1/1	0.99	0.05	26,26,26,26	1
4	RB	C	202	1/1	0.99	0.01	28,28,28,28	1
4	RB	C	205	1/1	1.00	0.11	45,45,45,45	1

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 B3H C 206:

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.