Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:00 AM GMT

PDB ID	:	3KJ6
Title	:	Crystal structure of a Methylated beta2 Adrenergic Receptor-Fab complex
Authors	:	Bokoch, M.P.; Zou, Y.; Rasmussen, S.G.F.; Liu, C.W.; Nygaard, R.; Rosenbaum, D.M.; Fung, J.J.; Choi, H.-J.; Thian, F.S.; Kobilka, T.S.; Puglisi, J.D.; Weis, W.I.; Pardo, L.; Prosser, S.; Mueller, L.; Kobilka, B.K.
Deposited on	:	2009-11-02
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

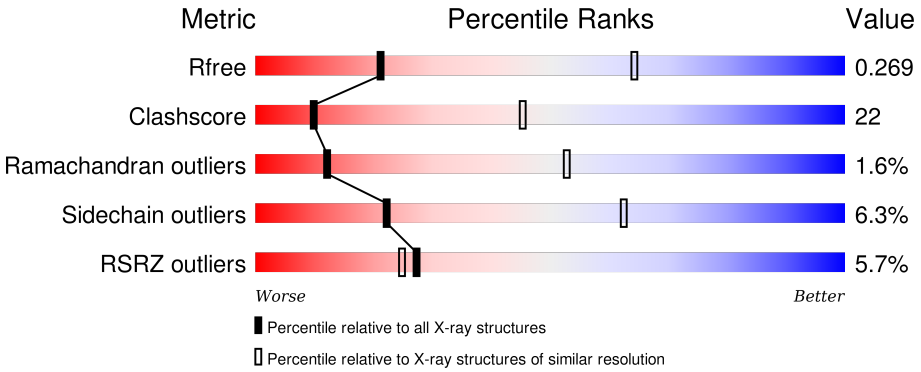
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	366	9%, 40%, 18%, 39%
2	L	214	57%, 37%, 6%
3	H	217	%, 55%, 39%, 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4974 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 Beta-2 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1656	1090	271	286	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P07550
A	1	PHE	-	EXPRESSION TAG	UNP P07550
A	16	ARG	GLY	VARIANT	UNP P07550
A	187	GLU	ASN	ENGINEERED	UNP P07550

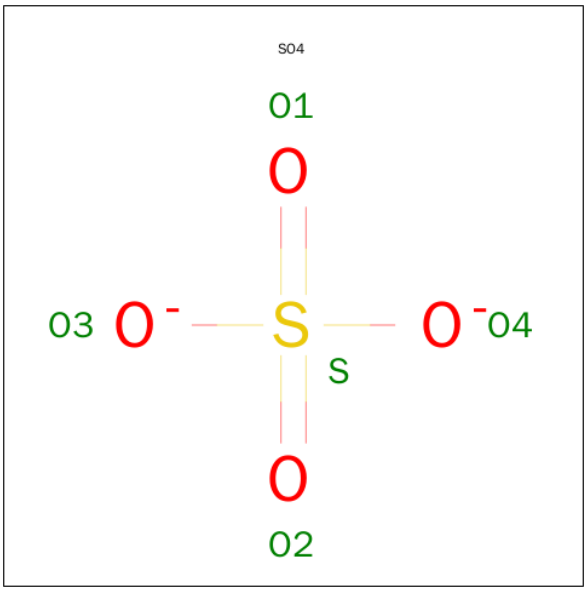
- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1678	1050	278	341	9			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1635	1031	269	328	7			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

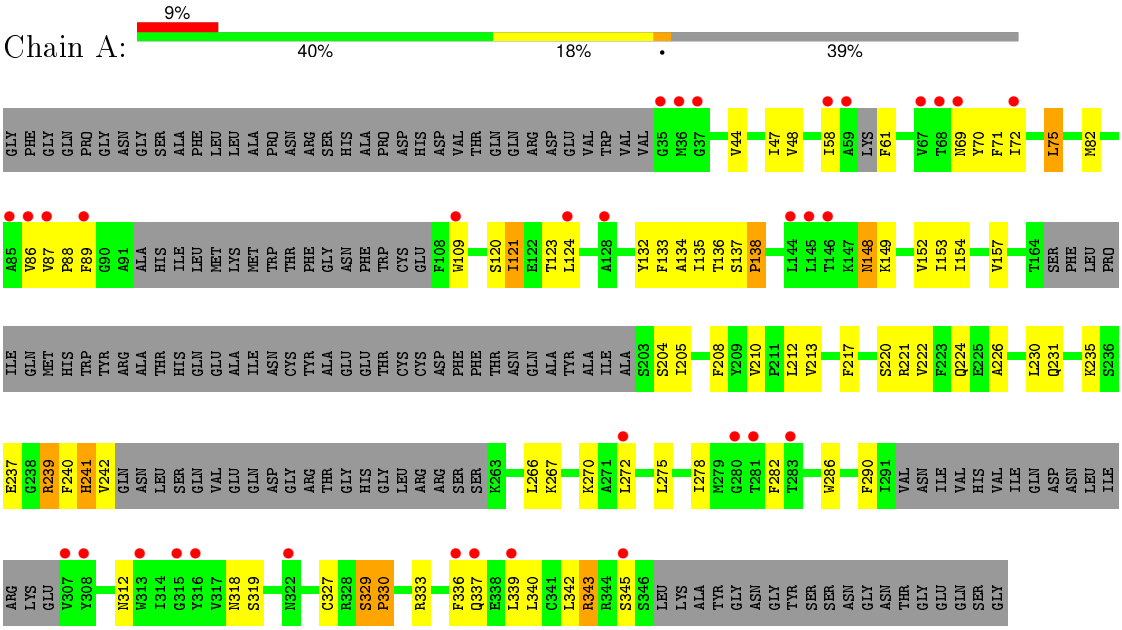


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

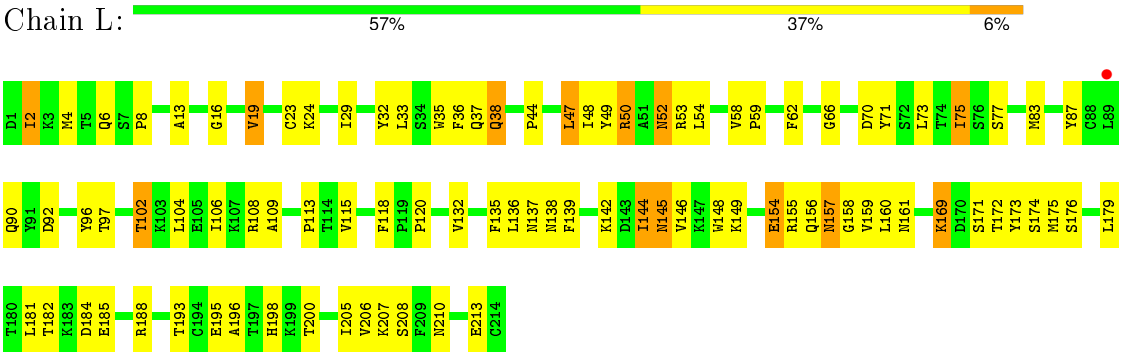
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

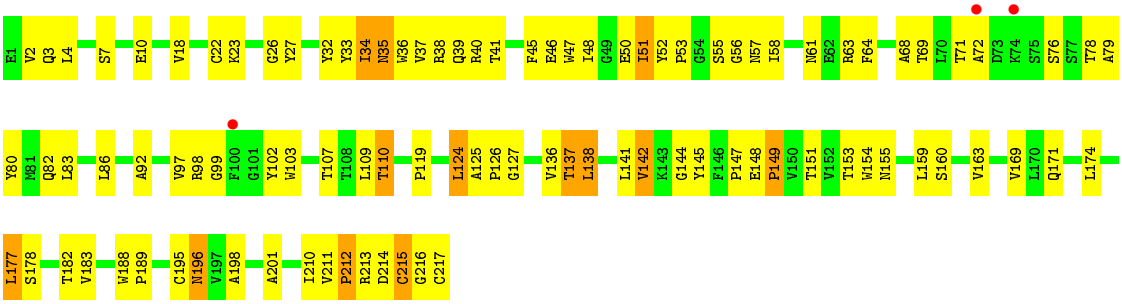
- Molecule 1: Beta-2 adrenergic receptor



- Molecule 2: Fab light chain



- Molecule 3: Fab heavy chain


E1 V2 Q3 L4 S7 E10 V18 C22 K23 G26 Y27 Y32 Y33 I34 N35 W36 V37 R38 Q39 R40 T41 F45 E46 W47 I48 G49 E50 I51 Y52 P53 G54 S55 G56 N57 I58 M61 E62 R63 F64 A68 T69 L70 T71 A72 D73 K74 S75 S76 S77 T78 A79
Y80 M81 Q82 L83 I86 A92 V97 R98 G99 F100 G101 Y102 W103 T107 T108 L109 T110 P119 L124 A125 P126 G127 V136 T137 L138 L141 V142 K143 G144 Y145 F146 P147 E148 P149 V150 T151 V152 T153 W154 N155 L159 S160 V163 V169 L170 Q171 L174
L177 S178 T182 V183 W188 P189 C195 N196 V197 A198 A201 I210 V211 P212 R213 D214 C215 G216 C217

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	338.60Å 48.60Å 88.90Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	44.41 – 3.40 44.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.41-3.40) 95.9 (44.41-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.238 , 0.280 0.228 , 0.269	Depositor DCC
R_{free} test set	1870 reflections (9.78%)	DCC
Wilson B-factor (Å^2)	102.1	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 105.8	EDS
Estimated twinning fraction	0.025 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 19567 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4974	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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	0.23	0/1686	0.36	0/2295
2	L	0.23	0/1716	0.42	0/2324
3	H	0.24	0/1677	0.45	0/2290
All	All	0.23	0/5079	0.41	0/6909

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	A	1656	0	1631	60	0
2	L	1678	0	1610	87	0
3	H	1635	0	1578	85	0
4	A	5	0	0	0	0
All	All	4974	0	4819	216	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 22.

All (216) 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)
3:H:214:ASP:O	3:H:215:CYS:HB2	1.65	0.93
2:L:19:VAL:HG13	2:L:75:ILE:HG23	1.62	0.82
2:L:38:GLN:HE21	3:H:39:GLN:HE22	1.25	0.81
3:H:214:ASP:C	3:H:216:GLY:HA3	2.02	0.80
1:A:241:HIS:O	1:A:242:VAL:HG23	1.83	0.79
1:A:235:LYS:O	1:A:239:ARG:HD3	1.85	0.76
2:L:108:ARG:HG2	2:L:109:ALA:H	1.52	0.75
2:L:169:LYS:HD2	2:L:169:LYS:H	1.51	0.73
1:A:231:GLN:HE21	1:A:235:LYS:HD2	1.53	0.73
3:H:214:ASP:O	3:H:216:GLY:HA3	1.91	0.70
1:A:148:ASN:HD22	1:A:149:LYS:N	1.90	0.70
2:L:38:GLN:NE2	3:H:39:GLN:HE22	1.89	0.69
3:H:34:ILE:HG13	3:H:34:ILE:O	1.93	0.69
3:H:119:PRO:HB2	3:H:142:VAL:HG23	1.75	0.69
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.75	0.69
1:A:71:PHE:HD2	1:A:154:ILE:HD11	1.58	0.68
2:L:44:PRO:HG2	3:H:103:TRP:CD2	2.28	0.68
1:A:329:SER:HB2	1:A:330:PRO:HD3	1.75	0.68
3:H:69:THR:OG1	3:H:82:GLN:HB3	1.94	0.67
2:L:118:PHE:CD2	3:H:124:LEU:HB3	2.30	0.67
3:H:213:ARG:HG2	3:H:214:ASP:H	1.59	0.66
1:A:75:LEU:HD11	1:A:123:THR:HB	1.78	0.66
1:A:266:LEU:HD21	3:H:57:ASN:HB2	1.79	0.63
3:H:35:ASN:ND2	3:H:50:GLU:HG3	2.14	0.62
1:A:213:VAL:O	1:A:217:PHE:HD1	1.82	0.62
1:A:226:ALA:O	1:A:230:LEU:HB2	2.00	0.61
3:H:154:TRP:CD1	3:H:163:VAL:HG21	2.36	0.61
2:L:29:ILE:HG22	2:L:92:ASP:HB3	1.83	0.61
3:H:213:ARG:CG	3:H:214:ASP:H	2.14	0.61
2:L:50:ARG:HH21	2:L:53:ARG:NH1	1.98	0.60
1:A:89:PHE:HB2	1:A:109:TRP:HE1	1.66	0.60
3:H:215:CYS:N	3:H:216:GLY:HA3	2.14	0.59
2:L:144:ILE:HD13	2:L:145:ASN:H	1.66	0.59
1:A:120:SER:O	1:A:124:LEU:HD23	2.03	0.58
1:A:231:GLN:NE2	1:A:235:LYS:HD2	2.17	0.58
2:L:36:PHE:HA	2:L:47:LEU:HD22	1.85	0.58
1:A:267:LYS:C	1:A:267:LYS:HD3	2.23	0.58
1:A:89:PHE:HB2	1:A:109:TRP:NE1	2.19	0.57
2:L:29:ILE:HG13	2:L:71:TYR:OH	2.05	0.57
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.86	0.57
2:L:50:ARG:HH21	2:L:53:ARG:HH12	1.52	0.57
2:L:138:ASN:HA	2:L:172:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:110:THR:HG21	3:H:147:PRO:HB2	1.86	0.56
3:H:211:VAL:HG13	3:H:212:PRO:HD2	1.87	0.56
3:H:18:VAL:HG22	3:H:86:LEU:HD11	1.87	0.56
3:H:188:TRP:CE3	3:H:189:PRO:HD3	2.41	0.56
2:L:139:PHE:CE1	2:L:144:ILE:HB	2.41	0.56
1:A:239:ARG:HB2	3:H:99:GLY:O	2.05	0.55
1:A:69:ASN:O	1:A:72:ILE:HG22	2.07	0.55
3:H:56:GLY:O	3:H:58:ILE:HG13	2.07	0.55
2:L:108:ARG:HG2	2:L:109:ALA:N	2.22	0.55
2:L:13:ALA:O	2:L:106:ILE:HA	2.07	0.55
1:A:134:ALA:O	1:A:137:SER:HB3	2.07	0.54
2:L:137:ASN:HD22	2:L:174:SER:HB3	1.72	0.54
1:A:153:ILE:O	1:A:157:VAL:HG23	2.07	0.54
2:L:59:PRO:HG2	2:L:62:PHE:CD1	2.43	0.53
3:H:35:ASN:HD22	3:H:35:ASN:N	2.06	0.53
3:H:23:LYS:HG3	3:H:78:THR:HG22	1.91	0.53
2:L:52:ASN:HD22	2:L:53:ARG:N	2.07	0.53
3:H:52:TYR:HD2	3:H:55:SER:H	1.56	0.53
1:A:135:ILE:HD12	1:A:222:VAL:HG13	1.90	0.53
1:A:337:GLN:HG3	1:A:343:ARG:HB3	1.89	0.53
3:H:33:TYR:CD2	3:H:52:TYR:HB2	2.44	0.53
1:A:121:ILE:HD11	1:A:212:LEU:HB2	1.91	0.53
3:H:34:ILE:HD13	3:H:79:ALA:HB3	1.91	0.52
1:A:71:PHE:HZ	1:A:153:ILE:HD11	1.74	0.52
1:A:286:TRP:O	1:A:290:PHE:HD1	1.93	0.52
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.91	0.52
2:L:149:LYS:HG2	2:L:154:GLU:HB3	1.91	0.52
2:L:157:ASN:C	2:L:157:ASN:HD22	2.13	0.52
2:L:44:PRO:HG2	3:H:103:TRP:CG	2.45	0.52
3:H:153:THR:HG23	3:H:196:ASN:HB2	1.91	0.52
2:L:193:THR:HG23	2:L:208:SER:HB2	1.92	0.52
2:L:142:LYS:HD2	2:L:173:TYR:CE1	2.44	0.52
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.76	0.51
1:A:337:GLN:HE22	1:A:345:SER:H	1.59	0.51
3:H:124:LEU:HD21	3:H:141:LEU:HB2	1.92	0.51
2:L:181:LEU:HB3	2:L:185:GLU:HB2	1.92	0.51
1:A:121:ILE:HD13	1:A:121:ILE:O	2.10	0.51
3:H:177:LEU:HD12	3:H:178:SER:N	2.26	0.51
2:L:138:ASN:HA	2:L:172:THR:CG2	2.40	0.51
3:H:188:TRP:CH2	3:H:212:PRO:HA	2.46	0.51
3:H:61:ASN:HD21	3:H:63:ARG:NH2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:148:TRP:O	2:L:154:GLU:HB2	2.11	0.50
1:A:235:LYS:HE3	2:L:92:ASP:O	2.11	0.50
3:H:142:VAL:HG13	3:H:177:LEU:HG	1.94	0.50
3:H:137:THR:HG22	3:H:182:THR:HG23	1.93	0.50
1:A:71:PHE:CD2	1:A:154:ILE:HD11	2.43	0.50
2:L:136:LEU:HD21	2:L:146:VAL:HG11	1.92	0.50
1:A:148:ASN:HD22	1:A:149:LYS:H	1.56	0.50
3:H:188:TRP:CZ2	3:H:212:PRO:HA	2.47	0.50
2:L:96:TYR:HD1	3:H:47:TRP:CD1	2.30	0.50
2:L:113:PRO:HG2	2:L:205:ILE:HD12	1.94	0.50
2:L:144:ILE:HD13	2:L:145:ASN:N	2.27	0.49
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.93	0.49
3:H:4:LEU:HB3	3:H:22:CYS:SG	2.52	0.49
3:H:183:VAL:HG21	3:H:188:TRP:HB2	1.95	0.49
3:H:213:ARG:HG2	3:H:214:ASP:N	2.27	0.49
3:H:35:ASN:HD21	3:H:50:GLU:HG3	1.78	0.49
2:L:155:ARG:HG2	2:L:156:GLN:H	1.77	0.49
2:L:118:PHE:CG	3:H:124:LEU:HB3	2.48	0.49
1:A:135:ILE:HD11	1:A:272:LEU:HD11	1.95	0.49
2:L:160:LEU:HD21	3:H:169:VAL:HB	1.95	0.49
3:H:155:ASN:HD22	3:H:159:LEU:HD13	1.78	0.48
1:A:275:LEU:HA	1:A:278:ILE:HG22	1.94	0.48
3:H:68:ALA:HA	3:H:82:GLN:O	2.12	0.48
1:A:337:GLN:NE2	1:A:345:SER:H	2.12	0.48
1:A:204:SER:O	1:A:208:PHE:HB3	2.12	0.48
2:L:59:PRO:HG2	2:L:62:PHE:CE1	2.47	0.48
2:L:160:LEU:HD23	2:L:160:LEU:C	2.34	0.48
1:A:220:SER:O	1:A:224:GLN:HG2	2.13	0.48
2:L:148:TRP:CE2	2:L:179:LEU:HD22	2.48	0.48
2:L:157:ASN:HD22	2:L:158:GLY:N	2.11	0.48
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.95	0.48
3:H:38:ARG:HD2	3:H:46:GLU:OE2	2.14	0.48
2:L:132:VAL:HB	2:L:179:LEU:CD2	2.44	0.47
1:A:235:LYS:HB2	2:L:32:TYR:CZ	2.48	0.47
1:A:132:TYR:CE1	1:A:221:ARG:HG2	2.50	0.47
1:A:282:PHE:HD1	1:A:318:ASN:HD22	1.62	0.47
2:L:83:MET:HE3	2:L:106:ILE:HD12	1.96	0.47
2:L:159:VAL:HG12	2:L:161:ASN:HD21	1.79	0.47
3:H:40:ARG:HA	3:H:92:ALA:HB1	1.97	0.47
3:H:136:VAL:HG12	3:H:138:LEU:HD23	1.96	0.47
2:L:24:LYS:HG2	2:L:70:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:138:LEU:HD12	3:H:210:ILE:HD12	1.97	0.47
1:A:87:VAL:HB	1:A:88:PRO:HD3	1.97	0.47
2:L:8:PRO:O	2:L:102:THR:HB	2.15	0.47
2:L:136:LEU:HD11	2:L:196:ALA:HB2	1.97	0.47
3:H:76:SER:O	3:H:78:THR:HG23	2.15	0.46
2:L:4:MET:HE2	2:L:23:CYS:SG	2.55	0.46
3:H:119:PRO:CB	3:H:142:VAL:HG23	2.44	0.46
1:A:132:TYR:HE1	1:A:221:ARG:HG2	1.80	0.46
1:A:82:MET:O	1:A:87:VAL:HG23	2.15	0.46
2:L:2:ILE:HG23	2:L:97:THR:OG1	2.15	0.46
2:L:184:ASP:O	2:L:188:ARG:HG3	2.16	0.46
2:L:16:GLY:O	2:L:77:SER:HA	2.15	0.46
2:L:198:HIS:HB3	2:L:200:THR:HG22	1.98	0.46
2:L:49:TYR:CD1	2:L:50:ARG:HB2	2.50	0.46
1:A:327:CYS:O	1:A:333:ARG:HB2	2.15	0.46
3:H:71:THR:HG23	3:H:80:TYR:HB2	1.98	0.46
2:L:36:PHE:CZ	2:L:87:TYR:HB2	2.51	0.46
2:L:33:LEU:HD13	2:L:71:TYR:CD1	2.51	0.46
1:A:47:ILE:HD12	1:A:319:SER:CB	2.46	0.46
2:L:48:ILE:HG12	2:L:54:LEU:HA	1.98	0.46
1:A:240:PHE:O	1:A:241:HIS:C	2.53	0.46
2:L:29:ILE:HG22	2:L:92:ASP:CB	2.44	0.46
3:H:214:ASP:O	3:H:215:CYS:CB	2.49	0.46
3:H:151:THR:HB	3:H:198:ALA:HB3	1.98	0.46
2:L:75:ILE:HG12	2:L:75:ILE:O	2.15	0.46
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.51	0.46
2:L:108:ARG:HD2	2:L:171:SER:O	2.16	0.46
3:H:215:CYS:N	3:H:216:GLY:CA	2.80	0.45
2:L:29:ILE:HG21	2:L:90:GLN:HB2	1.98	0.45
1:A:71:PHE:CZ	1:A:153:ILE:HD11	2.52	0.45
2:L:19:VAL:HG11	2:L:104:LEU:HD11	1.98	0.45
3:H:40:ARG:HA	3:H:92:ALA:CB	2.47	0.45
3:H:148:GLU:OE1	3:H:149:PRO:HA	2.17	0.45
3:H:213:ARG:CG	3:H:214:ASP:N	2.78	0.45
3:H:125:ALA:HB1	3:H:126:PRO:HD2	1.99	0.45
3:H:160:SER:O	3:H:163:VAL:HG12	2.17	0.44
2:L:29:ILE:HA	2:L:92:ASP:OD2	2.16	0.44
2:L:2:ILE:O	2:L:2:ILE:HG12	2.16	0.44
3:H:27:TYR:CZ	3:H:98:ARG:HD2	2.52	0.44
1:A:133:PHE:O	1:A:137:SER:HB2	2.18	0.44
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:34:ILE:HD11	3:H:36:TRP:HE1	1.83	0.44
2:L:115:VAL:HG11	2:L:205:ILE:HG22	2.00	0.44
1:A:47:ILE:HD12	1:A:319:SER:HB3	2.00	0.44
1:A:241:HIS:HB2	3:H:32:TYR:CE1	2.54	0.43
1:A:137:SER:OG	1:A:138:PRO:HD2	2.18	0.43
2:L:44:PRO:HG2	3:H:103:TRP:CE3	2.53	0.43
3:H:52:TYR:HA	3:H:53:PRO:HD2	1.84	0.43
2:L:115:VAL:HG13	2:L:207:LYS:HG2	2.01	0.43
3:H:51:ILE:C	3:H:51:ILE:HD13	2.39	0.43
1:A:132:TYR:O	1:A:136:THR:HG22	2.19	0.43
2:L:149:LYS:HG2	2:L:154:GLU:CB	2.49	0.43
2:L:47:LEU:HA	2:L:58:VAL:HG21	2.01	0.43
3:H:142:VAL:O	3:H:142:VAL:HG22	2.19	0.42
2:L:52:ASN:HD21	2:L:53:ARG:HH11	1.66	0.42
1:A:82:MET:HG2	1:A:86:VAL:HB	2.00	0.42
3:H:38:ARG:CZ	3:H:64:PHE:HE2	2.32	0.42
2:L:136:LEU:N	2:L:136:LEU:HD22	2.35	0.42
3:H:155:ASN:ND2	3:H:159:LEU:HD13	2.34	0.42
1:A:44:VAL:O	1:A:48:VAL:HG23	2.20	0.42
1:A:205:ILE:O	1:A:210:VAL:HG23	2.20	0.42
2:L:19:VAL:HG21	2:L:104:LEU:HD11	2.02	0.42
3:H:37:VAL:CG1	3:H:45:PHE:HB3	2.50	0.42
1:A:267:LYS:O	1:A:267:LYS:HD3	2.20	0.42
1:A:154:ILE:HD13	1:A:154:ILE:HA	1.94	0.41
3:H:147:PRO:HD2	3:H:201:ALA:HB1	2.02	0.41
3:H:41:THR:O	3:H:41:THR:HG23	2.20	0.41
2:L:132:VAL:HB	2:L:179:LEU:HD21	2.02	0.41
3:H:51:ILE:HD12	3:H:72:ALA:HB2	2.01	0.41
2:L:210:ASN:HB3	2:L:213:GLU:HG2	2.02	0.41
3:H:110:THR:HG21	3:H:147:PRO:CB	2.50	0.41
2:L:175:MET:HG2	2:L:176:SER:N	2.35	0.41
1:A:61:PHE:HE1	1:A:339:LEU:HD21	1.86	0.41
3:H:83:LEU:HA	3:H:83:LEU:HD12	1.85	0.41
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.55	0.41
1:A:149:LYS:HA	1:A:152:VAL:HG22	2.02	0.41
2:L:37:GLN:HB2	2:L:47:LEU:HD21	2.03	0.41
2:L:137:ASN:ND2	2:L:174:SER:HB3	2.34	0.41
3:H:144:GLY:C	3:H:174:LEU:HD12	2.41	0.41
3:H:7:SER:HB2	3:H:107:THR:HG23	2.02	0.41
1:A:266:LEU:HD11	3:H:57:ASN:CG	2.42	0.40
2:L:139:PHE:CD2	2:L:173:TYR:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:160:LEU:HD12	3:H:171:GLN:HB2	2.03	0.40
1:A:336:PHE:O	1:A:340:LEU:HG	2.21	0.40
1:A:270:LYS:HA	1:A:270:LYS:HD3	1.82	0.40
2:L:115:VAL:HA	2:L:135:PHE:O	2.20	0.40
3:H:10:GLU:O	3:H:109:LEU:HD12	2.21	0.40
1:A:75:LEU:HD21	1:A:124:LEU:HD22	2.03	0.40
2:L:142:LYS:HB2	2:L:173:TYR:CE2	2.56	0.40
2:L:159:VAL:HG12	2:L:161:ASN:ND2	2.36	0.40
3:H:154:TRP:CZ3	3:H:195:CYS:HB3	2.56	0.40
3:H:3:GLN:HA	3:H:102:TYR:CE2	2.57	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	210/366 (57%)	190 (90%)	15 (7%)	5 (2%)	7 44
2	L	212/214 (99%)	190 (90%)	21 (10%)	1 (0%)	34 75
3	H	215/217 (99%)	184 (86%)	27 (13%)	4 (2%)	10 49
All	All	637/797 (80%)	564 (88%)	63 (10%)	10 (2%)	12 53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	215	CYS
3	H	212	PRO
1	A	329	SER
1	A	343	ARG
3	H	127	GLY
1	A	241	HIS
1	A	330	PRO

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Mol	Chain	Res	Type
1	A	138	PRO
2	L	2	ILE
3	H	149	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/317 (53%)	160 (95%)	9 (5%)	28	67
2	L	191/191 (100%)	178 (93%)	13 (7%)	20	60
3	H	183/183 (100%)	171 (93%)	12 (7%)	21	61
All	All	543/691 (79%)	509 (94%)	34 (6%)	22	62

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ILE
1	A	70	TYR
1	A	75	LEU
1	A	121	ILE
1	A	148	ASN
1	A	237	GLU
1	A	239	ARG
1	A	312	ASN
1	A	342	LEU
2	L	19	VAL
2	L	38	GLN
2	L	47	LEU
2	L	50	ARG
2	L	52	ASN
2	L	75	ILE
2	L	102	THR
2	L	144	ILE
2	L	145	ASN
2	L	154	GLU

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Mol	Chain	Res	Type
2	L	157	ASN
2	L	169	LYS
2	L	182	THR
3	H	34	ILE
3	H	35	ASN
3	H	51	ILE
3	H	97	VAL
3	H	110	THR
3	H	124	LEU
3	H	137	THR
3	H	138	LEU
3	H	142	VAL
3	H	177	LEU
3	H	196	ASN
3	H	217	CYS

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

Mol	Chain	Res	Type
1	A	148	ASN
1	A	231	GLN
1	A	312	ASN
1	A	318	ASN
1	A	337	GLN
2	L	30	ASN
2	L	38	GLN
2	L	52	ASN
2	L	137	ASN
2	L	145	ASN
2	L	157	ASN
2	L	161	ASN
2	L	198	HIS
3	H	35	ASN
3	H	133	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	SO4	A	1001	-	4,4,4	0.23	0	6,6,6	0.07	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	SO4	A	1001	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	222/366 (60%)	0.72	33 (14%) 3 3	82, 220, 283, 334	0
2	L	214/214 (100%)	0.12	1 (0%) 91 89	65, 102, 149, 268	0
3	H	217/217 (100%)	0.12	3 (1%) 78 73	65, 104, 181, 282	0
All	All	653/797 (81%)	0.32	37 (5%) 27 25	65, 120, 264, 334	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	PHE	5.6
1	A	109	TRP	5.4
1	A	308	TYR	4.3
1	A	313	TRP	4.1
1	A	339	LEU	3.9
1	A	307	VAL	3.6
1	A	89	PHE	3.4
1	A	272	LEU	3.4
1	A	36	MET	3.2
1	A	87	VAL	3.1
1	A	144	LEU	3.1
1	A	128	ALA	3.0
1	A	37	GLY	3.0
1	A	337	GLN	2.9
1	A	124	LEU	2.7
1	A	316	TYR	2.7
1	A	68	THR	2.7
1	A	67	VAL	2.7
1	A	59	ALA	2.7
1	A	281	THR	2.6
1	A	85	ALA	2.6
1	A	322	ASN	2.6
1	A	86	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	58	ILE	2.5
3	H	72	ALA	2.4
1	A	280	GLY	2.4
1	A	146	THR	2.4
1	A	72	ILE	2.4
1	A	283	THR	2.3
1	A	69	ASN	2.3
3	H	100	PHE	2.3
1	A	145	LEU	2.3
1	A	35	GLY	2.2
3	H	74	LYS	2.2
1	A	315	GLY	2.1
1	A	345	SER	2.1
2	L	89	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	1001	5/5	0.84	0.22	-2.29	153,154,163,167	0

6.5 Other polymers (i)

There are no such residues in this entry.