Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:46 PM GMT

PDB ID	:	1YNK
Title	:	Identification of Key residues of the NC6.8 Fab antibody fragment binding to synthetic sweeteners: Crystal structure of NC6.8 co-crystalized with high potency sweetener compound SC45647
Authors	:	Gokulan, K.; Khare, S.; Ronning, D.R.; Linthicum, S.D.; Sacchettini, J.C.; Rupp, B.
Deposited on	:	2005-01-24
Resolution	:	2.10 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:

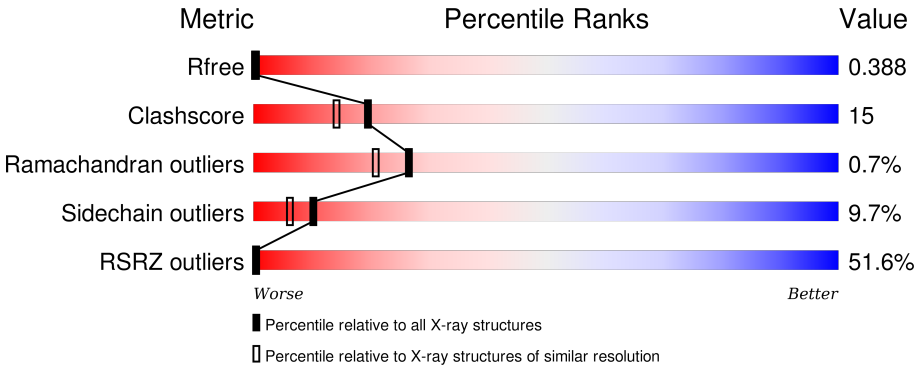
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	L	219	48% 63% 28% 8%
2	H	219	55% 71% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SC5	H	501	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3495 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.

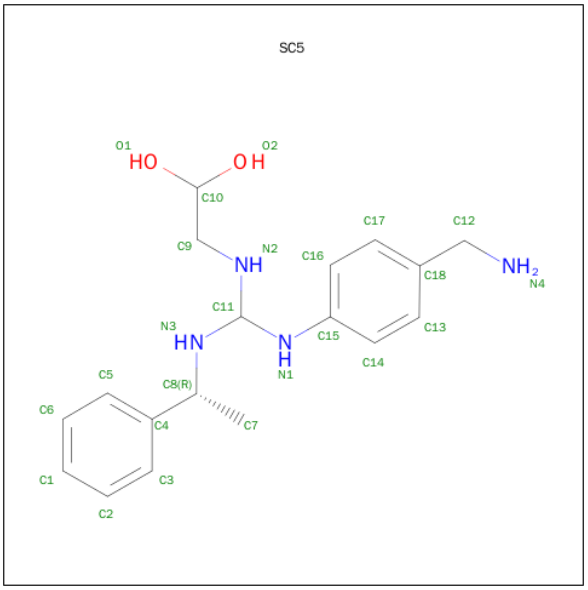
- Molecule 1 is a protein called immunoglobulin kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1696	1059	291	339	7			

- Molecule 2 is a protein called Ig gamma heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	2	0
			1649	1037	268	335	9			

- Molecule 3 is 2-[((R)-{[4-(AMINOMETHYL)PHENYL]AMINO}{[(1R)-1-PHENYLETHYL]AMINO}METHYL)AMINO]ETHANE-1,1-DIOL (three-letter code: SC5) (formula: $C_{18}H_{26}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			24	18	4	2		

- Molecule 4 is water.

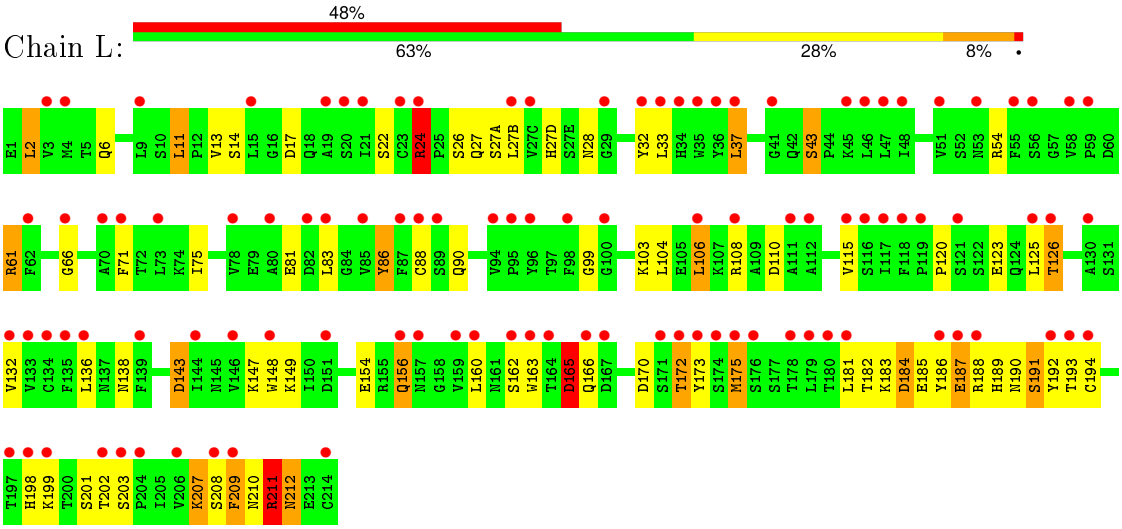
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	67	Total O 67 67	0	0
4	L	59	Total O 59 59	0	0

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.

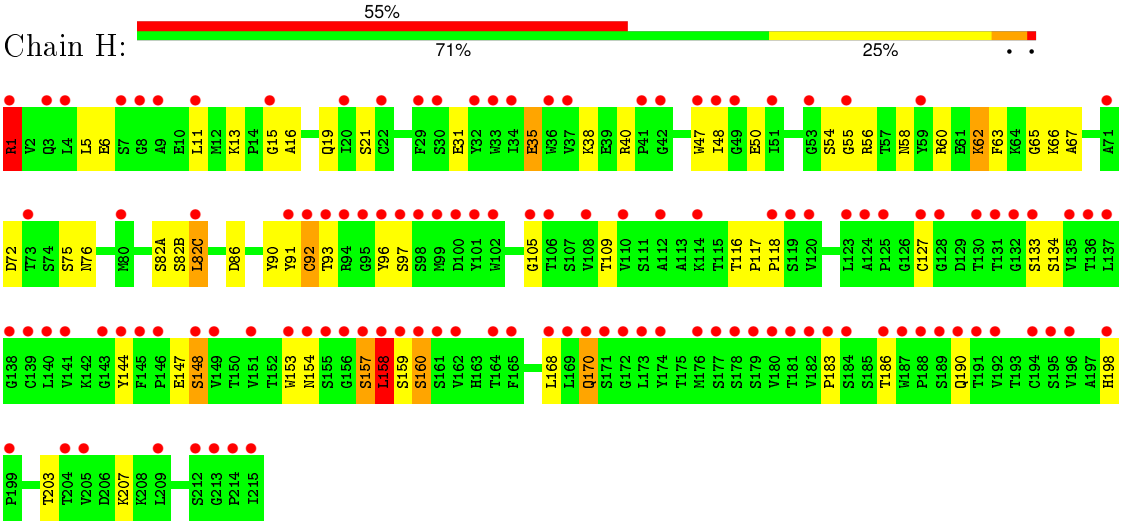
- Molecule 1: immunoglobulin kappa light chain

Chain L:



- Molecule 2: Ig gamma heavy chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	135.60Å 48.19Å 75.35Å 90.00° 109.04° 90.00°	Depositor
Resolution (Å)	23.64 – 2.10 24.09 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.7 (23.64-2.10) 91.5 (24.09-2.10)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.277 0.378 , 0.388	Depositor DCC
R_{free} test set	1246 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 24844 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	3495	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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: SC5

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	L	1.31	4/1736 (0.2%)	1.15	7/2355 (0.3%)
2	H	1.33	4/1704 (0.2%)	1.14	5/2325 (0.2%)
All	All	1.32	8/3440 (0.2%)	1.15	12/4680 (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	H	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	194	CYS	CB-SG	-6.57	1.71	1.82
1	L	88	CYS	CB-SG	-6.57	1.71	1.82
1	L	209	PHE	CE2-CZ	5.96	1.48	1.37
1	L	86	TYR	CD1-CE1	-5.49	1.31	1.39
2	H	92	CYS	C-O	5.35	1.33	1.23
2	H	127	CYS	CB-SG	-5.24	1.73	1.81
2	H	35	GLU	C-O	5.06	1.32	1.23
2	H	67	ALA	CA-CB	-5.05	1.41	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	2	LEU	CB-CG-CD1	-8.16	97.12	111.00
2	H	62	LYS	CD-CE-NZ	-7.55	94.34	111.70
2	H	158	LEU	CA-CB-CG	7.02	131.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	40	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	L	61	ARG	NE-CZ-NH1	-6.35	117.12	120.30
2	H	1	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	L	24	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	L	211	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	L	24	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	L	37	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	L	165	ASP	CB-CG-OD2	-5.56	113.30	118.30
2	H	47	TRP	CA-CB-CG	5.13	123.45	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	54	SER	Peptide

5.2 Too-close contacts (i)

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	L	1696	0	1637	61	1
2	H	1649	0	1590	45	2
3	H	24	0	17	2	0
4	H	67	0	0	1	0
4	L	59	0	0	0	1
All	All	3495	0	3244	99	4

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 15.

All (99) 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:H:1:ARG:H3	2:H:1:ARG:HD2	1.11	1.14
2:H:1:ARG:CD	2:H:1:ARG:H3	1.73	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:ARG:N	2:H:1:ARG:CD	2.26	0.95
1:L:32:TYR:CE1	2:H:97:SER:HB2	2.02	0.94
2:H:198:HIS:HB3	2:H:203:THR:CG2	2.00	0.91
1:L:27(D):HIS:HD2	1:L:28:ASN:H	1.25	0.84
2:H:159:SER:N	2:H:160:SER:HA	1.98	0.77
1:L:32:TYR:HE1	2:H:97:SER:HB2	1.49	0.77
2:H:1:ARG:N	2:H:1:ARG:HD2	1.83	0.77
1:L:27(D):HIS:CD2	1:L:28:ASN:H	2.04	0.75
1:L:182:THR:OG1	1:L:185:GLU:HG3	1.89	0.72
2:H:60:ARG:HD3	2:H:62:LYS:HD3	1.72	0.70
1:L:138:ASN:HD22	1:L:172:THR:HG21	1.56	0.70
1:L:138:ASN:HA	1:L:172:THR:HG23	1.74	0.69
1:L:110:ASP:OD2	1:L:199:LYS:HD3	1.91	0.69
2:H:198:HIS:HB3	2:H:203:THR:HG22	1.74	0.68
1:L:170:ASP:OD1	1:L:172:THR:HB	1.94	0.68
1:L:138:ASN:HA	1:L:172:THR:CG2	2.24	0.68
1:L:147:LYS:HG3	1:L:154:GLU:HG3	1.76	0.68
2:H:96:TYR:O	3:H:501:SC5:H8	1.93	0.67
2:H:198:HIS:HB3	2:H:203:THR:HG23	1.76	0.67
1:L:24:ARG:HG3	1:L:24:ARG:HH11	1.60	0.67
1:L:43:SER:HB2	2:H:91:TYR:CE1	2.31	0.66
1:L:27(B):LEU:CD1	1:L:33:LEU:HD23	2.25	0.66
1:L:187:GLU:HG3	1:L:211:ARG:HH21	1.61	0.65
2:H:1:ARG:NE	2:H:1:ARG:N	2.46	0.64
2:H:35:GLU:O	2:H:92:CYS:HA	1.99	0.63
2:H:117:PRO:HB3	2:H:203:THR:HG21	1.80	0.61
2:H:158:LEU:C	2:H:160:SER:HA	2.22	0.60
1:L:103:LYS:NZ	1:L:165:ASP:OD1	2.34	0.60
1:L:125:LEU:O	1:L:183:LYS:HD2	2.00	0.60
2:H:170:GLN:HE21	2:H:170:GLN:HA	1.65	0.60
1:L:184:ASP:O	1:L:188:ARG:HG3	2.03	0.59
1:L:190:ASN:HD21	1:L:212:ASN:ND2	2.01	0.58
1:L:11:LEU:HB3	1:L:104:LEU:HD12	1.86	0.58
1:L:189:HIS:O	1:L:211:ARG:HD3	2.04	0.57
2:H:50:GLU:OE2	2:H:58:ASN:ND2	2.34	0.56
1:L:32:TYR:CE2	3:H:501:SC5:H6	2.41	0.56
1:L:162:SER:HB2	2:H:168:LEU:HD13	1.88	0.56
2:H:72:ASP:HB3	2:H:75:SER:OG	2.05	0.55
1:L:170:ASP:CG	1:L:172:THR:HB	2.27	0.54
1:L:32:TYR:CD1	2:H:97:SER:HB2	2.42	0.54
1:L:83:LEU:HD21	1:L:106:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:201:SER:OG	1:L:203:SER:O	2.22	0.53
1:L:27(B):LEU:HD11	1:L:33:LEU:HD23	1.90	0.53
2:H:16:ALA:O	2:H:82(C):LEU:HD22	2.08	0.53
1:L:138:ASN:ND2	1:L:172:THR:HG21	2.24	0.52
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.91	0.52
1:L:166:GLN:HB2	1:L:173:TYR:OH	2.09	0.52
2:H:1:ARG:NE	2:H:1:ARG:H1	2.08	0.51
1:L:115:VAL:O	1:L:207:LYS:HD2	2.10	0.51
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.92	0.50
1:L:147:LYS:HD3	1:L:149:LYS:HE3	1.94	0.49
2:H:1:ARG:NE	2:H:1:ARG:H3	2.07	0.48
1:L:43:SER:HB2	2:H:91:TYR:HE1	1.78	0.48
2:H:170:GLN:NE2	2:H:170:GLN:HA	2.29	0.48
2:H:147:GLU:HA	2:H:148:SER:HA	1.60	0.48
2:H:19:GLN:HG3	4:H:546:HOH:O	2.13	0.48
1:L:37:LEU:HD13	1:L:86:TYR:CZ	2.48	0.48
1:L:163:TRP:CZ2	1:L:175:MET:HE2	2.49	0.48
2:H:50:GLU:HG2	2:H:58:ASN:HB2	1.97	0.46
2:H:118:PRO:HB3	2:H:144:TYR:HB3	1.98	0.46
1:L:108:ARG:HD2	1:L:170:ASP:O	2.16	0.46
1:L:6:GLN:OE1	1:L:99:GLY:HA3	2.16	0.45
2:H:48:ILE:HG23	2:H:63:PHE:CG	2.51	0.45
1:L:2:LEU:HA	1:L:2:LEU:HD13	1.64	0.45
1:L:166:GLN:HB2	1:L:173:TYR:CZ	2.52	0.45
1:L:138:ASN:HA	1:L:172:THR:HG21	1.99	0.45
2:H:66:LYS:NZ	2:H:86:ASP:OD2	2.46	0.45
1:L:191:SER:HB2	1:L:210:ASN:OD1	2.17	0.45
1:L:187:GLU:HG3	1:L:211:ARG:NH2	2.30	0.44
2:H:153:TRP:HB2	2:H:157:SER:HB3	1.99	0.44
2:H:1:ARG:H1	2:H:1:ARG:CD	2.21	0.44
1:L:190:ASN:ND2	1:L:210:ASN:HB3	2.33	0.44
1:L:14:SER:O	1:L:17:ASP:HB2	2.18	0.44
2:H:90:TYR:O	2:H:105:GLY:HA2	2.18	0.43
1:L:123:GLU:N	1:L:123:GLU:OE1	2.35	0.43
1:L:183:LYS:O	1:L:187:GLU:HB2	2.17	0.43
1:L:32:TYR:O	1:L:90:GLN:HA	2.18	0.43
2:H:117:PRO:CB	2:H:203:THR:HG21	2.47	0.43
1:L:136:LEU:N	1:L:136:LEU:HD12	2.34	0.43
1:L:181:LEU:HB3	1:L:185:GLU:HB2	2.01	0.43
2:H:134:SER:HA	2:H:183:PRO:HA	2.01	0.42
2:H:6:GLU:HA	2:H:21:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:ARG:HG2	1:L:61:ARG:HH11	1.84	0.42
1:L:143:ASP:O	1:L:198:HIS:HD2	2.02	0.41
1:L:192:TYR:HB2	1:L:209:PHE:CZ	2.55	0.41
2:H:183:PRO:O	2:H:186:THR:OG1	2.37	0.41
1:L:61:ARG:O	1:L:75:ILE:HA	2.21	0.41
2:H:11:LEU:HD23	2:H:109:THR:HB	2.01	0.41
1:L:160:LEU:HD11	2:H:170:GLN:HG2	2.02	0.41
1:L:66:GLY:HA3	1:L:71:PHE:HA	2.03	0.41
2:H:116:THR:HA	2:H:117:PRO:HD2	1.93	0.41
1:L:81:GLU:CD	1:L:81:GLU:H	2.24	0.41
1:L:24:ARG:CG	1:L:24:ARG:HH11	2.31	0.41
1:L:148:TRP:HA	1:L:193:THR:O	2.21	0.40
1:L:126:THR:CG2	1:L:126:THR:O	2.69	0.40
1:L:186:TYR:OH	1:L:211:ARG:HG3	2.22	0.40

All (4) 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)
2:H:82(A):SER:OG	2:H:82(B):SER:OG[2_556]	1.54	0.66
4:L:243:HOH:O	4:L:264:HOH:O[2_556]	2.06	0.14
2:H:15:GLY:N	2:H:65:GLY:CA[2_556]	2.10	0.10
1:L:26:SER:O	1:L:156:GLN:CG[2_556]	2.18	0.02

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	L	217/219 (99%)	211 (97%)	5 (2%)	1 (0%)	34	30
2	H	219/219 (100%)	207 (94%)	10 (5%)	2 (1%)	21	15
All	All	436/438 (100%)	418 (96%)	15 (3%)	3 (1%)	26	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	154	ASN
2	H	55	GLY
1	L	126	THR

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	L	195/195 (100%)	173 (89%)	22 (11%)	7 4
2	H	188/186 (101%)	172 (92%)	16 (8%)	13 9
All	All	383/381 (100%)	345 (90%)	38 (10%)	10 6

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	L	13	VAL
1	L	22	SER
1	L	24	ARG
1	L	27	GLN
1	L	27(A)	SER
1	L	43	SER
1	L	54	ARG
1	L	106	LEU
1	L	143	ASP
1	L	156	GLN
1	L	165	ASP
1	L	172	THR
1	L	175	MET
1	L	184	ASP
1	L	187	GLU
1	L	191	SER
1	L	202	THR
1	L	207	LYS
1	L	208	SER

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Mol	Chain	Res	Type
1	L	211	ARG
1	L	212	ASN
2	H	1	ARG
2	H	5	LEU
2	H	13	LYS
2	H	56[A]	ARG
2	H	56[B]	ARG
2	H	76	ASN
2	H	82(C)	LEU
2	H	93	THR
2	H	133	SER
2	H	148	SER
2	H	157	SER
2	H	158	LEU
2	H	160	SER
2	H	170	GLN
2	H	190	GLN
2	H	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27(D)	HIS
1	L	138	ASN
1	L	212	ASN
2	H	3	GLN
2	H	170	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
3	SC5	H	501	-	20,25,25	2.05	9 (45%)	26,32,32	3.06	5 (19%)

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	SC5	H	501	-	1/1/3/6	0/13/19/19	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	SC5	C12-C18	-3.03	1.41	1.51
3	H	501	SC5	C11-N1	-2.16	1.30	1.41
3	H	501	SC5	C12-N4	-2.03	1.16	1.39
3	H	501	SC5	C14-C13	2.01	1.42	1.38
3	H	501	SC5	C5-C4	2.38	1.42	1.39
3	H	501	SC5	C15-N1	2.53	1.44	1.39
3	H	501	SC5	C14-C15	2.61	1.43	1.39
3	H	501	SC5	C16-C15	3.11	1.44	1.39
3	H	501	SC5	C3-C4	3.35	1.44	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	501	SC5	C9-N2-C11	2.86	124.68	114.85
3	H	501	SC5	N3-C11-N2	4.10	116.13	109.75
3	H	501	SC5	N3-C11-N1	7.81	121.91	109.75
3	H	501	SC5	N2-C11-N1	7.82	121.93	109.75
3	H	501	SC5	C11-N3-C8	9.41	132.95	116.74

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	501	SC5	C11

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	501	SC5	2	0

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, 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	L	219/219 (100%)	2.15	105 (47%)	0	0	21, 34, 47, 50	0
2	H	219/219 (100%)	2.36	121 (55%)	0	0	19, 33, 53, 71	0
All	All	438/438 (100%)	2.25	226 (51%)	0	0	19, 34, 49, 71	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	158	LEU	13.8
2	H	155	SER	8.3
2	H	215	ILE	7.8
2	H	160	SER	7.3
2	H	159	SER	6.6
2	H	42	GLY	6.5
2	H	157	SER	6.1
1	L	87	PHE	5.8
1	L	133	VAL	5.4
1	L	173	TYR	5.4
1	L	125	LEU	5.3
2	H	7	SER	5.0
1	L	148	TRP	5.0
1	L	35	TRP	5.0
2	H	55	GLY	4.9
1	L	135	PHE	4.8
1	L	146	VAL	4.8
1	L	88	CYS	4.8
2	H	22	CYS	4.8
1	L	36	TYR	4.7
2	H	143	GLY	4.7
1	L	188	ARG	4.6
2	H	173	LEU	4.5
2	H	144	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	L	115	VAL	4.4
2	H	168	LEU	4.4
2	H	171	SER	4.4
2	H	47	TRP	4.3
1	L	37	LEU	4.3
1	L	9	LEU	4.3
1	L	33	LEU	4.2
1	L	179	LEU	4.2
1	L	55	PHE	4.2
2	H	169	LEU	4.2
1	L	157	ASN	4.2
2	H	120	VAL	4.0
2	H	199	PRO	4.0
1	L	85	VAL	4.0
1	L	117	ILE	4.0
2	H	180	VAL	4.0
2	H	194	CYS	4.0
2	H	161	SER	3.9
1	L	204	PRO	3.9
1	L	206	VAL	3.9
2	H	98	SER	3.9
1	L	126	THR	3.9
2	H	53	GLY	3.9
2	H	93	THR	3.8
2	H	102	TRP	3.8
2	H	164	THR	3.8
1	L	98	PHE	3.8
1	L	82	ASP	3.8
1	L	106	LEU	3.8
2	H	123	LEU	3.8
2	H	132	GLY	3.8
1	L	59	PRO	3.7
2	H	41	PRO	3.7
2	H	135	VAL	3.7
1	L	139	PHE	3.6
1	L	71	PHE	3.6
2	H	191	THR	3.5
1	L	48	ILE	3.5
1	L	89	SER	3.5
2	H	37	VAL	3.5
1	L	15	LEU	3.5
1	L	73	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	15	GLY	3.5
2	H	187	TRP	3.4
1	L	151	ASP	3.4
2	H	189	SER	3.4
1	L	181	LEU	3.4
2	H	29	PHE	3.4
2	H	165	PHE	3.4
2	H	156	GLY	3.4
2	H	141	VAL	3.3
2	H	188	PRO	3.3
1	L	172	THR	3.3
2	H	71	ALA	3.3
1	L	175	MET	3.3
2	H	145	PHE	3.3
2	H	149	VAL	3.3
1	L	178	THR	3.2
1	L	32	TYR	3.2
1	L	23	CYS	3.2
1	L	94	VAL	3.2
2	H	138	GLY	3.2
2	H	96	TYR	3.2
1	L	58	VAL	3.2
2	H	48	ILE	3.2
1	L	96	TYR	3.2
1	L	130	ALA	3.1
2	H	148	SER	3.1
1	L	209	PHE	3.1
1	L	51	VAL	3.1
1	L	78	VAL	3.1
2	H	204	THR	3.1
2	H	95	GLY	3.1
1	L	116	SER	3.1
2	H	162	VAL	3.0
1	L	163	TRP	3.0
2	H	195	SER	3.0
1	L	134	CYS	3.0
2	H	30	SER	3.0
2	H	205	VAL	3.0
1	L	193	THR	3.0
2	H	105	GLY	3.0
1	L	198	HIS	3.0
1	L	29	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	118	PRO	3.0
1	L	47	LEU	3.0
1	L	27(B)	LEU	3.0
2	H	183	PRO	2.9
1	L	27(C)	VAL	2.9
1	L	24	ARG	2.9
1	L	112	ALA	2.9
2	H	182	VAL	2.9
1	L	46	LEU	2.9
2	H	11	LEU	2.9
2	H	73	THR	2.9
2	H	94	ARG	2.9
1	L	34	HIS	2.9
2	H	100	ASP	2.9
2	H	106	THR	2.9
2	H	192	VAL	2.9
2	H	9	ALA	2.9
2	H	153	TRP	2.9
2	H	1	ARG	2.8
1	L	160	LEU	2.8
2	H	108	VAL	2.8
2	H	91	TYR	2.8
2	H	112	ALA	2.8
1	L	132	VAL	2.8
2	H	196	VAL	2.8
2	H	174	TYR	2.8
1	L	66	GLY	2.8
2	H	80	MET	2.7
2	H	99	MET	2.7
1	L	192	TYR	2.7
2	H	32	TYR	2.7
1	L	3	VAL	2.7
1	L	166	GLN	2.7
1	L	194	CYS	2.7
1	L	83	LEU	2.7
2	H	101	TYR	2.7
2	H	179	SER	2.7
1	L	100	GLY	2.7
1	L	121	SER	2.7
2	H	8	GLY	2.7
2	H	140	LEU	2.6
1	L	167	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	19	ALA	2.6
2	H	136	THR	2.6
2	H	114	LYS	2.6
1	L	202	THR	2.6
2	H	33	TRP	2.6
2	H	4	LEU	2.6
2	H	137	LEU	2.6
2	H	130	THR	2.6
2	H	176	MET	2.6
2	H	82(C)	LEU	2.6
2	H	97	SER	2.5
1	L	95	PRO	2.5
2	H	127	CYS	2.5
1	L	80	ALA	2.5
1	L	176	SER	2.5
2	H	170	GLN	2.5
1	L	136	LEU	2.5
2	H	190	GLN	2.5
2	H	128	GLY	2.5
2	H	146	PRO	2.5
1	L	171	SER	2.5
1	L	111	ALA	2.5
1	L	186	TYR	2.5
1	L	144	ILE	2.5
2	H	154	ASN	2.4
2	H	198	HIS	2.4
2	H	139	CYS	2.4
2	H	36	TRP	2.4
2	H	184	SER	2.4
1	L	53	ASN	2.4
2	H	186	THR	2.4
2	H	212	SER	2.4
2	H	3	GLN	2.4
1	L	214	CYS	2.4
1	L	41	GLY	2.4
2	H	151	VAL	2.4
1	L	119	PRO	2.4
1	L	174	SER	2.4
2	H	213	GLY	2.4
2	H	178	SER	2.4
2	H	34	ILE	2.3
1	L	187	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	199	LYS	2.3
1	L	4	MET	2.3
1	L	118	PHE	2.3
1	L	180	THR	2.3
2	H	172	GLY	2.3
2	H	209	LEU	2.3
2	H	214	PRO	2.3
2	H	20	ILE	2.3
1	L	62	PHE	2.2
2	H	125	PRO	2.2
1	L	45	LYS	2.2
1	L	21	ILE	2.2
1	L	203	SER	2.2
1	L	108	ARG	2.2
1	L	56	SER	2.2
1	L	208	SER	2.2
1	L	159	VAL	2.2
1	L	164	THR	2.2
2	H	131	THR	2.1
2	H	59	TYR	2.1
1	L	162	SER	2.1
2	H	177	SER	2.1
2	H	92	CYS	2.1
2	H	110	VAL	2.1
1	L	20	SER	2.1
2	H	133	SER	2.1
1	L	156	GLN	2.1
2	H	124	ALA	2.1
2	H	119	SER	2.1
1	L	197	THR	2.0
2	H	49	GLY	2.0
2	H	51	ILE	2.0
1	L	70	ALA	2.0
2	H	181	THR	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
3	SC5	H	501	24/24	0.65	0.29	0.95	32,34,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.