



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 01:43 AM EDT

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-crystallized with high potency sweetener compound SC45647
Authors : Gokulan, K.; Khare, S.; Ronning, D.R.; Linthicum, S.D.; Sacchettini, J.C.; Rupp, B.
Deposited on : unknown
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

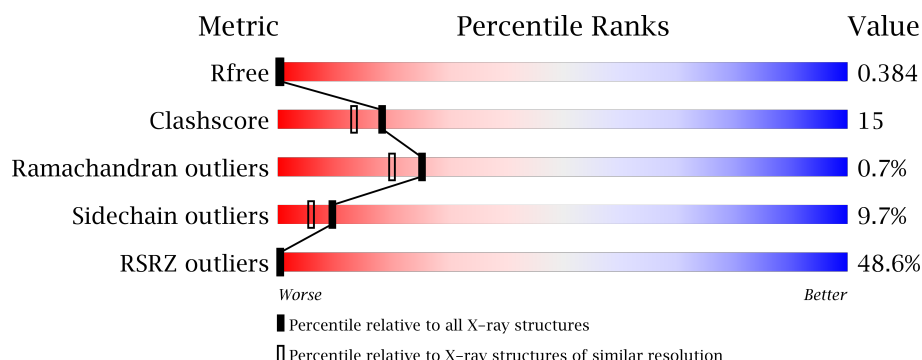
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 $\leq 5\%$. 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	L	219	<div> <div>46%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>8%</div> <div>.</div> </div> </div>
2	H	219	<div> <div>51%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> <div>.</div> </div> </div>

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 [i](#)

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.

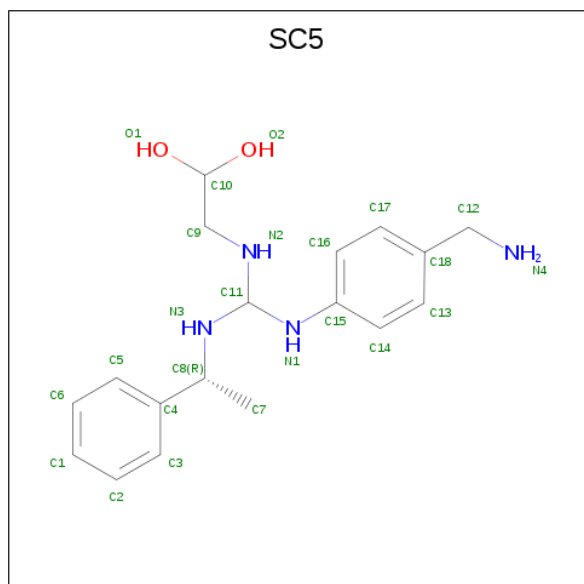
- Molecule 1 is a protein called immunoglobulin kappa light chain.

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: C₁₈H₂₆N₄O₂).



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

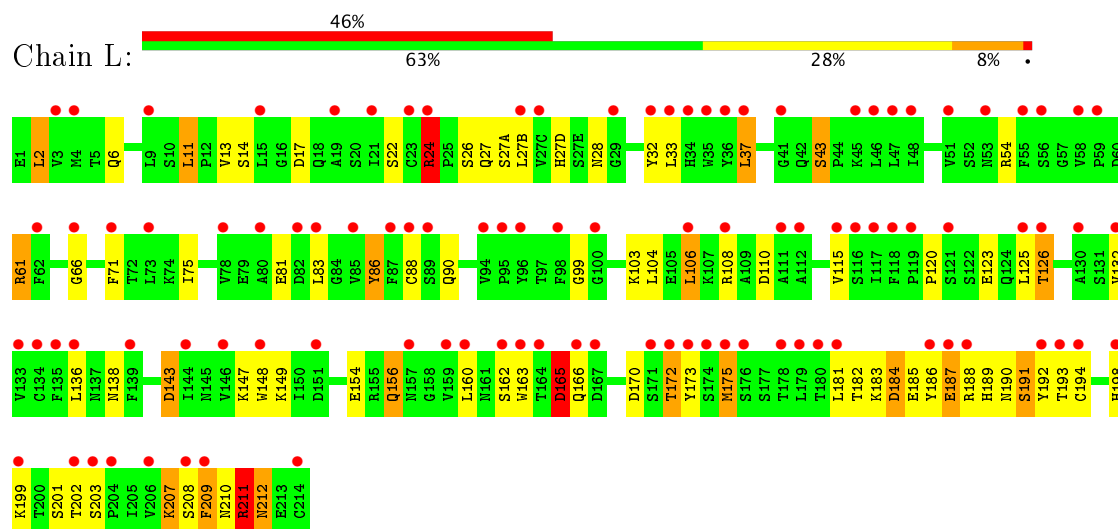
- Molecule 4 is water.

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

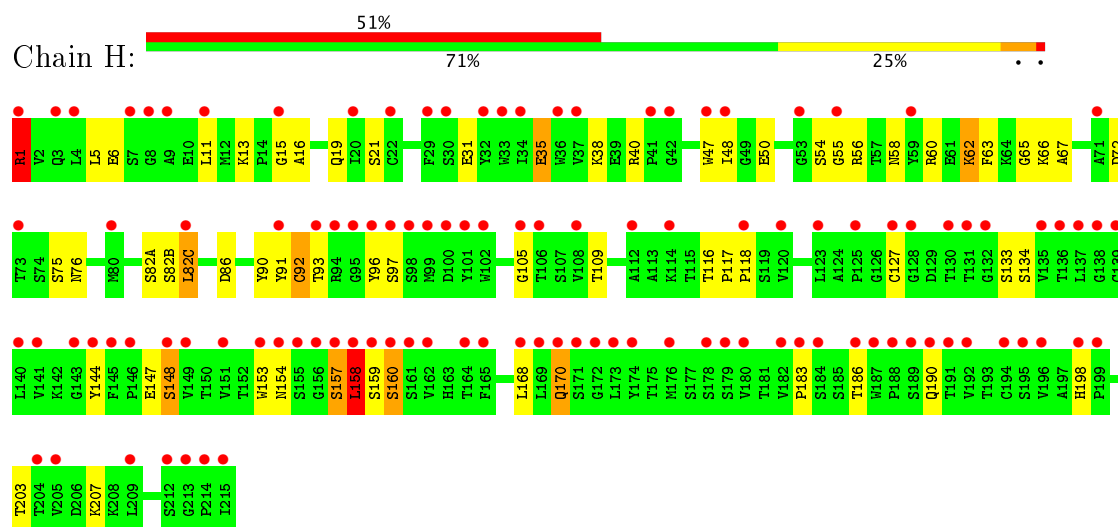
3 Residue-property plots [i](#)

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



- Molecule 2: Ig gamma heavy chain



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.213 , 0.277 0.375 , 0.384	Depositor DCC
R_{free} test set	1246 reflections (5.02%)	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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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: 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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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:H3	2:H:1:ARG:CD	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:163:TRP:CZ2	1:L:175:MET:HE2	2.49	0.48
1:L:37:LEU:HD13	1:L:86:TYR:CZ	2.48	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
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:32:TYR:O	1:L:90:GLN:HA	2.18	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:11:LEU:HD23	2:H:109:THR:HB	2.01	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
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:126:THR:CG2	1:L:126:THR:O	2.69	0.40
1:L:148:TRP:HA	1:L:193:THR:O	2.21	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%)	32	28
2	H	219/219 (100%)	207 (94%)	10 (5%)	2 (1%)	20	14
All	All	436/438 (100%)	418 (96%)	15 (3%)	3 (1%)	25	20

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	3
2	H	188/186 (101%)	172 (92%)	16 (8%)	12	8
All	All	383/381 (100%)	345 (90%)	38 (10%)	9	5

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 ⓘ

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	-	22,25,25	2.42	9 (40%)	29,32,32	3.78	6 (20%)

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	0/15/19/19	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	O1-C10	-6.73	1.24	1.40
3	H	501	SC5	C12-C18	-3.04	1.41	1.51
3	H	501	SC5	C12-N4	-2.24	1.16	1.40
3	H	501	SC5	C14-C13	2.02	1.42	1.38
3	H	501	SC5	C5-C4	2.40	1.42	1.39
3	H	501	SC5	C14-C15	2.53	1.43	1.39
3	H	501	SC5	C15-N1	2.55	1.44	1.39
3	H	501	SC5	C16-C15	3.02	1.44	1.39
3	H	501	SC5	C3-C4	3.39	1.44	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	501	SC5	N3-C11-N2	4.10	116.13	109.75
3	H	501	SC5	O1-C10-C9	7.21	123.91	109.63
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	501	SC5	C18-C12-N4	11.25	179.61	115.47

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, 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	L	219/219 (100%)	2.02	101 (46%) 0 0	21, 34, 47, 50	0
2	H	219/219 (100%)	2.23	112 (51%) 0 0	19, 33, 53, 71	0
All	All	438/438 (100%)	2.13	213 (48%) 0 0	19, 34, 49, 71	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	158	LEU	13.2
2	H	155	SER	8.0
2	H	215	ILE	7.4
2	H	160	SER	7.1
2	H	159	SER	6.4
2	H	42	GLY	6.2
2	H	157	SER	5.9
1	L	87	PHE	5.6
1	L	173	TYR	5.2
1	L	125	LEU	5.1
1	L	133	VAL	5.1
2	H	7	SER	4.8
1	L	35	TRP	4.7
1	L	148	TRP	4.7
2	H	55	GLY	4.6
1	L	135	PHE	4.6
1	L	88	CYS	4.6
2	H	22	CYS	4.6
1	L	36	TYR	4.5
1	L	146	VAL	4.5
2	H	143	GLY	4.5
1	L	188	ARG	4.4
2	H	144	TYR	4.3
2	H	173	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	171	SER	4.2
2	H	168	LEU	4.2
1	L	115	VAL	4.2
2	H	47	TRP	4.1
1	L	9	LEU	4.0
1	L	37	LEU	4.0
1	L	33	LEU	4.0
1	L	179	LEU	4.0
1	L	157	ASN	4.0
1	L	55	PHE	4.0
2	H	169	LEU	3.9
2	H	199	PRO	3.8
2	H	120	VAL	3.8
1	L	117	ILE	3.8
2	H	194	CYS	3.8
1	L	204	PRO	3.8
2	H	161	SER	3.8
1	L	85	VAL	3.8
2	H	98	SER	3.7
2	H	180	VAL	3.7
1	L	126	THR	3.7
2	H	53	GLY	3.7
1	L	206	VAL	3.7
2	H	93	THR	3.7
2	H	102	TRP	3.6
2	H	164	THR	3.6
1	L	82	ASP	3.6
1	L	98	PHE	3.6
1	L	59	PRO	3.6
2	H	132	GLY	3.6
1	L	106	LEU	3.6
2	H	123	LEU	3.6
2	H	41	PRO	3.5
1	L	139	PHE	3.4
1	L	71	PHE	3.4
2	H	135	VAL	3.4
2	H	191	THR	3.4
1	L	89	SER	3.3
1	L	73	LEU	3.3
2	H	15	GLY	3.3
2	H	189	SER	3.3
1	L	15	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	48	ILE	3.3
2	H	187	TRP	3.3
1	L	151	ASP	3.3
2	H	37	VAL	3.3
1	L	181	LEU	3.2
2	H	188	PRO	3.2
2	H	29	PHE	3.2
1	L	175	MET	3.2
2	H	156	GLY	3.2
2	H	165	PHE	3.2
1	L	172	THR	3.2
2	H	71	ALA	3.1
2	H	141	VAL	3.1
1	L	32	TYR	3.1
1	L	178	THR	3.1
2	H	145	PHE	3.1
1	L	23	CYS	3.1
2	H	96	TYR	3.1
1	L	96	TYR	3.0
2	H	149	VAL	3.0
2	H	138	GLY	3.0
2	H	148	SER	3.0
1	L	94	VAL	3.0
1	L	130	ALA	3.0
1	L	58	VAL	2.9
1	L	209	PHE	2.9
2	H	48	ILE	2.9
2	H	204	THR	2.9
1	L	116	SER	2.9
2	H	95	GLY	2.9
1	L	134	CYS	2.9
1	L	198	HIS	2.9
1	L	51	VAL	2.9
2	H	30	SER	2.9
2	H	195	SER	2.9
1	L	163	TRP	2.9
1	L	193	THR	2.9
1	L	78	VAL	2.9
2	H	118	PRO	2.9
2	H	105	GLY	2.9
1	L	29	GLY	2.8
1	L	24	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	162	VAL	2.8
2	H	183	PRO	2.8
1	L	47	LEU	2.8
2	H	205	VAL	2.8
1	L	27(B)	LEU	2.8
2	H	94	ARG	2.8
1	L	34	HIS	2.8
1	L	112	ALA	2.7
2	H	100	ASP	2.7
2	H	73	THR	2.7
2	H	1	ARG	2.7
1	L	46	LEU	2.7
2	H	11	LEU	2.7
1	L	27(C)	VAL	2.7
2	H	106	THR	2.7
2	H	91	TYR	2.7
2	H	182	VAL	2.7
2	H	153	TRP	2.7
2	H	9	ALA	2.7
1	L	160	LEU	2.7
2	H	174	TYR	2.7
2	H	80	MET	2.7
2	H	99	MET	2.7
2	H	192	VAL	2.6
2	H	112	ALA	2.6
1	L	192	TYR	2.6
2	H	32	TYR	2.6
2	H	108	VAL	2.6
1	L	66	GLY	2.6
1	L	166	GLN	2.6
1	L	132	VAL	2.6
2	H	196	VAL	2.6
1	L	194	CYS	2.6
2	H	101	TYR	2.6
2	H	179	SER	2.6
1	L	121	SER	2.5
1	L	83	LEU	2.5
1	L	3	VAL	2.5
1	L	100	GLY	2.5
2	H	114	LYS	2.5
2	H	8	GLY	2.5
1	L	167	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	140	LEU	2.5
2	H	136	THR	2.5
1	L	202	THR	2.5
2	H	176	MET	2.5
1	L	19	ALA	2.5
2	H	130	THR	2.4
2	H	33	TRP	2.4
1	L	95	PRO	2.4
2	H	170	GLN	2.4
2	H	4	LEU	2.4
2	H	137	LEU	2.4
2	H	97	SER	2.4
2	H	127	CYS	2.4
1	L	176	SER	2.4
2	H	82(C)	LEU	2.4
2	H	190	GLN	2.4
1	L	80	ALA	2.4
2	H	146	PRO	2.4
1	L	136	LEU	2.4
1	L	171	SER	2.4
2	H	128	GLY	2.4
1	L	186	TYR	2.4
2	H	154	ASN	2.3
2	H	198	HIS	2.3
1	L	111	ALA	2.3
1	L	53	ASN	2.3
2	H	3	GLN	2.3
2	H	184	SER	2.3
2	H	139	CYS	2.3
2	H	212	SER	2.3
2	H	36	TRP	2.3
2	H	186	THR	2.3
1	L	214	CYS	2.3
1	L	119	PRO	2.3
1	L	144	ILE	2.3
1	L	41	GLY	2.3
1	L	174	SER	2.3
1	L	187	GLU	2.3
1	L	4	MET	2.2
2	H	178	SER	2.2
2	H	213	GLY	2.2
1	L	199	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	151	VAL	2.2
1	L	180	THR	2.2
2	H	214	PRO	2.2
1	L	118	PHE	2.2
2	H	34	ILE	2.2
2	H	172	GLY	2.2
1	L	45	LYS	2.2
2	H	209	LEU	2.1
1	L	108	ARG	2.1
2	H	125	PRO	2.1
1	L	203	SER	2.1
1	L	56	SER	2.1
1	L	62	PHE	2.1
1	L	208	SER	2.1
2	H	20	ILE	2.1
1	L	21	ILE	2.1
1	L	164	THR	2.0
2	H	59	TYR	2.0
2	H	131	THR	2.0
1	L	159	VAL	2.0
1	L	162	SER	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, 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	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.