



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:53 PM UTC

PDB ID : 1YNK / pdb_00001ynk
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

<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](#) ①) 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

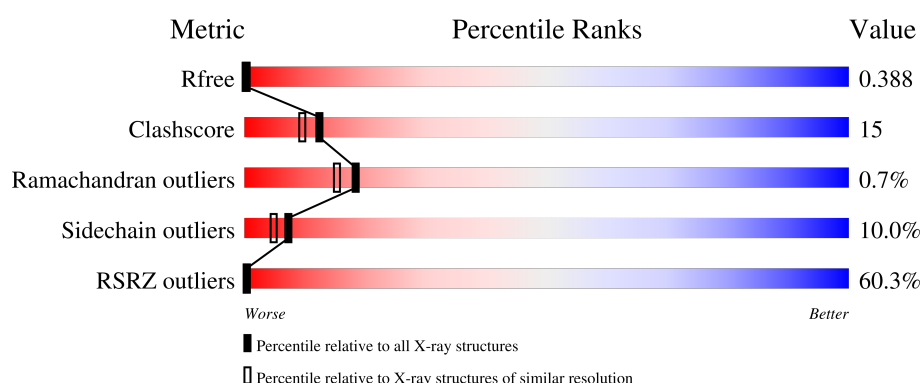
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	L	219	56% 58% 33% 7% .
2	H	219	65% 66% 26% 8%

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.

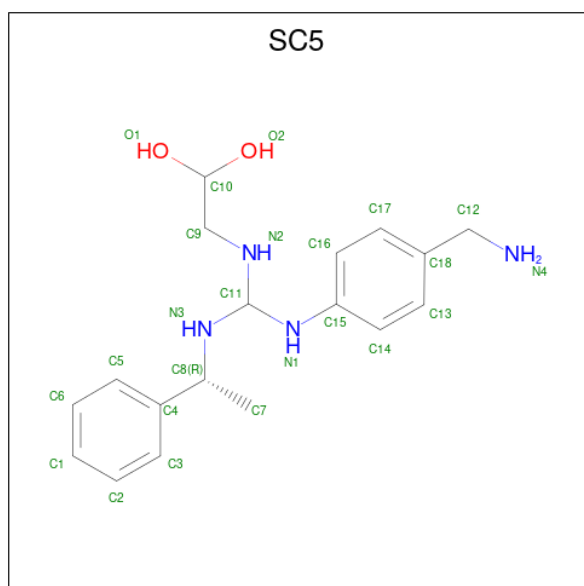
- Molecule 1 is a protein called immunoglobulin kappa light chain.

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 (CCD ID: SC5) (formula: C₁₈H₂₆N₄O₂).



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

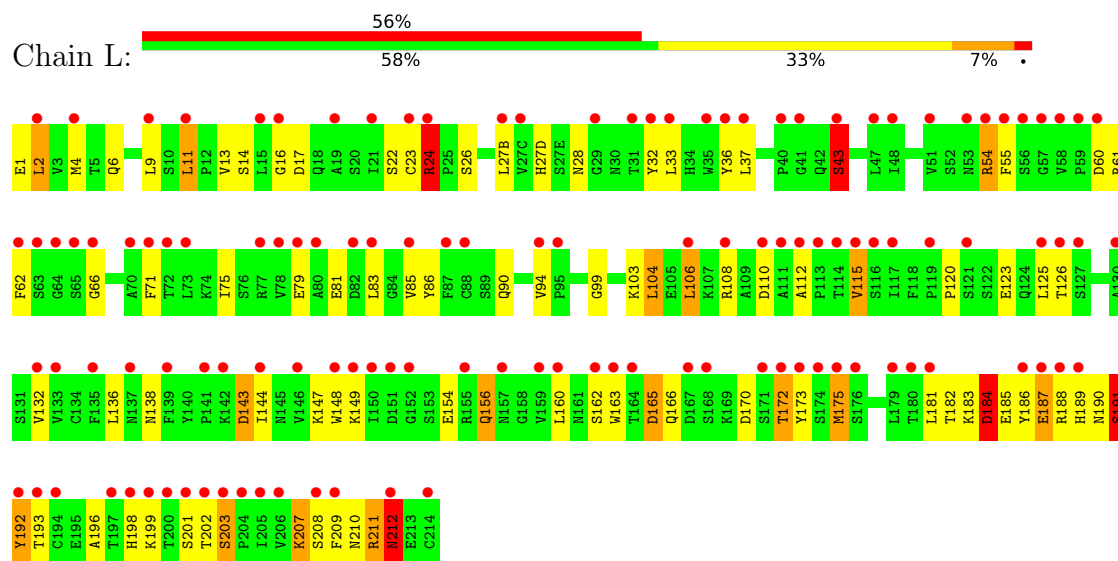
- Molecule 4 is water.

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

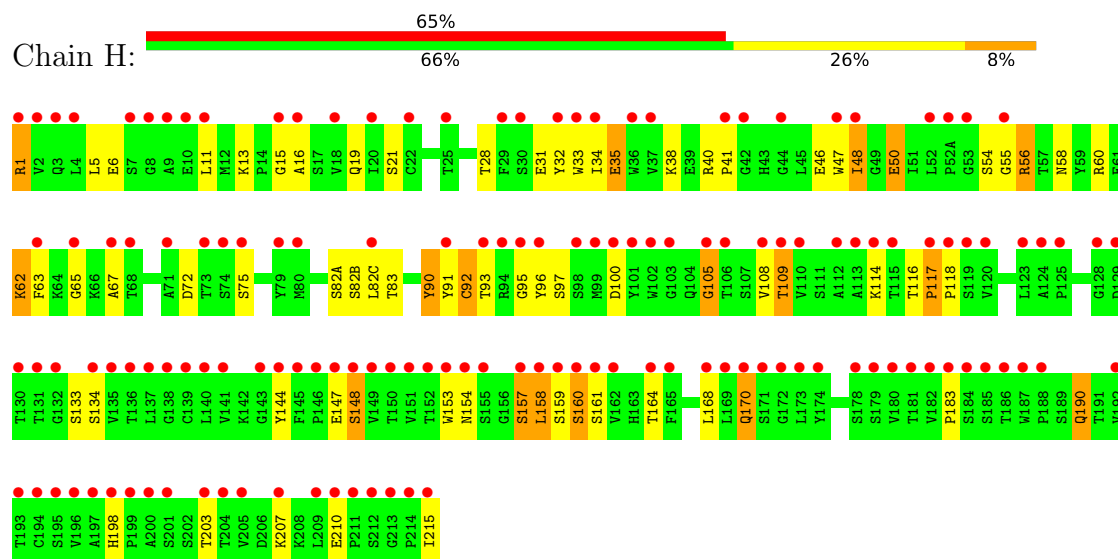
3 Residue-property plots

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: 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 23.64 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.7 (23.64-2.10) 91.4 (23.64-2.10)	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 0.376 , 0.388	Depositor DCC
R_{free} test set	1246 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.9	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	1.60	12/1736 (0.7%)	1.39	12/2355 (0.5%)
2	H	1.66	19/1704 (1.1%)	1.40	7/2325 (0.3%)
All	All	1.63	31/3440 (0.9%)	1.40	19/4680 (0.4%)

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 (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	92	CYS	C-O	8.28	1.33	1.23
2	H	35	GLU	C-O	7.81	1.32	1.23
2	H	67	ALA	CA-CB	-7.50	1.41	1.53
2	H	48	ILE	C-O	7.40	1.31	1.23
2	H	34	ILE	CA-CB	7.08	1.62	1.54
2	H	210	GLU	N-CA	-6.84	1.40	1.45
1	L	196	ALA	CA-CB	-6.78	1.44	1.53
1	L	203	SER	CA-C	6.51	1.59	1.52
1	L	24	ARG	C-O	-6.37	1.18	1.24
2	H	108	VAL	CA-CB	6.23	1.62	1.54
2	H	83	THR	CA-CB	-6.18	1.45	1.53
2	H	105	GLY	C-O	6.05	1.31	1.23
1	L	55	PHE	N-CA	-6.01	1.37	1.45
2	H	50	GLU	C-O	5.91	1.31	1.23
2	H	100	ASP	N-CA	-5.89	1.38	1.46
2	H	109	THR	CA-C	-5.75	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	28	THR	N-CA	-5.59	1.39	1.46
1	L	192	TYR	C-O	-5.56	1.17	1.24
2	H	117	PRO	CA-C	5.56	1.55	1.52
1	L	85	VAL	CA-CB	5.53	1.60	1.54
2	H	164	THR	C-O	-5.43	1.17	1.24
1	L	16	GLY	C-O	-5.41	1.16	1.24
2	H	95	GLY	C-O	-5.34	1.17	1.23
1	L	79	GLU	C-O	-5.25	1.17	1.23
1	L	43	SER	CA-C	5.22	1.59	1.52
2	H	32	TYR	C-O	-5.18	1.17	1.23
1	L	62	PHE	N-CA	-5.18	1.39	1.46
2	H	46	GLU	CA-C	5.13	1.58	1.52
2	H	95	GLY	N-CA	5.13	1.50	1.45
1	L	36	TYR	C-O	-5.05	1.17	1.23
1	L	115	VAL	CA-CB	-5.00	1.48	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	43	SER	CA-C-N	-7.23	112.18	119.92
1	L	43	SER	C-N-CA	-7.23	112.18	119.92
2	H	56[A]	ARG	N-CA-C	-7.15	97.59	109.24
2	H	56[B]	ARG	N-CA-C	-7.15	97.59	109.24
2	H	114	LYS	N-CA-C	-6.63	100.70	110.52
2	H	190	GLN	N-CA-C	6.36	119.48	110.14
1	L	112	ALA	CA-C-N	5.81	125.57	119.76
1	L	112	ALA	C-N-CA	5.81	125.57	119.76
1	L	94	VAL	N-CA-C	-5.80	103.64	108.63
1	L	212	ASN	N-CA-C	5.58	119.83	113.19
2	H	62	LYS	CD-CE-NZ	-5.49	94.34	111.90
1	L	54	ARG	CB-CA-C	5.39	118.64	109.80
1	L	104	LEU	N-CA-C	-5.39	99.95	108.73
2	H	47	TRP	CA-CB-CG	5.18	123.45	113.60
1	L	55	PHE	N-CA-C	-5.14	103.74	110.53
1	L	184	ASP	N-CA-C	5.10	116.52	111.07
1	L	191	SER	CB-CA-C	5.07	118.41	110.19
2	H	90	TYR	CA-CB-CG	-5.07	104.77	113.90
1	L	60	ASP	N-CA-C	5.02	118.18	111.75

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	64	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	102	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 (102) 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:HD2	2:H:1:ARG:H3	1.17	1.07
2:H:1:ARG:N	2:H:1:ARG:CD	2.26	0.98
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
2:H:1:ARG:H3	2:H:1:ARG:CD	1.82	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
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
1:L:163:TRP:CZ2	1:L:175:MET:HE2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:158:LEU:C	2:H:160:SER:HA	2.22	0.65
1:L:187:GLU:HG3	1:L:211:ARG:HH21	1.61	0.65
2:H:1:ARG:N	2:H:1:ARG:NE	2.46	0.64
2:H:35:GLU:O	2:H:92:CYS:HA	1.99	0.63
2:H:1:ARG:CD	2:H:1:ARG:H1	2.11	0.62
2:H:117:PRO:HB3	2:H:203:THR:HG21	1.80	0.61
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
2:H:1:ARG:NE	2:H:1:ARG:H1	2.00	0.59
1:L:184:ASP:O	1:L:188:ARG:HG3	2.03	0.59
1:L:170:ASP:CG	1:L:172:THR:HB	2.27	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
2:H:1:ARG:HD2	2:H:1:ARG:N	1.83	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: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
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
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:4:MET:HE3	1:L:23:CYS:SG	2.53	0.49
1:L:147:LYS:HD3	1:L:149:LYS:HE3	1.94	0.49
1:L:43:SER:HB2	2:H:91:TYR:HE1	1.78	0.48
2:H:170:GLN:HA	2:H:170:GLN:NE2	2.29	0.48
2:H:147:GLU:HA	2:H:148:SER:HA	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:LEU:HD13	1:L:86:TYR:CZ	2.48	0.48
2:H:19:GLN:HG3	4:H:546:HOH:O	2.13	0.48
2:H:33:TRP:H	2:H:33:TRP:CD1	2.30	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
1:L:81:GLU:H	1:L:81:GLU:CD	2.24	0.45
1:L:2:LEU:HA	1:L:2:LEU:HD13	1.64	0.45
2:H:48:ILE:HG23	2:H:63:PHE:CG	2.51	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
1:L:144:ILE:HG23	1:L:175:MET:HE3	1.97	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:157:SER:C	2:H:159:SER:N	2.76	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:OE1	1:L:123:GLU:N	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
1:L:136:LEU:HD12	1:L:136:LEU:N	2.34	0.43
2:H:117:PRO:CB	2:H:203:THR:HG21	2.47	0.43
1:L:181:LEU:HB3	1:L:185:GLU:HB2	2.01	0.43
1:L:185:GLU:O	1:L:186:TYR:C	2.61	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
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
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:81:GLU:CD	1:L:81:GLU:N	2.79	0.41
1:L:66:GLY:HA3	1:L:71:PHE:HA	2.03	0.41
1:L:160:LEU:HD11	2:H:170:GLN:HG2	2.02	0.41
2:H:40:ARG:O	2:H:41:PRO:C	2.62	0.41
2:H:116:THR:HA	2:H:117:PRO:HD2	1.93	0.41
1:L:24:ARG:HH11	1:L:24:ARG:CG	2.31	0.41
1:L:148:TRP:HA	1:L:193:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	22
2	H	219/219 (100%)	207 (94%)	10 (5%)	2 (1%)	14	10
All	All	436/438 (100%)	418 (96%)	15 (3%)	3 (1%)	18	15

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 [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	L	195/195 (100%)	172 (88%)	23 (12%)	5	3
2	H	188/186 (101%)	172 (92%)	16 (8%)	10	7
All	All	383/381 (100%)	344 (90%)	39 (10%)	7	4

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLU
1	L	2	LEU
1	L	9	LEU
1	L	11	LEU
1	L	13	VAL
1	L	22	SER
1	L	24	ARG
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
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	93	THR
2	H	133	SER
2	H	148	SER
2	H	157	SER
2	H	158	LEU

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Mol	Chain	Res	Type
2	H	160	SER
2	H	161	SER
2	H	170	GLN
2	H	190	GLN
2	H	207	LYS
2	H	215	ILE

Sometimes 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 oligosaccharides 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	-	22,25,25	2.13	10 (45%)	31,32,32	3.91	8 (25%)

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	3/15/19/19	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	SC5	O1-C10	-4.22	1.24	1.39
3	H	501	SC5	C3-C4	3.43	1.44	1.39
3	H	501	SC5	C16-C15	3.01	1.44	1.39
3	H	501	SC5	C12-C18	-2.86	1.41	1.51
3	H	501	SC5	C15-N1	2.60	1.44	1.39
3	H	501	SC5	C14-C15	2.52	1.43	1.39
3	H	501	SC5	C5-C4	2.41	1.42	1.39
3	H	501	SC5	C14-C13	2.20	1.42	1.38
3	H	501	SC5	C17-C16	2.03	1.42	1.38
3	H	501	SC5	C13-C18	2.02	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	501	SC5	C18-C12-N4	11.88	179.61	114.90
3	H	501	SC5	C8-N3-C11	9.91	132.95	116.72
3	H	501	SC5	N1-C11-N2	7.81	121.93	109.87
3	H	501	SC5	N1-C11-N3	7.79	121.91	109.87
3	H	501	SC5	O1-C10-C9	7.13	123.91	109.59
3	H	501	SC5	O2-C10-O1	5.06	124.08	111.70
3	H	501	SC5	N2-C11-N3	4.05	116.13	109.87
3	H	501	SC5	C9-N2-C11	3.33	124.68	115.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	501	SC5	C11

All (3) torsion outliers are listed below:

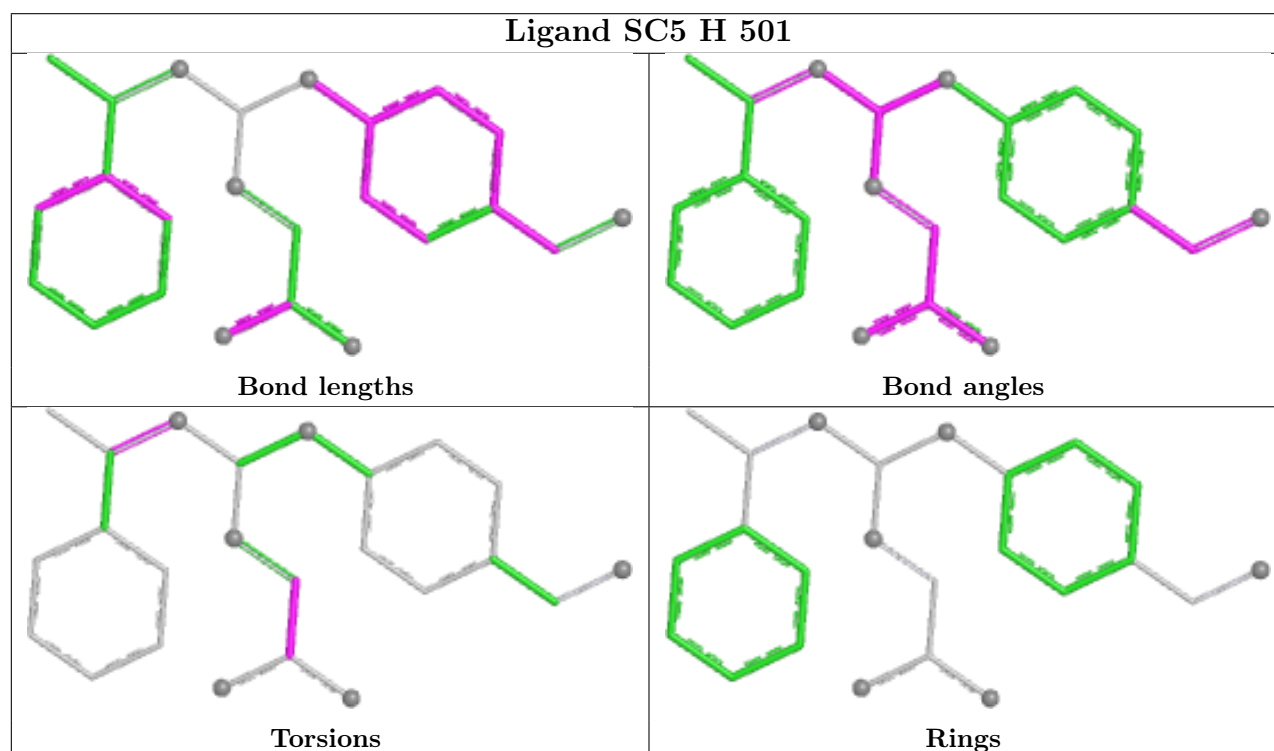
Mol	Chain	Res	Type	Atoms
3	H	501	SC5	C4-C8-N3-C11
3	H	501	SC5	C7-C8-N3-C11
3	H	501	SC5	O1-C10-C9-N2

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

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	L	219/219 (100%)	2.37	122 (55%) 0 0	21, 34, 47, 50	0
2	H	219/219 (100%)	2.59	142 (64%) 0 0	19, 33, 53, 71	2 (0%)
All	All	438/438 (100%)	2.48	264 (60%) 0 0	19, 34, 49, 71	2 (0%)

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	158	LEU	10.4
2	H	157	SER	6.8
2	H	215	ILE	6.2
1	L	173	TYR	5.8
1	L	146	VAL	5.8
1	L	148	TRP	5.7
2	H	169	LEU	5.4
1	L	125	LEU	5.2
2	H	144	TYR	5.1
2	H	162	VAL	4.9
2	H	199	PRO	4.9
2	H	138	GLY	4.8
2	H	95	GLY	4.8
2	H	22	CYS	4.8
1	L	111	ALA	4.8
2	H	192	VAL	4.7
1	L	15	LEU	4.6
2	H	160	SER	4.6
2	H	205	VAL	4.6
1	L	33	LEU	4.6
1	L	82	ASP	4.6
1	L	37	LEU	4.5
1	L	157	ASN	4.5
1	L	115	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	L	55	PHE	4.5
1	L	202	THR	4.4
2	H	179	SER	4.4
2	H	180	VAL	4.4
2	H	131	THR	4.3
1	L	87	PHE	4.3
1	L	58	VAL	4.3
1	L	85	VAL	4.3
1	L	181	LEU	4.3
1	L	139	PHE	4.3
2	H	7	SER	4.3
2	H	120	VAL	4.3
1	L	130	ALA	4.2
2	H	106	THR	4.2
2	H	164	THR	4.2
2	H	73	THR	4.1
1	L	204	PRO	4.1
1	L	59	PRO	4.1
2	H	29	PHE	4.1
1	L	35	TRP	4.0
2	H	161	SER	4.0
1	L	71	PHE	4.0
1	L	57	GLY	4.0
2	H	130	THR	3.9
2	H	183	PRO	3.9
1	L	152	GLY	3.9
2	H	47	TRP	3.9
2	H	113	ALA	3.9
1	L	106	LEU	3.9
1	L	151	ASP	3.8
2	H	143	GLY	3.8
2	H	209	LEU	3.8
2	H	153	TRP	3.8
1	L	48	ILE	3.8
2	H	91	TYR	3.8
1	L	133	VAL	3.7
1	L	179	LEU	3.7
2	H	173	LEU	3.7
2	H	102	TRP	3.7
2	H	105	GLY	3.7
1	L	27(C)	VAL	3.7
2	H	196	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	117	ILE	3.6
1	L	209	PHE	3.6
1	L	192	TYR	3.6
1	L	199	LYS	3.6
1	L	78	VAL	3.6
2	H	165	PHE	3.6
2	H	136	THR	3.6
2	H	118	PRO	3.6
2	H	211	PRO	3.6
2	H	174	TYR	3.6
2	H	171	SER	3.6
1	L	80	ALA	3.5
2	H	194	CYS	3.5
2	H	204	THR	3.5
2	H	182	VAL	3.5
1	L	47	LEU	3.5
2	H	55	GLY	3.5
2	H	15	GLY	3.4
2	H	42	GLY	3.4
1	L	51	VAL	3.4
2	H	93	THR	3.4
2	H	187	TRP	3.4
2	H	32	TYR	3.4
1	L	32	TYR	3.4
2	H	149	VAL	3.4
2	H	124	ALA	3.4
1	L	174	SER	3.3
2	H	188	PRO	3.3
1	L	23	CYS	3.3
2	H	125	PRO	3.3
2	H	141	VAL	3.3
2	H	198	HIS	3.3
1	L	135	PHE	3.3
1	L	188	ARG	3.3
1	L	149	LYS	3.3
2	H	195	SER	3.3
2	H	146	PRO	3.3
2	H	168	LEU	3.3
2	H	30	SER	3.2
2	H	213	GLY	3.2
2	H	71	ALA	3.2
1	L	19	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	112	ALA	3.2
2	H	96	TYR	3.2
1	L	56	SER	3.2
2	H	155	SER	3.2
2	H	154	ASN	3.2
1	L	94	VAL	3.2
2	H	9	ALA	3.2
1	L	54	ARG	3.2
2	H	145	PHE	3.2
1	L	198	HIS	3.2
2	H	53	GLY	3.2
2	H	41	PRO	3.2
1	L	110	ASP	3.1
1	L	171	SER	3.1
1	L	88	CYS	3.1
2	H	82(C)	LEU	3.1
1	L	208	SER	3.1
1	L	164	THR	3.1
1	L	73	LEU	3.1
1	L	206	VAL	3.1
1	L	175	MET	3.1
2	H	101	TYR	3.0
1	L	126	THR	3.0
1	L	167	ASP	3.0
2	H	16	ALA	3.0
1	L	27(B)	LEU	3.0
2	H	4	LEU	3.0
1	L	205	ILE	3.0
2	H	181	THR	3.0
1	L	163	TRP	3.0
2	H	11	LEU	3.0
2	H	137	LEU	3.0
1	L	16	GLY	3.0
2	H	115	THR	3.0
2	H	94	ARG	2.9
2	H	20	ILE	2.9
1	L	200	THR	2.9
2	H	214	PRO	2.9
2	H	123	LEU	2.9
1	L	66	GLY	2.9
1	L	63	SER	2.9
1	L	112	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	139	CYS	2.9
2	H	80	MET	2.8
1	L	194	CYS	2.8
2	H	151	VAL	2.8
1	L	168	SER	2.8
1	L	70	ALA	2.8
1	L	141	PRO	2.8
1	L	144	ILE	2.8
2	H	52(A)	PRO	2.8
2	H	201	SER	2.8
2	H	67	ALA	2.8
1	L	214	CYS	2.8
2	H	159	SER	2.8
1	L	64	GLY	2.8
2	H	110	VAL	2.8
2	H	128	GLY	2.7
1	L	197	THR	2.7
1	L	43	SER	2.7
1	L	162	SER	2.7
2	H	210	GLU	2.7
2	H	108	VAL	2.7
2	H	36	TRP	2.7
1	L	62	PHE	2.6
1	L	114	THR	2.6
1	L	113	PRO	2.6
1	L	116	SER	2.6
1	L	121	SER	2.6
2	H	148	SER	2.6
1	L	180	THR	2.6
2	H	150	THR	2.6
2	H	152	THR	2.6
2	H	212	SER	2.6
1	L	155	ARG	2.6
2	H	18	VAL	2.6
1	L	201	SER	2.6
1	L	159	VAL	2.6
2	H	193	THR	2.6
1	L	40	PRO	2.6
2	H	1	ARG	2.5
1	L	31	THR	2.5
1	L	60	ASP	2.5
2	H	25	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	68	THR	2.5
2	H	37	VAL	2.5
2	H	48	ILE	2.5
2	H	132	GLY	2.5
2	H	172	GLY	2.5
1	L	36	TYR	2.5
1	L	77	ARG	2.5
2	H	134	SER	2.5
2	H	197	ALA	2.5
2	H	52	LEU	2.5
2	H	33	TRP	2.5
2	H	79	TYR	2.5
2	H	170	GLN	2.5
1	L	193	THR	2.5
2	H	98	SER	2.5
1	L	95	PRO	2.5
1	L	83	LEU	2.5
1	L	132	VAL	2.4
1	L	150	ILE	2.5
1	L	65	SER	2.4
2	H	99	MET	2.4
1	L	176	SER	2.4
2	H	114	LYS	2.4
1	L	2	LEU	2.4
1	L	160	LEU	2.4
2	H	135	VAL	2.4
1	L	127	SER	2.4
1	L	172	THR	2.4
1	L	11	LEU	2.3
2	H	2	VAL	2.3
2	H	75	SER	2.3
2	H	185	SER	2.3
1	L	21	ILE	2.3
1	L	137	ASN	2.3
2	H	74	SER	2.3
2	H	34	ILE	2.3
1	L	119	PRO	2.3
1	L	108	ARG	2.3
2	H	8	GLY	2.3
1	L	186	TYR	2.3
2	H	207	LYS	2.2
1	L	9	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	189	HIS	2.2
2	H	178	SER	2.2
1	L	24	ARG	2.2
1	L	53	ASN	2.2
2	H	63	PHE	2.2
2	H	103	GLY	2.2
1	L	4	MET	2.2
2	H	129	ASP	2.2
1	L	79	GLU	2.1
1	L	142	LYS	2.1
2	H	186	THR	2.1
1	L	41	GLY	2.1
2	H	65	GLY	2.1
1	L	187	GLU	2.1
2	H	147	GLU	2.1
2	H	3	GLN	2.1
2	H	184	SER	2.1
2	H	10	GLU	2.1
1	L	72	THR	2.1
2	H	109	THR	2.1
1	L	29	GLY	2.1
2	H	200	ALA	2.1
2	H	140	LEU	2.0
2	H	203	THR	2.0
2	H	44	GLY	2.0
1	L	203	SER	2.0
2	H	119	SER	2.0
1	L	212	ASN	2.0
2	H	100	ASP	2.0
2	H	117	PRO	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](#)

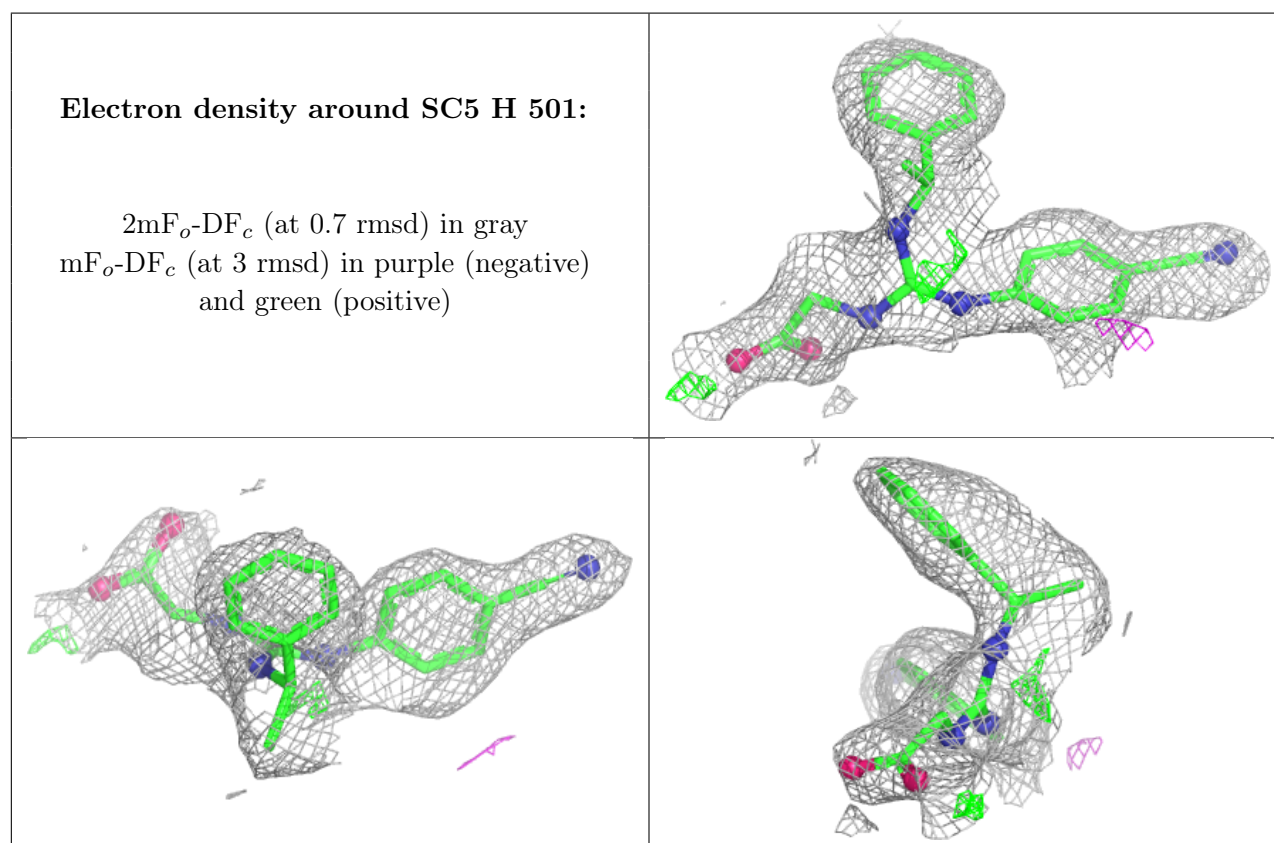
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	SC5	H	501	24/24	0.72	0.19	32,34,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.