



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:15 AM UTC

PDB ID : 1UB5 / pdb_00001ub5
Title : Crystal structure of Antibody 19G2 with hapten at 100K
Authors : Beuscher, A.B.; Wirsching, P.; Lerner, R.A.; Janda, K.; Stevens, R.C.
Deposited on : 2003-03-30
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

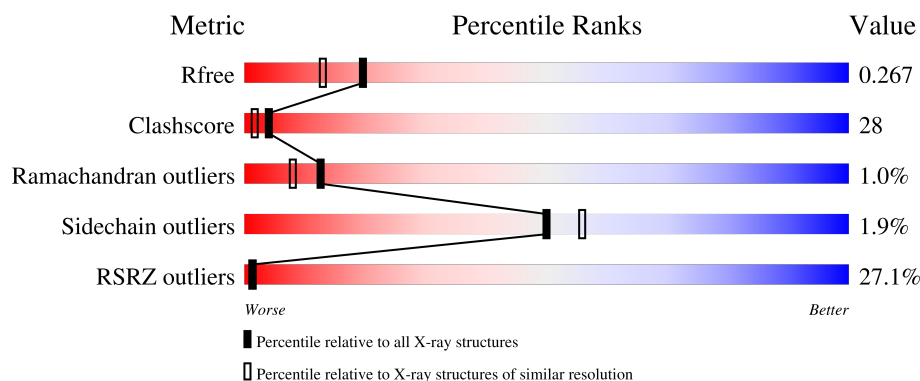
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	209	25% 57% 39% .
1	H	209	22% 63% 34% .
2	B	214	34% 59% 39% .
2	L	214	27% 60% 38% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7017 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.

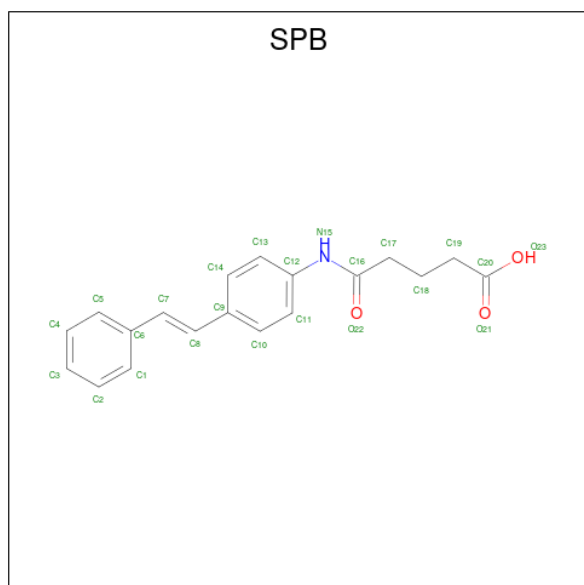
- Molecule 1 is a protein called antibody 19G2, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	209	Total	C	N	O	S	0	0	0
			1560	985	261	306	8			
1	A	209	Total	C	N	O	S	0	0	0
			1560	985	261	306	8			

- Molecule 2 is a protein called antibody 19G2, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1647	1032	275	333	7			
2	B	214	Total	C	N	O	S	0	0	0
			1647	1032	275	333	7			

- Molecule 3 is 4-(4-STYRYL-PHENYL-CARBAMOYL)-BUTYRIC ACID (CCD ID: SPB) (formula: C₁₉H₁₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			23	19	1	3		
3	B	1	Total	C	N	O	0	0
			23	19	1	3		

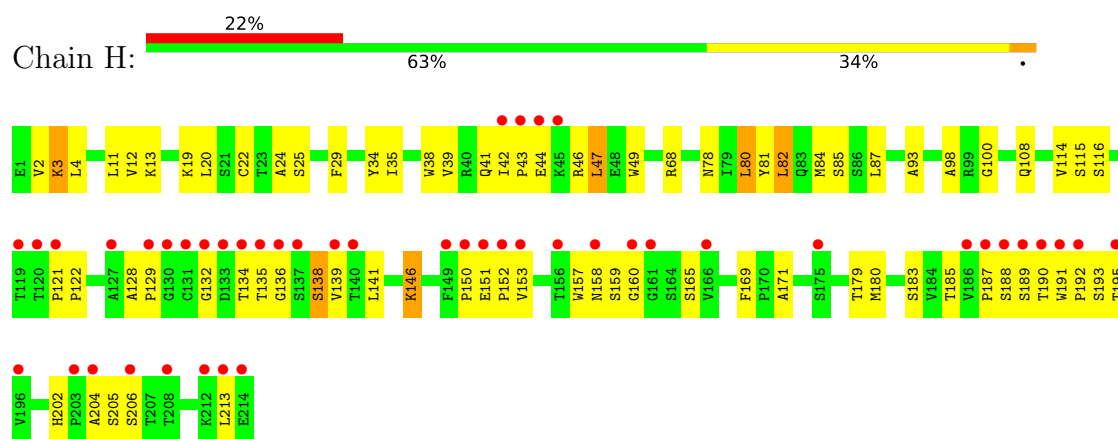
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	92	Total	O	0	0
			92	92		
4	L	163	Total	O	0	0
			163	163		
4	A	145	Total	O	0	0
			145	145		
4	B	157	Total	O	0	0
			157	157		

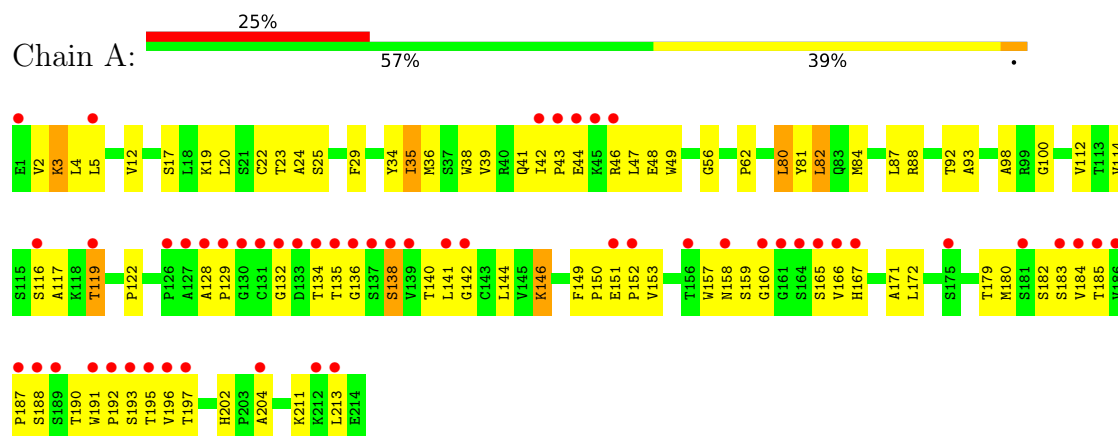
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

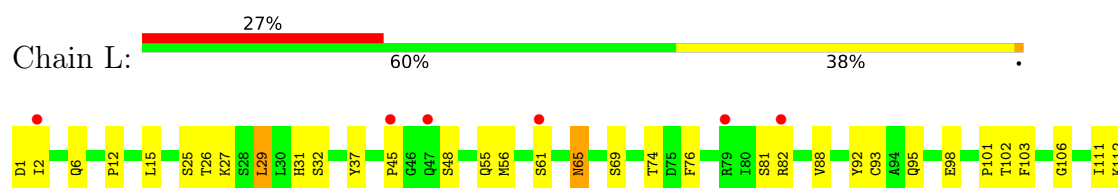
- Molecule 1: antibody 19G2, alpha chain

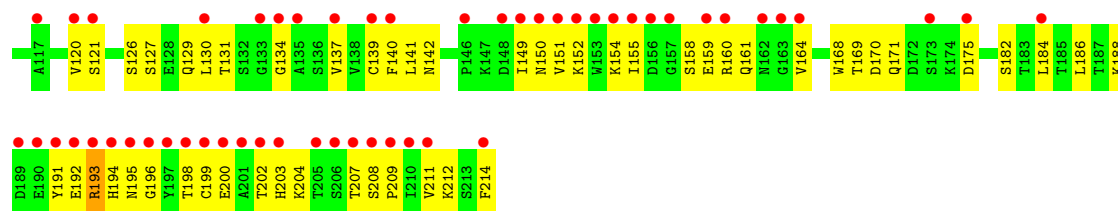


- Molecule 1: antibody 19G2, alpha chain

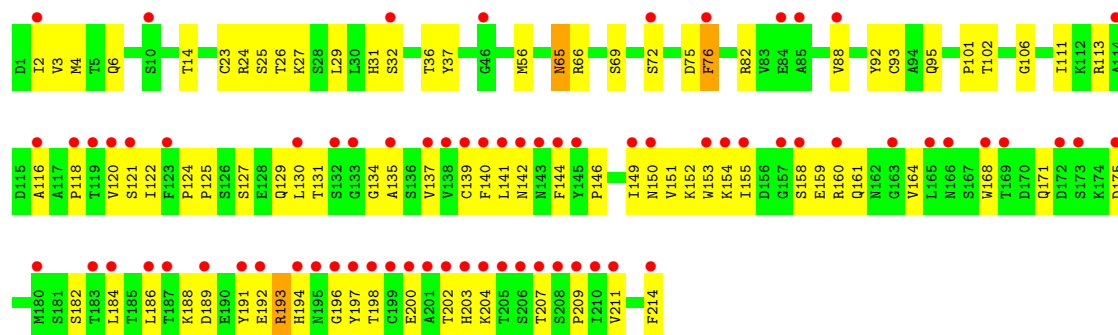


- Molecule 2: antibody 19G2, beta chain





● Molecule 2: antibody 19G2, beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.93Å 61.06Å 92.59Å 90.00° 117.05° 90.00°	Depositor
Resolution (Å)	19.89 – 2.00 19.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.89-2.00) 96.0 (19.89-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.267 0.247 , 0.267	Depositor DCC
R_{free} test set	3207 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: SPB

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	0.39	0/1599	0.87	6/2182 (0.3%)
1	H	0.36	0/1599	0.86	6/2182 (0.3%)
2	B	0.34	0/1684	0.81	3/2288 (0.1%)
2	L	0.36	0/1684	0.81	2/2288 (0.1%)
All	All	0.36	0/6566	0.84	17/8940 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	100	GLY	N-CA-C	7.09	122.74	114.16
1	A	35	ILE	N-CA-C	-6.49	97.60	107.73
1	A	100	GLY	N-CA-C	6.43	121.94	114.16
1	H	35	ILE	N-CA-C	-6.04	98.30	107.73
1	A	116	SER	N-CA-C	-5.93	106.38	113.97
1	H	98	ALA	N-CA-C	5.60	118.33	108.75
1	A	98	ALA	N-CA-C	5.48	118.12	108.75
2	B	66	ARG	N-CA-C	-5.46	105.88	112.54
1	A	34	TYR	N-CA-C	5.41	118.09	109.81
1	H	47	LEU	N-CA-C	5.41	117.86	110.24
1	H	34	TYR	N-CA-C	5.36	118.01	109.81
2	L	37	TYR	N-CA-C	5.23	117.71	109.39
1	A	62	PRO	N-CA-C	-5.19	103.10	111.77
2	B	37	TYR	N-CA-C	5.17	117.60	109.39
2	L	93	CYS	N-CA-C	-5.16	102.14	110.14
2	B	93	CYS	N-CA-C	-5.12	102.21	110.14
1	H	29	PHE	N-CA-C	5.08	117.47	111.33

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	1560	0	1546	100	0
1	H	1560	0	1546	75	0
2	B	1647	0	1596	101	0
2	L	1647	0	1596	86	1
3	B	23	0	18	1	0
3	H	23	0	18	0	0
4	A	145	0	0	41	0
4	B	157	0	0	44	0
4	H	92	0	0	16	0
4	L	163	0	0	31	1
All	All	7017	0	6320	357	1

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 28.

All (357) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ARG:HA	4:B:843:HOH:O	1.60	0.99
2:L:175:ASP:HB3	4:L:295:HOH:O	1.63	0.98
2:B:175:ASP:HB3	4:B:752:HOH:O	1.65	0.94
2:B:2:ILE:HG13	4:B:851:HOH:O	1.68	0.94
1:H:11:LEU:HD11	1:H:150:PRO:HG2	1.51	0.90
1:A:144:LEU:HG	4:A:299:HOH:O	1.75	0.86
2:B:139:CYS:HB2	4:B:832:HOH:O	1.75	0.84
2:L:2:ILE:HD11	2:L:25:SER:OG	1.78	0.84
1:A:166:VAL:HG22	4:A:271:HOH:O	1.78	0.83
2:B:2:ILE:HD11	2:B:25:SER:OG	1.80	0.82
2:L:102:THR:HB	4:L:350:HOH:O	1.80	0.81
2:L:98:GLU:HG3	4:L:323:HOH:O	1.81	0.81
1:A:4:LEU:HD23	1:A:24:ALA:HB2	1.63	0.80
2:L:25:SER:HB3	4:L:349:HOH:O	1.82	0.80
2:B:189:ASP:HB3	4:B:829:HOH:O	1.83	0.79
1:H:4:LEU:HD23	1:H:24:ALA:HB2	1.65	0.78
1:H:44:GLU:HG3	1:H:46:ARG:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:GLN:HG3	4:H:644:HOH:O	1.82	0.78
2:L:2:ILE:HD13	2:L:27:LYS:HB3	1.67	0.76
2:B:75:ASP:HA	4:B:843:HOH:O	1.84	0.76
2:B:129:GLN:HG3	4:B:824:HOH:O	1.83	0.76
2:L:126:SER:HB3	4:L:348:HOH:O	1.85	0.76
1:A:44:GLU:HG3	1:A:46:ARG:H	1.49	0.76
1:A:146:LYS:HD2	4:B:850:HOH:O	1.85	0.76
2:L:188:LYS:O	2:L:192:GLU:HG2	1.86	0.75
1:A:22:CYS:SG	4:A:331:HOH:O	2.43	0.75
1:H:24:ALA:HB3	4:H:633:HOH:O	1.87	0.75
2:B:2:ILE:HD13	2:B:27:LYS:HB3	1.68	0.74
4:A:334:HOH:O	2:B:124:PRO:HD2	1.86	0.74
2:B:188:LYS:O	2:B:192:GLU:HG2	1.86	0.74
1:A:39:VAL:HG12	1:A:47:LEU:HD12	1.71	0.71
2:B:24:ARG:HD3	4:B:825:HOH:O	1.91	0.71
2:L:12:PRO:HB2	2:L:112:LYS:HB2	1.71	0.71
1:H:11:LEU:HD11	1:H:150:PRO:CG	2.20	0.70
2:B:2:ILE:HG22	4:B:728:HOH:O	1.91	0.70
1:H:39:VAL:HG12	1:H:47:LEU:HD12	1.72	0.70
1:A:144:LEU:HD21	4:B:850:HOH:O	1.91	0.70
1:H:189:SER:HB2	4:H:649:HOH:O	1.91	0.70
2:B:113:ARG:NH1	2:B:113:ARG:HB2	2.07	0.70
2:B:200:GLU:HG3	2:B:211:VAL:HG12	1.74	0.69
2:B:111:ILE:H	2:B:171:GLN:HE22	1.39	0.69
2:B:203:HIS:HB3	4:B:807:HOH:O	1.93	0.69
1:A:136:GLY:O	1:A:188:SER:HB2	1.93	0.69
1:H:136:GLY:O	1:H:188:SER:HB2	1.93	0.69
1:A:41:GLN:HG3	4:A:287:HOH:O	1.93	0.69
1:H:141:LEU:HB3	1:H:213:LEU:HD13	1.76	0.68
1:H:121:PRO:HB3	4:H:678:HOH:O	1.93	0.68
1:H:108:GLN:HB2	4:H:687:HOH:O	1.93	0.68
1:A:141:LEU:HB3	1:A:213:LEU:HD13	1.75	0.68
2:B:111:ILE:HB	4:B:849:HOH:O	1.93	0.67
2:B:186:LEU:HG	4:B:827:HOH:O	1.93	0.67
2:L:200:GLU:HG3	2:L:211:VAL:HG12	1.75	0.67
1:A:157:TRP:HH2	4:A:319:HOH:O	1.77	0.67
2:B:135:ALA:HA	4:B:759:HOH:O	1.94	0.67
2:L:29:LEU:HD13	4:L:375:HOH:O	1.93	0.67
1:H:151:GLU:N	1:H:152:PRO:HD2	2.10	0.66
2:L:154:LYS:HB2	2:L:198:THR:HB	1.78	0.66
2:L:196:GLY:HA2	2:L:214:PHE:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:149:ILE:HG12	4:L:357:HOH:O	1.96	0.66
1:A:129:PRO:HA	4:A:320:HOH:O	1.94	0.66
2:B:154:LYS:HB2	2:B:198:THR:HB	1.78	0.66
2:B:196:GLY:HA2	2:B:214:PHE:O	1.96	0.66
1:A:213:LEU:HB2	4:A:341:HOH:O	1.96	0.66
1:A:112:VAL:HA	4:A:258:HOH:O	1.95	0.65
1:A:151:GLU:N	1:A:152:PRO:HD2	2.10	0.65
1:A:213:LEU:HD21	4:A:319:HOH:O	1.95	0.65
1:H:42:ILE:HB	1:H:43:PRO:HD2	1.78	0.65
2:L:81:SER:HA	4:L:345:HOH:O	1.96	0.65
1:H:4:LEU:HD23	1:H:24:ALA:CB	2.26	0.64
1:A:119:THR:HG22	4:A:337:HOH:O	1.96	0.64
1:A:47:LEU:HD22	4:A:287:HOH:O	1.97	0.64
1:A:196:VAL:HA	4:A:311:HOH:O	1.96	0.64
1:A:42:ILE:HB	1:A:43:PRO:HD2	1.79	0.64
1:A:166:VAL:HB	4:A:330:HOH:O	1.98	0.64
1:H:191:TRP:HB3	4:H:668:HOH:O	1.98	0.64
1:A:187:PRO:HG2	1:A:190:THR:HG22	1.79	0.64
1:H:47:LEU:HD23	4:L:245:HOH:O	1.99	0.63
1:H:187:PRO:HG2	1:H:190:THR:HG22	1.79	0.63
1:A:4:LEU:HD23	1:A:24:ALA:CB	2.27	0.63
2:B:72:SER:HB3	4:B:856:HOH:O	1.97	0.63
2:B:207:THR:O	2:B:209:PRO:HD3	1.99	0.63
1:H:150:PRO:HD2	1:H:204:ALA:HB1	1.80	0.63
1:A:196:VAL:HB	4:A:341:HOH:O	1.98	0.63
1:A:3:LYS:HB2	4:A:338:HOH:O	1.98	0.63
2:L:207:THR:O	2:L:209:PRO:HD3	1.99	0.62
1:A:172:LEU:HD12	4:B:838:HOH:O	1.99	0.62
2:B:6:GLN:NE2	2:B:106:GLY:H	1.97	0.62
1:A:150:PRO:HD2	1:A:204:ALA:HB1	1.80	0.62
2:L:6:GLN:NE2	2:L:106:GLY:H	1.97	0.61
2:L:129:GLN:N	4:L:348:HOH:O	2.33	0.61
1:H:68:ARG:HA	4:H:676:HOH:O	2.00	0.61
1:A:42:ILE:HG22	1:A:93:ALA:HB2	1.83	0.61
2:B:127:SER:O	2:B:131:THR:HG23	2.01	0.61
1:H:42:ILE:HG22	1:H:93:ALA:HB2	1.84	0.60
2:B:120:VAL:HG12	4:B:832:HOH:O	2.02	0.60
1:A:184:VAL:HB	4:A:286:HOH:O	2.00	0.60
1:A:39:VAL:CG1	1:A:47:LEU:HD12	2.32	0.59
1:A:211:LYS:HE2	4:A:285:HOH:O	2.03	0.59
2:B:125:PRO:HG3	4:B:815:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:127:SER:O	2:L:131:THR:HG23	2.02	0.59
2:L:208:SER:HB3	4:L:312:HOH:O	2.02	0.59
2:B:116:ALA:HB3	4:B:746:HOH:O	2.02	0.59
2:B:182:SER:HB3	4:B:848:HOH:O	2.02	0.58
2:L:76:PHE:HB3	4:L:334:HOH:O	2.02	0.58
2:L:111:ILE:H	2:L:171:GLN:HE22	1.51	0.58
2:L:137:VAL:CG1	2:L:184:LEU:HB3	2.33	0.58
1:A:138:SER:H	1:A:187:PRO:HA	1.68	0.58
1:A:213:LEU:HD11	4:A:319:HOH:O	2.02	0.58
2:L:151:VAL:HG11	2:L:182:SER:OG	2.04	0.58
2:L:193:ARG:HG3	2:L:194:HIS:ND1	2.19	0.57
1:H:42:ILE:HB	1:H:43:PRO:CD	2.34	0.57
1:H:138:SER:H	1:H:187:PRO:HA	1.69	0.57
2:B:151:VAL:HG11	2:B:182:SER:OG	2.04	0.57
1:A:20:LEU:HG	1:A:84:MET:HE2	1.87	0.57
2:B:137:VAL:CG1	2:B:184:LEU:HB3	2.34	0.57
2:B:3:VAL:C	4:B:851:HOH:O	2.47	0.57
1:H:187:PRO:O	1:H:190:THR:HG22	2.05	0.56
2:L:74:THR:HG22	4:L:349:HOH:O	2.05	0.56
2:B:193:ARG:HG3	2:B:194:HIS:ND1	2.19	0.56
1:A:42:ILE:HB	1:A:43:PRO:CD	2.35	0.56
1:H:39:VAL:CG1	1:H:47:LEU:HD12	2.35	0.56
1:H:42:ILE:HG13	1:H:44:GLU:HG2	1.88	0.56
4:H:686:HOH:O	2:L:48:SER:HB3	2.06	0.56
2:B:155:ILE:HD12	2:B:160:ARG:HH11	1.71	0.56
2:L:2:ILE:HG22	4:L:279:HOH:O	2.03	0.56
2:L:186:LEU:CD1	2:L:191:TYR:HB2	2.35	0.56
1:A:47:LEU:HD23	4:B:801:HOH:O	2.04	0.56
2:B:182:SER:HB2	4:B:766:HOH:O	2.06	0.56
1:H:3:LYS:NZ	1:H:3:LYS:HB2	2.20	0.56
1:A:187:PRO:O	1:A:190:THR:HG22	2.06	0.56
2:B:186:LEU:CD1	2:B:191:TYR:HB2	2.35	0.56
2:B:149:ILE:HG12	4:B:744:HOH:O	2.05	0.55
2:B:130:LEU:HD12	4:B:831:HOH:O	2.06	0.55
1:H:141:LEU:HB3	1:H:213:LEU:CD1	2.37	0.55
1:A:17:SER:HB3	4:A:354:HOH:O	2.05	0.55
2:B:168:TRP:HB3	4:B:835:HOH:O	2.06	0.55
1:A:153:VAL:HG12	4:A:254:HOH:O	2.07	0.55
2:L:150:ASN:OD1	2:L:202:THR:HB	2.07	0.55
2:L:155:ILE:HD12	2:L:160:ARG:HH11	1.71	0.55
1:A:141:LEU:HB3	1:A:213:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:GLU:C	2:B:194:HIS:H	2.15	0.54
2:L:192:GLU:C	2:L:194:HIS:H	2.15	0.54
2:B:188:LYS:HE3	4:B:846:HOH:O	2.08	0.54
1:A:213:LEU:HD22	4:A:345:HOH:O	2.07	0.54
2:L:137:VAL:HG12	2:L:184:LEU:HB3	1.89	0.54
1:A:183:SER:HB3	2:B:140:PHE:CE2	2.42	0.54
2:B:137:VAL:HG12	2:B:184:LEU:HB3	1.90	0.54
2:B:125:PRO:HB3	4:B:759:HOH:O	2.08	0.53
1:A:42:ILE:HG13	1:A:44:GLU:HG2	1.89	0.53
2:B:150:ASN:OD1	2:B:202:THR:HB	2.07	0.53
1:A:213:LEU:HD13	4:A:345:HOH:O	2.08	0.53
1:H:206:SER:HA	4:H:667:HOH:O	2.08	0.53
1:A:150:PRO:HD2	1:A:204:ALA:CB	2.38	0.53
1:A:150:PRO:HB2	1:A:152:PRO:HD2	1.89	0.53
1:H:150:PRO:HB2	1:H:152:PRO:HD2	1.91	0.53
1:H:146:LYS:HB3	1:H:179:THR:HG23	1.90	0.53
2:B:23:CYS:O	4:B:843:HOH:O	2.19	0.53
1:H:12:VAL:HG11	1:H:87:LEU:HD12	1.91	0.52
1:H:183:SER:HB3	2:L:140:PHE:CE2	2.43	0.52
1:A:195:THR:HA	4:A:317:HOH:O	2.09	0.52
2:B:171:GLN:CD	4:B:849:HOH:O	2.53	0.52
2:L:199:CYS:HB3	4:L:290:HOH:O	2.10	0.52
1:A:128:ALA:HB1	1:A:129:PRO:HD2	1.91	0.52
2:L:152:LYS:HE3	2:L:154:LYS:HE2	1.92	0.52
2:B:113:ARG:HB2	2:B:113:ARG:HH11	1.72	0.52
1:H:150:PRO:HD2	1:H:204:ALA:CB	2.40	0.52
2:L:103:PHE:N	4:L:350:HOH:O	2.43	0.52
1:A:146:LYS:HB3	1:A:179:THR:HG23	1.90	0.52
1:A:3:LYS:HB2	1:A:3:LYS:NZ	2.25	0.52
2:L:160:ARG:HD2	4:L:356:HOH:O	2.09	0.51
2:B:186:LEU:HD11	2:B:191:TYR:HB2	1.92	0.51
1:H:20:LEU:HG	1:H:84:MET:HE2	1.91	0.51
2:L:1:ASP:HA	4:L:341:HOH:O	2.10	0.51
2:B:72:SER:HB2	4:B:787:HOH:O	2.09	0.51
1:H:4:LEU:CD2	1:H:24:ALA:HB2	2.38	0.51
1:H:165:SER:OG	1:H:185:THR:HB	2.10	0.51
1:A:12:VAL:HG11	1:A:87:LEU:HD12	1.92	0.51
2:B:120:VAL:HG11	4:B:804:HOH:O	2.10	0.51
2:L:31:HIS:ND1	2:L:32:SER:N	2.58	0.51
1:A:4:LEU:CD2	1:A:24:ALA:HB2	2.37	0.51
1:A:165:SER:OG	1:A:185:THR:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LYS:HE3	2:B:154:LYS:HE2	1.92	0.51
1:H:128:ALA:HB1	1:H:129:PRO:HD2	1.92	0.50
2:L:88:VAL:HB	4:L:355:HOH:O	2.10	0.50
2:L:56:MET:O	2:L:69:SER:HB3	2.11	0.50
1:A:197:THR:HB	4:A:295:HOH:O	2.10	0.50
2:B:129:GLN:HG2	4:B:759:HOH:O	2.10	0.50
1:H:12:VAL:O	1:H:114:VAL:HA	2.11	0.50
1:H:13:LYS:CD	1:H:116:SER:HA	2.41	0.50
1:H:153:VAL:HG12	4:H:630:HOH:O	2.11	0.50
2:B:121:SER:O	2:B:139:CYS:HA	2.11	0.50
2:L:121:SER:O	2:L:139:CYS:HA	2.12	0.50
2:B:111:ILE:H	2:B:171:GLN:NE2	2.09	0.50
2:L:186:LEU:HD11	2:L:191:TYR:HB2	1.93	0.50
1:A:141:LEU:HD22	4:A:345:HOH:O	2.12	0.50
2:B:118:PRO:HB3	2:B:144:PHE:HB3	1.93	0.50
2:L:212:LYS:HB2	4:L:290:HOH:O	2.09	0.49
2:B:161:GLN:O	2:B:164:VAL:HG12	2.12	0.49
1:A:185:THR:HG23	4:A:291:HOH:O	2.11	0.49
2:L:2:ILE:HD12	2:L:26:THR:OG1	2.12	0.49
2:L:203:HIS:CD2	2:L:204:LYS:H	2.30	0.49
2:B:88:VAL:CG1	2:B:111:ILE:HG12	2.43	0.49
1:H:44:GLU:OE1	1:H:46:ARG:HB3	2.13	0.49
2:B:2:ILE:HD12	2:B:26:THR:OG1	2.12	0.49
2:L:168:TRP:HB3	4:L:272:HOH:O	2.13	0.49
1:A:35:ILE:HD12	3:B:701:SPB:H192	1.94	0.49
1:A:180:MET:HE3	4:A:254:HOH:O	2.13	0.49
2:L:161:GLN:O	2:L:164:VAL:HG12	2.14	0.48
1:A:44:GLU:OE1	1:A:46:ARG:HB3	2.13	0.48
2:L:12:PRO:HG2	4:L:358:HOH:O	2.12	0.48
2:B:31:HIS:ND1	2:B:32:SER:N	2.61	0.48
1:A:191:TRP:N	1:A:192:PRO:HD2	2.29	0.48
2:B:203:HIS:CD2	2:B:204:LYS:H	2.32	0.48
2:L:2:ILE:CD1	2:L:27:LYS:H	2.26	0.48
2:L:120:VAL:HA	2:L:140:PHE:O	2.14	0.48
1:A:2:VAL:HA	1:A:25:SER:O	2.14	0.48
2:B:154:LYS:HA	2:B:158:SER:O	2.13	0.48
1:A:46:ARG:HG2	4:A:343:HOH:O	2.14	0.48
1:A:22:CYS:HB3	1:A:80:LEU:HB3	1.94	0.48
1:A:142:GLY:C	4:A:319:HOH:O	2.56	0.47
1:A:182:SER:C	4:A:262:HOH:O	2.57	0.47
2:B:197:TYR:HD1	4:B:828:HOH:O	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:GLU:HG3	1:H:46:ARG:N	2.24	0.47
1:H:171:ALA:HA	1:H:180:MET:HB3	1.95	0.47
1:A:88:ARG:HD2	4:A:281:HOH:O	2.13	0.47
1:H:191:TRP:N	1:H:192:PRO:HD2	2.28	0.47
2:B:204:LYS:HB2	4:B:753:HOH:O	2.14	0.47
2:L:15:LEU:HD21	2:L:111:ILE:HD13	1.96	0.47
2:B:14:THR:HG23	4:B:748:HOH:O	2.14	0.47
2:L:154:LYS:HA	2:L:158:SER:O	2.13	0.47
1:A:49:TRP:CG	2:B:101:PRO:HD2	2.49	0.47
1:A:171:ALA:HA	1:A:180:MET:HB3	1.97	0.47
2:B:2:ILE:CD1	2:B:27:LYS:H	2.27	0.47
2:B:82:ARG:HG2	2:B:82:ARG:HH11	1.80	0.47
2:B:120:VAL:HA	2:B:140:PHE:O	2.14	0.47
2:L:2:ILE:HD11	2:L:27:LYS:H	1.79	0.47
2:L:195:ASN:HB2	4:L:373:HOH:O	2.14	0.47
2:B:56:MET:O	2:B:69:SER:HB3	2.15	0.47
1:H:22:CYS:HB3	1:H:80:LEU:HB3	1.97	0.47
1:H:136:GLY:C	1:H:188:SER:HB2	2.40	0.47
2:B:152:LYS:HD2	2:B:159:GLU:CD	2.40	0.46
2:L:81:SER:CA	4:L:345:HOH:O	2.59	0.46
2:L:82:ARG:HG2	2:L:82:ARG:HH11	1.80	0.46
1:A:39:VAL:HG13	1:A:48:GLU:O	2.16	0.46
2:B:2:ILE:HD11	2:B:27:LYS:H	1.79	0.46
2:L:45:PRO:HB3	2:L:170:ASP:OD2	2.15	0.46
2:L:152:LYS:HD2	2:L:159:GLU:CD	2.39	0.46
1:A:136:GLY:C	1:A:188:SER:HB2	2.41	0.46
2:L:25:SER:HB3	4:L:375:HOH:O	2.16	0.46
1:H:13:LYS:HD3	1:H:115:SER:O	2.15	0.46
1:A:3:LYS:NZ	4:A:338:HOH:O	2.49	0.46
1:A:141:LEU:HD13	1:A:213:LEU:HD12	1.98	0.46
2:B:82:ARG:HG2	2:B:82:ARG:NH1	2.30	0.45
2:B:146:PRO:HD3	4:B:762:HOH:O	2.16	0.45
1:H:157:TRP:C	1:H:159:SER:N	2.73	0.45
2:L:82:ARG:HG2	2:L:82:ARG:NH1	2.30	0.45
2:L:130:LEU:HD23	2:L:134:GLY:O	2.16	0.45
1:A:193:SER:O	1:A:195:THR:HB	2.17	0.45
2:L:6:GLN:HE22	2:L:92:TYR:HA	1.81	0.45
1:A:23:THR:N	4:A:331:HOH:O	2.49	0.45
2:B:184:LEU:HD13	2:B:184:LEU:C	2.42	0.45
1:A:167:HIS:N	4:A:330:HOH:O	2.49	0.45
1:H:3:LYS:HB2	1:H:3:LYS:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:MET:SD	4:B:851:HOH:O	2.61	0.45
1:H:193:SER:O	1:H:195:THR:HB	2.17	0.45
1:A:140:THR:HA	4:A:291:HOH:O	2.17	0.45
2:B:130:LEU:HD23	2:B:134:GLY:O	2.16	0.45
1:A:158:ASN:C	1:A:160:GLY:H	2.25	0.45
1:H:139:VAL:HA	4:H:639:HOH:O	2.16	0.44
1:A:5:LEU:N	4:A:331:HOH:O	2.39	0.44
2:B:2:ILE:HD13	2:B:27:LYS:CB	2.43	0.44
2:L:184:LEU:HD13	2:L:184:LEU:C	2.42	0.44
2:B:2:ILE:HG21	2:B:95:GLN:CD	2.42	0.44
2:L:202:THR:N	4:L:357:HOH:O	2.50	0.44
2:B:2:ILE:C	4:B:851:HOH:O	2.61	0.44
2:L:61:SER:HA	4:L:280:HOH:O	2.17	0.44
1:A:157:TRP:C	1:A:159:SER:H	2.26	0.44
1:A:157:TRP:C	1:A:159:SER:N	2.73	0.44
2:B:120:VAL:CG1	4:B:832:HOH:O	2.63	0.44
2:L:154:LYS:HG2	4:L:377:HOH:O	2.18	0.44
1:A:151:GLU:N	1:A:152:PRO:CD	2.81	0.44
1:A:141:LEU:HD13	1:A:213:LEU:CD1	2.48	0.43
2:B:193:ARG:NH2	4:B:829:HOH:O	2.50	0.43
2:L:76:PHE:HZ	4:L:375:HOH:O	2.00	0.43
1:H:202:HIS:NE2	1:H:204:ALA:HB3	2.33	0.43
1:A:38:TRP:CE2	1:A:82:LEU:HB2	2.53	0.43
1:H:158:ASN:C	1:H:160:GLY:H	2.26	0.43
1:A:134:THR:HG22	1:A:134:THR:O	2.18	0.43
1:A:158:ASN:O	1:A:159:SER:HB2	2.18	0.43
2:B:154:LYS:HE2	2:B:200:GLU:OE2	2.19	0.43
1:H:122:PRO:HD3	1:H:202:HIS:ND1	2.34	0.43
2:B:2:ILE:HG23	2:B:2:ILE:O	2.19	0.43
2:B:121:SER:C	4:B:832:HOH:O	2.60	0.43
1:H:157:TRP:C	1:H:159:SER:H	2.27	0.43
1:H:158:ASN:O	1:H:159:SER:HB2	2.19	0.43
1:H:141:LEU:HD11	1:H:191:TRP:NE1	2.34	0.43
2:L:25:SER:CB	4:L:375:HOH:O	2.67	0.43
2:B:2:ILE:HG23	2:B:102:THR:OG1	2.18	0.43
2:B:88:VAL:HG12	2:B:111:ILE:HG12	2.00	0.43
1:H:78:ASN:ND2	4:H:633:HOH:O	2.51	0.42
1:H:141:LEU:HD11	1:H:191:TRP:HE1	1.83	0.42
1:H:85:SER:HB2	4:H:676:HOH:O	2.19	0.42
1:H:187:PRO:HG2	1:H:190:THR:CG2	2.48	0.42
1:A:5:LEU:C	4:A:331:HOH:O	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ALA:HB2	4:A:345:HOH:O	2.19	0.42
1:A:141:LEU:HD11	1:A:191:TRP:HE1	1.85	0.42
2:L:140:PHE:C	2:L:141:LEU:HD12	2.44	0.42
1:H:134:THR:O	1:H:134:THR:HG22	2.19	0.42
2:L:154:LYS:HE2	2:L:200:GLU:OE2	2.19	0.42
1:H:141:LEU:HD13	1:H:213:LEU:HD12	2.01	0.42
2:L:2:ILE:HG21	2:L:95:GLN:CD	2.44	0.42
2:L:65:ASN:C	2:L:65:ASN:HD22	2.26	0.42
1:A:92:THR:O	1:A:93:ALA:HB2	2.20	0.42
1:H:192:PRO:HD3	4:H:668:HOH:O	2.20	0.42
2:L:2:ILE:HD13	2:L:27:LYS:CB	2.43	0.42
2:B:135:ALA:O	2:B:186:LEU:HD12	2.19	0.42
1:H:2:VAL:HA	1:H:25:SER:O	2.19	0.42
2:B:56:MET:HE1	2:B:76:PHE:HD2	1.85	0.42
2:B:75:ASP:CA	4:B:843:HOH:O	2.56	0.42
1:H:38:TRP:CE2	1:H:82:LEU:HB2	2.55	0.42
1:A:44:GLU:HG3	1:A:46:ARG:N	2.24	0.42
2:B:140:PHE:C	2:B:141:LEU:HD12	2.45	0.42
2:B:140:PHE:HB3	2:B:142:ASN:ND2	2.35	0.42
1:H:205:SER:HB2	4:H:678:HOH:O	2.19	0.41
2:L:29:LEU:HD22	4:L:375:HOH:O	2.20	0.41
2:L:2:ILE:CD1	2:L:27:LYS:N	2.84	0.41
1:A:12:VAL:O	1:A:114:VAL:HA	2.21	0.41
2:B:36:THR:HG21	2:B:56:MET:HE2	2.01	0.41
2:B:6:GLN:HE22	2:B:92:TYR:HA	1.84	0.41
1:H:169:PHE:CD1	2:L:169:THR:HG23	2.55	0.41
2:B:151:VAL:HA	2:B:200:GLU:O	2.20	0.41
2:L:2:ILE:HG23	2:L:2:ILE:O	2.21	0.41
1:A:56:GLY:HA3	4:A:251:HOH:O	2.19	0.41
2:B:2:ILE:CD1	2:B:27:LYS:N	2.84	0.41
1:A:141:LEU:HD11	1:A:191:TRP:NE1	2.36	0.41
1:H:19:LYS:HE3	1:H:81:TYR:CD2	2.55	0.41
2:L:140:PHE:HB3	2:L:142:ASN:ND2	2.35	0.41
1:A:29:PHE:CE2	1:A:36:MET:HE2	2.56	0.41
1:H:115:SER:HB2	4:H:640:HOH:O	2.20	0.41
2:B:193:ARG:HG3	2:B:194:HIS:CE1	2.56	0.41
1:H:42:ILE:CG1	1:H:44:GLU:HG2	2.51	0.41
1:H:141:LEU:HD13	1:H:213:LEU:CD1	2.51	0.41
2:B:65:ASN:C	2:B:65:ASN:HD22	2.28	0.41
1:H:49:TRP:CG	2:L:101:PRO:HD2	2.56	0.41
1:A:122:PRO:HD3	1:A:202:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:HIS:NE2	1:A:204:ALA:HB3	2.36	0.41
2:B:137:VAL:HG13	2:B:153:TRP:CH2	2.56	0.41
1:A:19:LYS:HE3	1:A:81:TYR:CD2	2.56	0.40
2:L:151:VAL:HA	2:L:200:GLU:O	2.20	0.40
2:L:207:THR:O	2:L:207:THR:HG22	2.21	0.40
2:L:2:ILE:HG23	2:L:102:THR:OG1	2.20	0.40
1:A:117:ALA:HB3	1:A:149:PHE:CE2	2.57	0.40
1:A:166:VAL:HG12	4:A:286:HOH:O	2.22	0.40
2:B:122:ILE:HG13	2:B:139:CYS:HB3	2.03	0.40
1:H:157:TRP:O	1:H:159:SER:N	2.55	0.40
2:L:55:GLN:O	2:L:56:MET:HB3	2.21	0.40
2:L:193:ARG:HG3	2:L:194:HIS:CE1	2.56	0.40

All (1) 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:L:32:SER:OG	4:L:345:HOH:O[4_544]	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	A	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	9	4
1	H	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	9	4
2	B	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	24	21
2	L	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	24	21
All	All	838/846 (99%)	784 (94%)	46 (6%)	8 (1%)	12	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	135	THR
1	A	135	THR
2	L	193	ARG
2	B	193	ARG
1	H	138	SER
1	A	138	SER
1	H	132	GLY
1	A	132	GLY

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	177/177 (100%)	172 (97%)	5 (3%)	38	41
1	H	177/177 (100%)	173 (98%)	4 (2%)	44	49
2	B	188/188 (100%)	185 (98%)	3 (2%)	55	62
2	L	188/188 (100%)	186 (99%)	2 (1%)	65	73
All	All	730/730 (100%)	716 (98%)	14 (2%)	50	56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	LYS
1	H	80	LEU
1	H	82	LEU
1	H	146	LYS
2	L	29	LEU
2	L	65	ASN
1	A	3	LYS
1	A	80	LEU
1	A	82	LEU
1	A	119	THR
1	A	146	LYS
2	B	29	LEU
2	B	65	ASN
2	B	76	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	174	GLN
2	L	6	GLN
2	L	65	ASN
2	L	142	ASN
2	L	166	ASN
2	L	171	GLN
2	L	203	HIS
1	A	108	GLN
1	A	174	GLN
2	B	6	GLN
2	B	65	ASN
2	B	142	ASN
2	B	171	GLN
2	B	203	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	SPB	B	701	-	24,24,24	2.00	9 (37%)	30,30,30	1.20	3 (10%)
3	SPB	H	601	-	24,24,24	1.91	9 (37%)	30,30,30	1.26	3 (10%)

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	SPB	B	701	-	-	6/15/15/15	0/2/2/2
3	SPB	H	601	-	-	3/15/15/15	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	SPB	O21-C20	4.85	1.38	1.22
3	H	601	SPB	O21-C20	4.61	1.37	1.22
3	H	601	SPB	C11-C12	2.75	1.43	1.39
3	B	701	SPB	C11-C12	2.68	1.43	1.39
3	H	601	SPB	C5-C6	2.50	1.44	1.39
3	B	701	SPB	C5-C6	2.44	1.44	1.39
3	B	701	SPB	C14-C9	2.42	1.44	1.39
3	B	701	SPB	C13-C12	2.39	1.43	1.39
3	H	601	SPB	C14-C9	2.35	1.44	1.39
3	B	701	SPB	O23-C20	-2.29	1.23	1.30
3	B	701	SPB	C4-C5	2.20	1.42	1.38
3	H	601	SPB	C6-C7	2.19	1.53	1.47
3	B	701	SPB	C9-C8	2.12	1.53	1.47
3	H	601	SPB	O23-C20	-2.07	1.24	1.30
3	B	701	SPB	C6-C7	2.03	1.53	1.47
3	H	601	SPB	C4-C3	2.02	1.42	1.38
3	H	601	SPB	C1-C6	2.02	1.43	1.39
3	H	601	SPB	C2-C1	2.00	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	601	SPB	O21-C20-C19	-3.64	111.56	123.09
3	B	701	SPB	O21-C20-C19	-3.31	112.60	123.09
3	B	701	SPB	C12-N15-C16	3.20	133.19	127.52
3	H	601	SPB	O23-C20-C19	3.05	123.64	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	601	SPB	C12-N15-C16	2.91	132.68	127.52
3	B	701	SPB	O23-C20-C19	2.86	123.02	114.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

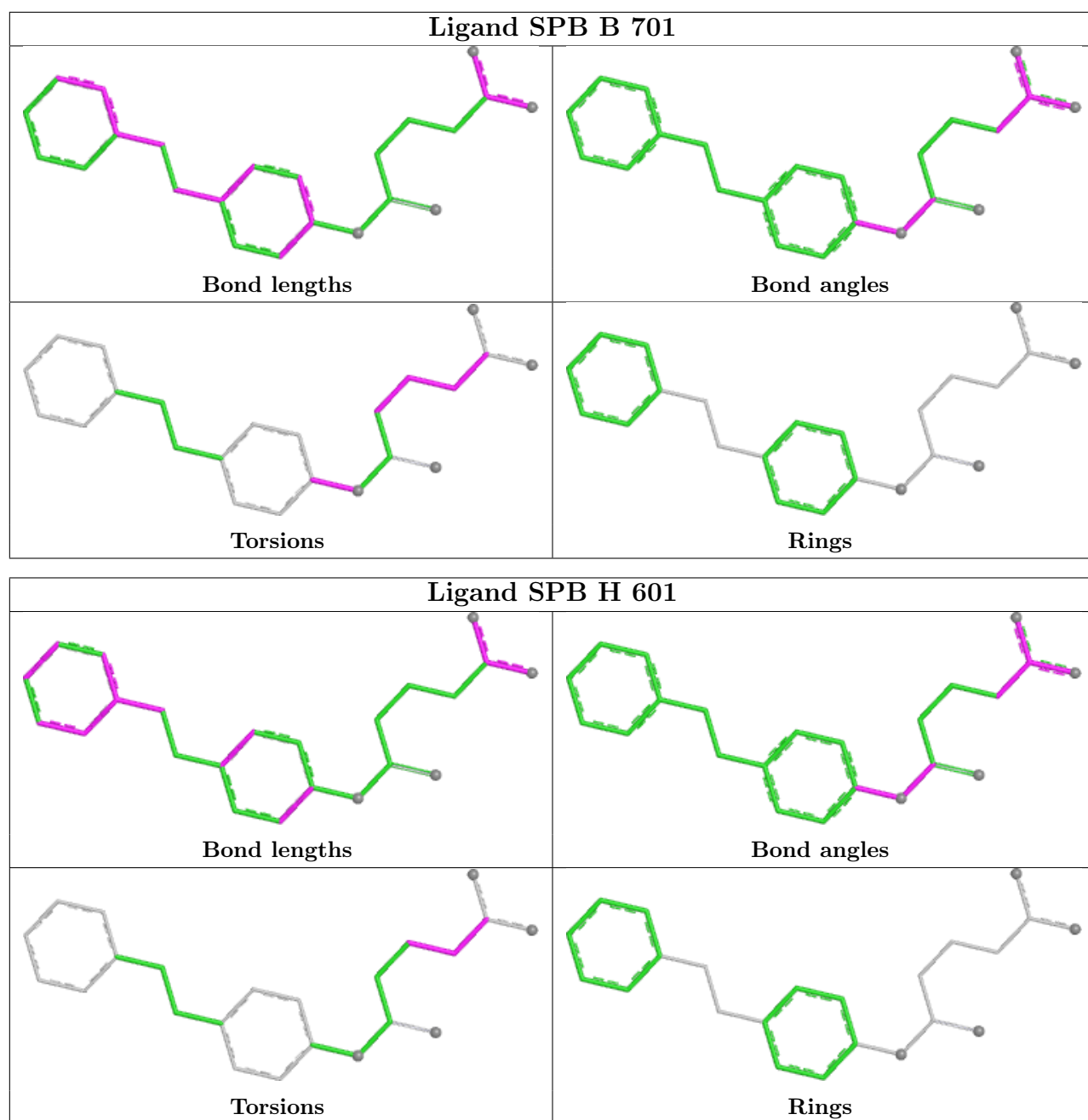
Mol	Chain	Res	Type	Atoms
3	B	701	SPB	C16-C17-C18-C19
3	H	601	SPB	C17-C18-C19-C20
3	B	701	SPB	C17-C18-C19-C20
3	B	701	SPB	C13-C12-N15-C16
3	B	701	SPB	C18-C19-C20-O23
3	B	701	SPB	C18-C19-C20-O21
3	H	601	SPB	C18-C19-C20-O23
3	B	701	SPB	C11-C12-N15-C16
3	H	601	SPB	C18-C19-C20-O21

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	SPB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/209 (100%)	1.10	53 (25%) 1 1	16, 42, 83, 96	0
1	H	209/209 (100%)	1.15	46 (22%) 2 2	17, 43, 84, 96	0
2	B	214/214 (100%)	1.33	72 (33%) 1 1	17, 42, 83, 90	0
2	L	214/214 (100%)	1.14	58 (27%) 1 1	15, 36, 83, 90	0
All	All	846/846 (100%)	1.18	229 (27%) 1 1	15, 42, 83, 96	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	191	TRP	7.2
1	A	191	TRP	6.9
2	B	196	GLY	6.0
1	A	129	PRO	5.8
2	L	197	TYR	5.5
2	L	214	PHE	5.3
2	L	160	ARG	5.2
1	A	186	VAL	5.1
2	B	72	SER	4.9
2	B	197	TYR	4.9
1	H	132	GLY	4.9
1	H	136	GLY	4.8
1	A	127	ALA	4.8
2	B	208	SER	4.7
2	L	196	GLY	4.6
2	L	209	PRO	4.6
1	H	135	THR	4.5
2	B	207	THR	4.5
2	L	201	ALA	4.5
2	B	210	ILE	4.5
2	B	214	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	45	LYS	4.3
2	L	184	LEU	4.2
1	A	43	PRO	4.2
1	A	135	THR	4.1
2	L	202	THR	4.1
2	B	202	THR	4.1
2	L	155	ILE	4.1
2	L	195	ASN	4.0
1	A	212	LYS	4.0
2	B	140	PHE	4.0
1	A	141	LEU	4.0
1	H	192	PRO	4.0
2	L	193	ARG	4.0
1	H	189	SER	3.9
2	L	189	ASP	3.9
1	A	137	SER	3.8
2	B	194	HIS	3.8
1	A	44	GLU	3.8
1	A	133	ASP	3.8
1	A	187	PRO	3.8
2	B	175	ASP	3.8
1	A	196	VAL	3.7
1	H	42	ILE	3.7
2	B	187	THR	3.7
1	H	119	THR	3.7
1	H	129	PRO	3.7
1	H	188	SER	3.7
2	L	190	GLU	3.7
1	A	204	ALA	3.6
2	B	209	PRO	3.6
2	L	203	HIS	3.5
1	H	213	LEU	3.5
2	B	189	ASP	3.5
1	A	160	GLY	3.5
2	B	145	TYR	3.5
1	A	128	ALA	3.5
1	A	138	SER	3.4
1	H	196	VAL	3.4
2	B	144	PHE	3.4
2	B	116	ALA	3.4
2	B	120	VAL	3.4
1	H	43	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	208	SER	3.3
2	L	175	ASP	3.3
1	H	130	GLY	3.3
2	L	157	GLY	3.3
2	B	195	ASN	3.3
2	B	201	ALA	3.2
1	H	206	SER	3.2
1	A	161	GLY	3.2
2	B	46	GLY	3.2
2	L	2	ILE	3.2
1	H	134	THR	3.2
1	A	134	THR	3.2
2	L	210	ILE	3.1
1	A	192	PRO	3.1
1	H	166	VAL	3.1
2	L	164	VAL	3.1
1	A	42	ILE	3.1
1	A	130	GLY	3.1
1	H	186	VAL	3.1
1	A	197	THR	3.0
2	L	194	HIS	3.0
1	A	131	CYS	3.0
2	B	199	CYS	3.0
2	B	205	THR	3.0
1	H	152	PRO	3.0
1	A	116	SER	3.0
2	B	186	LEU	3.0
1	A	126	PRO	3.0
2	L	152	LYS	3.0
2	L	191	TYR	3.0
1	H	131	CYS	2.9
2	L	163	GLY	2.9
2	L	156	ASP	2.9
2	L	130	LEU	2.9
2	L	139	CYS	2.9
2	L	149	ILE	2.9
1	H	195	THR	2.9
2	L	205	THR	2.9
1	A	189	SER	2.9
2	B	173	SER	2.9
2	L	199	CYS	2.9
1	H	160	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	132	GLY	2.9
2	L	47	GLN	2.8
2	B	160	ARG	2.8
2	B	206	SER	2.8
2	L	121	SER	2.8
2	L	173	SER	2.8
2	B	191	TYR	2.8
1	A	119	THR	2.8
2	L	120	VAL	2.8
2	L	192	GLU	2.8
1	A	136	GLY	2.8
2	B	163	GLY	2.8
2	B	143	ASN	2.7
2	B	84	GLU	2.7
1	A	45	LYS	2.7
2	B	114	ALA	2.7
1	H	120	THR	2.7
2	B	150	ASN	2.7
2	B	32	SER	2.7
2	B	168	TRP	2.7
2	L	140	PHE	2.7
2	B	149	ILE	2.7
2	B	121	SER	2.7
2	B	132	SER	2.7
1	H	161	GLY	2.7
1	A	164	SER	2.7
2	L	151	VAL	2.7
1	H	133	ASP	2.7
1	A	1	GLU	2.6
2	B	135	ALA	2.6
1	A	142	GLY	2.6
2	L	207	THR	2.6
2	B	184	LEU	2.6
1	H	212	LYS	2.6
2	B	85	ALA	2.6
2	B	118	PRO	2.6
2	B	139	CYS	2.5
2	L	150	ASN	2.5
2	B	88	VAL	2.5
1	H	140	THR	2.5
1	H	190	THR	2.5
2	L	198	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	44	GLU	2.5
1	H	137	SER	2.5
2	L	45	PRO	2.5
2	B	10	SER	2.5
1	A	213	LEU	2.5
2	B	76	PHE	2.5
1	A	175	SER	2.5
1	A	185	THR	2.5
2	L	206	SER	2.5
1	H	149	PHE	2.5
2	B	133	GLY	2.5
2	L	162	ASN	2.5
2	B	192	GLU	2.4
2	B	154	LYS	2.4
2	L	137	VAL	2.4
2	L	211	VAL	2.4
2	B	172	ASP	2.4
2	L	200	GLU	2.4
1	H	187	PRO	2.4
2	L	135	ALA	2.3
2	L	159	GLU	2.3
2	B	141	LEU	2.3
1	A	184	VAL	2.3
1	H	151	GLU	2.3
1	A	152	PRO	2.3
2	B	169	THR	2.3
2	B	119	THR	2.3
2	L	148	ASP	2.3
2	B	130	LEU	2.3
2	L	154	LYS	2.3
1	A	165	SER	2.3
2	B	158	SER	2.3
2	B	203	HIS	2.3
1	H	153	VAL	2.3
2	B	138	VAL	2.3
1	A	195	THR	2.3
2	L	117	ALA	2.3
1	A	167	HIS	2.2
1	A	139	VAL	2.2
1	A	166	VAL	2.2
1	H	204	ALA	2.2
2	L	133	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	181	SER	2.2
1	A	183	SER	2.2
1	H	158	ASN	2.2
2	B	198	THR	2.2
1	H	127	ALA	2.2
1	A	188	SER	2.2
2	L	61	SER	2.2
2	B	204	LYS	2.2
1	A	158	ASN	2.2
1	H	121	PRO	2.1
1	H	150	PRO	2.1
2	B	183	THR	2.2
2	B	200	GLU	2.1
2	B	142	ASN	2.1
2	B	180	MET	2.1
1	H	214	GLU	2.1
2	L	153	TRP	2.1
2	B	2	ILE	2.1
2	L	79	ARG	2.1
2	B	165	LEU	2.1
1	A	151	GLU	2.1
2	B	155	ILE	2.1
1	H	175	SER	2.1
2	B	157	GLY	2.1
2	B	153	TRP	2.1
1	A	193	SER	2.1
1	A	46	ARG	2.0
1	H	156	THR	2.0
1	H	203	PRO	2.0
1	H	208	THR	2.0
1	A	156	THR	2.0
2	L	146	PRO	2.0
2	L	134	GLY	2.0
1	H	139	VAL	2.0
2	B	123	PHE	2.0
2	B	137	VAL	2.0
2	B	211	VAL	2.0
2	B	166	ASN	2.0
1	A	5	LEU	2.0
2	L	82	ARG	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](#)

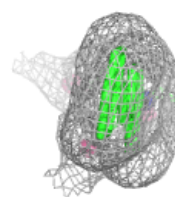
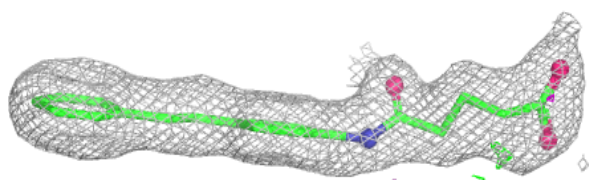
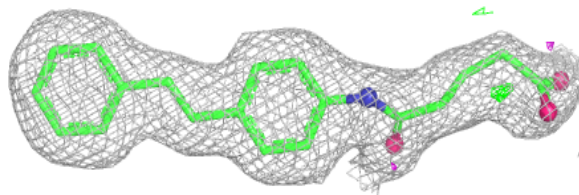
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SPB	H	601	23/23	0.93	0.08	15,22,46,48	0
3	SPB	B	701	23/23	0.93	0.09	15,21,45,54	0

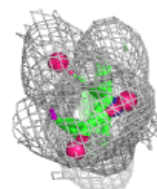
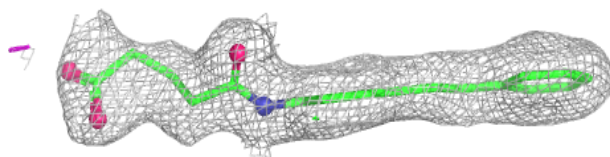
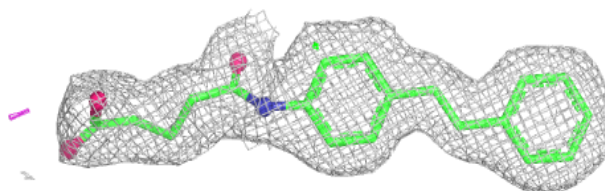
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SPB H 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SPB B 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.