



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:48 PM UTC

PDB ID : 1KFA / pdb_00001kfa
Title : Crystal structure of Fab fragment complexed with gibberellin A4
Authors : Murata, T.; Fushinobu, S.; Nakajima, M.; Asami, O.; Sassa, T.; Wakagi, T.; Yamaguchi, I.
Deposited on : 2001-11-20
Resolution : 2.80 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

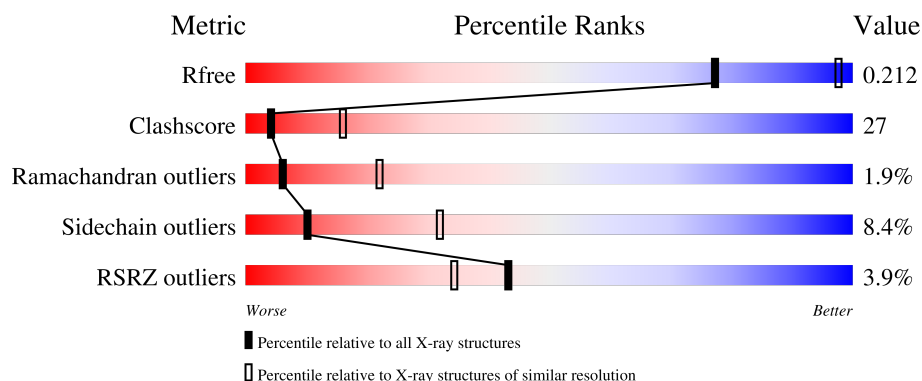
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	217	3% 55% 40% 5%
1	M	217	6% 50% 42% 6%
2	H	221	2% 53% 34% 8%
2	I	221	4% 51% 35% 8% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6677 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.

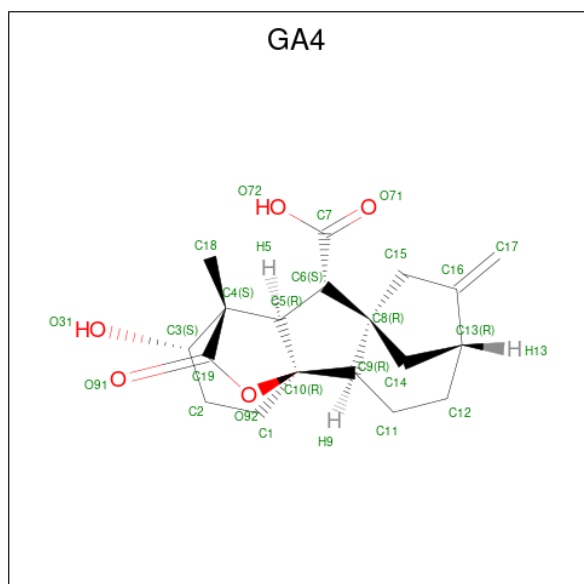
- Molecule 1 is a protein called monoclonal antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1671	1043	284	338	6			
1	M	213	Total	C	N	O	S	0	0	0
			1635	1021	276	332	6			

- Molecule 2 is a protein called monoclonal antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1616	1021	268	317	10			
2	I	209	Total	C	N	O	S	0	0	0
			1589	1006	264	309	10			

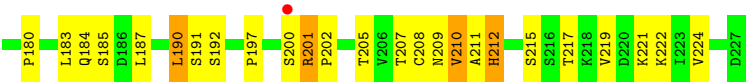
- Molecule 3 is GIBBERELLIN A4 (CCD ID: GA4) (formula: $C_{19}H_{24}O_5$).



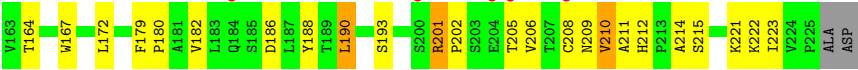
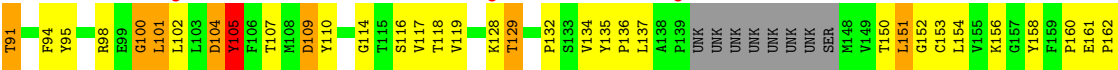
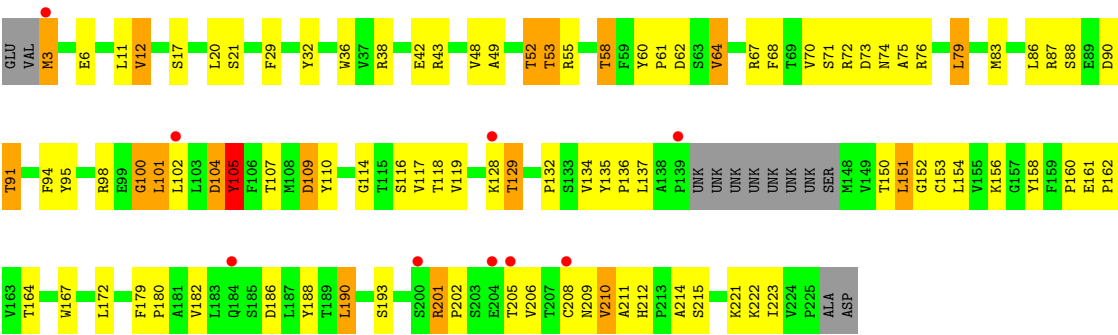
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	24	0
			24	19	5		
3	I	1	Total	C	O	24	0
			24	19	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	26	Total	O	0	0
			26	26		
4	H	44	Total	O	0	0
			44	44		
4	M	18	Total	O	0	0
			18	18		
4	I	30	Total	O	0	0
			30	30		



● Molecule 2: monoclonal antibody heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.08Å 150.15Å 106.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 2.80 39.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.62-2.80) 99.9 (39.62-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.313 0.222 , 0.212	Depositor DCC
R_{free} test set	1340 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.75% 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: GA4

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	0.43	0/1710	0.90	4/2316 (0.2%)
1	M	0.39	0/1673	0.87	3/2268 (0.1%)
2	H	0.50	0/1655	1.01	11/2256 (0.5%)
2	I	0.46	0/1628	1.01	7/2220 (0.3%)
All	All	0.45	0/6666	0.95	25/9060 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	100	GLY	N-CA-C	10.11	124.23	112.50
2	H	100	GLY	N-CA-C	9.37	125.50	114.16
1	L	62	GLY	N-CA-C	-6.47	97.84	113.18
2	H	70	VAL	CB-CA-C	-6.29	104.67	111.59
1	M	142	ASN	N-CA-C	6.16	118.66	110.53
2	H	33	ALA	N-CA-C	-6.13	101.40	110.48
2	H	105	TYR	N-CA-C	5.95	123.48	110.80
2	I	161	GLU	N-CA-C	-5.91	102.45	110.36
2	I	62	ASP	N-CA-C	5.86	118.15	111.11
2	I	105	TYR	N-CA-C	5.76	123.06	110.80
1	L	142	ASN	N-CA-C	5.60	119.22	110.32
2	H	42	GLU	N-CA-C	-5.51	106.63	113.19
2	H	217	THR	N-CA-C	5.46	117.99	108.76
2	H	212	HIS	CA-C-N	5.39	125.46	119.32
2	H	212	HIS	C-N-CA	5.39	125.46	119.32
1	M	66	ARG	N-CA-C	-5.37	106.70	113.20
2	I	156	LYS	N-CA-C	5.37	118.31	109.72
1	L	63	PHE	CA-C-N	5.34	125.81	120.52
1	L	63	PHE	C-N-CA	5.34	125.81	120.52
2	H	60	TYR	N-CA-C	5.27	114.20	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	78	THR	N-CA-C	5.25	117.64	108.76
1	M	93	CYS	N-CA-C	-5.11	102.22	110.14
2	I	116	SER	N-CA-C	5.10	117.92	109.46
2	I	186	ASP	N-CA-C	-5.10	105.37	112.30
2	H	155	VAL	N-CA-C	-5.04	100.64	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1671	0	1607	83	0
1	M	1635	0	1574	97	1
2	H	1616	0	1589	90	0
2	I	1589	0	1566	92	0
3	H	24	0	24	0	0
3	I	24	0	24	0	0
4	H	44	0	0	3	0
4	I	30	0	0	1	0
4	L	26	0	0	0	0
4	M	18	0	0	0	0
All	All	6677	0	6384	351	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 27.

All (351) 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:201:ARG:HG2	2:H:202:PRO:HA	1.10	1.10
2:H:201:ARG:HH11	2:H:201:ARG:HB3	1.13	1.09
2:I:201:ARG:HH11	2:I:201:ARG:HB3	1.18	1.04
2:I:201:ARG:HG2	2:I:202:PRO:HA	1.36	1.01
1:L:21:ILE:HD12	1:L:107:THR:HG21	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:HIS:HD2	1:M:33:ASN:H	1.12	0.89
1:L:120:VAL:HA	1:L:140:PHE:O	1.71	0.88
1:M:95:GLN:HE22	1:M:98:HIS:H	1.15	0.87
1:L:95:GLN:HE22	1:L:98:HIS:H	1.15	0.86
2:H:201:ARG:HB3	2:H:201:ARG:NH1	1.90	0.86
2:H:134:VAL:HG21	2:H:210:VAL:HG11	1.55	0.86
2:H:201:ARG:CG	2:H:202:PRO:HA	2.03	0.85
2:H:151:LEU:HD21	2:H:201:ARG:HD3	1.58	0.85
2:H:100:GLY:HA3	2:H:109:ASP:OD2	1.76	0.85
2:H:201:ARG:HG2	2:H:202:PRO:CA	2.03	0.85
1:M:31:HIS:CD2	1:M:33:ASN:H	1.95	0.84
2:I:88:SER:O	2:I:91:THR:HG23	1.78	0.83
1:L:85:ALA:HA	1:L:111:ILE:CD1	2.10	0.82
1:M:52:LEU:HD23	1:M:53:ILE:HG13	1.64	0.80
1:L:31:HIS:HD2	1:L:33:ASN:H	1.30	0.80
2:H:49:ALA:HB1	2:H:70:VAL:HG22	1.66	0.78
1:L:85:ALA:HA	1:L:111:ILE:HD11	1.67	0.77
2:I:12:VAL:HG21	2:I:86:LEU:HD13	1.65	0.77
1:M:8:PRO:HG3	1:M:11:LEU:HD13	1.67	0.76
1:M:38:LEU:HD22	1:M:76:PHE:CG	2.22	0.74
2:I:151:LEU:HD21	2:I:201:ARG:HD3	1.68	0.73
1:M:189:ASP:HB3	1:M:193:ARG:HH21	1.54	0.72
2:I:49:ALA:HB1	2:I:70:VAL:CG2	2.19	0.72
2:I:83:MET:HE2	2:I:86:LEU:HD21	1.70	0.72
2:H:72:ARG:HE	2:H:74:ASN:HD21	1.34	0.72
2:I:72:ARG:HE	2:I:74:ASN:HD21	1.38	0.72
1:L:17:ASP:O	1:L:83:VAL:HG23	1.90	0.72
2:I:201:ARG:HB3	2:I:201:ARG:NH1	2.01	0.72
1:L:120:VAL:HB	1:L:141:LEU:HD13	1.72	0.71
1:M:156:ASP:HA	1:M:196:SER:HB3	1.73	0.71
1:M:13:VAL:HG11	1:M:83:VAL:HG21	1.72	0.71
2:I:132:PRO:HB3	2:I:158:TYR:HB3	1.71	0.71
1:L:155:ILE:CD1	1:L:160:ARG:HG3	2.21	0.71
1:M:138:VAL:HG22	1:M:183:THR:HG23	1.73	0.70
2:I:128:LYS:HD3	2:I:129:THR:H	1.55	0.70
1:L:31:HIS:CD2	1:L:33:ASN:H	2.10	0.70
1:M:88:LEU:HD23	1:M:88:LEU:O	1.91	0.70
1:M:31:HIS:HD2	1:M:33:ASN:N	1.88	0.69
1:M:14:SER:O	1:M:17:ASP:HB2	1.92	0.69
2:H:52:THR:HG22	2:H:55:ARG:H	1.58	0.69
2:H:49:ALA:HB1	2:H:70:VAL:CG2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:52:THR:HG22	2:I:55:ARG:H	1.59	0.68
1:L:197:TYR:O	1:L:213:SER:HB2	1.92	0.67
1:M:110:GLU:HG2	1:M:111:ILE:N	2.08	0.67
1:M:66:ARG:HH22	1:M:87:ASP:CG	2.02	0.67
2:H:212:HIS:HD2	2:H:215:SER:OG	1.78	0.66
1:L:129:GLN:HG2	1:L:134:GLY:O	1.95	0.66
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.26	0.66
2:H:190:LEU:HD12	2:H:190:LEU:C	2.21	0.66
1:L:203:HIS:HD2	1:L:205:THR:OG1	1.78	0.66
2:H:132:PRO:HB3	2:H:158:TYR:HB3	1.79	0.66
2:H:3:MET:HB3	2:H:25:SER:OG	1.95	0.65
2:H:58:THR:HG23	2:H:60:TYR:CE1	2.31	0.65
1:M:111:ILE:H	1:M:171:GLN:HE22	1.45	0.64
2:I:137:LEU:HB2	2:I:152:GLY:C	2.21	0.64
2:I:201:ARG:CG	2:I:202:PRO:HA	2.21	0.64
1:L:154:LYS:HA	1:L:158:SER:O	1.98	0.64
1:L:137:VAL:CG1	1:L:184:LEU:HB3	2.27	0.64
1:M:39:HIS:HB3	1:M:54:TYR:HA	1.80	0.64
1:L:155:ILE:HD12	1:L:160:ARG:HG3	1.79	0.63
1:M:85:ALA:HA	1:M:111:ILE:CD1	2.28	0.63
2:I:212:HIS:HD2	2:I:215:SER:OG	1.81	0.63
1:L:120:VAL:HG22	1:L:212:LYS:HG3	1.81	0.63
2:H:88:SER:O	2:H:91:THR:HG23	1.99	0.63
1:M:155:ILE:CD1	1:M:160:ARG:HG3	2.27	0.62
1:L:198:THR:HG23	1:L:213:SER:HB3	1.80	0.62
1:L:85:ALA:HA	1:L:111:ILE:HD13	1.80	0.62
2:I:49:ALA:HB1	2:I:70:VAL:HG21	1.82	0.62
2:H:52:THR:HG22	2:H:55:ARG:N	2.15	0.61
2:I:201:ARG:HH11	2:I:201:ARG:CB	2.02	0.61
1:M:127:SER:O	1:M:131:THR:HG23	2.00	0.61
1:L:14:SER:O	1:L:17:ASP:HB2	2.01	0.61
2:H:12:VAL:CG2	2:H:119:VAL:HG22	2.31	0.61
2:I:67:ARG:NH2	2:I:90:ASP:OD2	2.34	0.60
1:M:140:PHE:C	1:M:141:LEU:HD22	2.25	0.60
1:L:126:SER:OG	2:H:135:TYR:HB3	2.01	0.60
2:H:160:PRO:HB2	4:H:312:HOH:O	2.00	0.60
2:I:190:LEU:C	2:I:190:LEU:HD12	2.26	0.60
1:L:111:ILE:H	1:L:171:GLN:HE22	1.48	0.60
2:H:134:VAL:CG2	2:H:210:VAL:HG11	2.27	0.60
2:I:43:ARG:HA	2:I:43:ARG:HH11	1.66	0.60
1:M:156:ASP:OD2	1:M:194:HIS:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:88:SER:O	2:I:91:THR:CG2	2.48	0.59
1:M:110:GLU:HG2	1:M:111:ILE:H	1.67	0.59
2:I:164:THR:OG1	2:I:211:ALA:HB3	2.02	0.59
2:H:154:LEU:HD22	2:H:156:LYS:HB2	1.82	0.59
2:I:52:THR:CG2	2:I:55:ARG:H	2.15	0.59
1:L:88:LEU:HD12	1:L:171:GLN:HB3	1.83	0.58
1:M:57:SER:HB3	1:M:69:GLY:O	2.03	0.58
2:I:136:PRO:HG3	2:I:221:LYS:HE2	1.85	0.58
1:L:12:SER:O	1:L:112:LYS:HE3	2.03	0.58
2:H:134:VAL:HG21	2:H:210:VAL:CG1	2.29	0.58
1:L:110:GLU:HG2	1:L:111:ILE:N	2.17	0.58
1:M:9:LEU:C	1:M:107:THR:HG23	2.29	0.58
2:I:52:THR:HG22	2:I:55:ARG:N	2.18	0.58
2:H:83:MET:HE1	2:H:94:PHE:CZ	2.39	0.57
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.87	0.57
1:L:38:LEU:HD22	1:L:76:PHE:CG	2.39	0.57
1:M:175:ASP:OD1	1:M:177:THR:HG22	2.04	0.57
2:I:206:VAL:O	2:I:223:ILE:HG12	2.05	0.57
2:I:201:ARG:HG2	2:I:202:PRO:CA	2.23	0.56
1:L:44:LYS:HE2	1:L:86:GLU:O	2.04	0.56
2:H:68:PHE:CZ	2:H:83:MET:HE2	2.41	0.56
1:M:197:TYR:O	1:M:213:SER:HB2	2.05	0.56
2:I:151:LEU:HD23	2:I:206:VAL:HG11	1.88	0.56
1:M:137:VAL:CG1	1:M:184:LEU:HB3	2.35	0.56
2:H:12:VAL:HG23	2:H:119:VAL:HG22	1.87	0.56
1:M:120:VAL:HA	1:M:140:PHE:O	2.05	0.56
2:I:87:ARG:C	2:I:119:VAL:HG11	2.31	0.56
2:I:134:VAL:HG21	2:I:210:VAL:HG11	1.88	0.56
1:M:111:ILE:N	1:M:171:GLN:HE22	2.02	0.56
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.88	0.56
1:M:4:MET:HE3	1:M:23:CYS:SG	2.46	0.55
2:I:128:LYS:HD3	2:I:129:THR:N	2.21	0.55
1:L:95:GLN:HE22	1:L:98:HIS:N	1.96	0.55
2:H:177:HIS:O	2:H:192:SER:HA	2.07	0.55
1:M:13:VAL:CG1	1:M:83:VAL:HG21	2.35	0.55
1:M:189:ASP:HB3	1:M:193:ARG:NH2	2.20	0.55
2:I:134:VAL:CG2	2:I:210:VAL:HG11	2.36	0.55
1:L:153:TRP:O	1:L:159:GLU:HA	2.06	0.55
2:H:201:ARG:HH11	2:H:201:ARG:CB	2.02	0.55
2:I:58:THR:CG2	2:I:60:TYR:CE1	2.90	0.55
2:I:64:VAL:HG13	2:I:68:PHE:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:88:LEU:O	1:L:88:LEU:HD23	2.05	0.55
2:I:67:ARG:C	2:I:68:PHE:HD1	2.16	0.55
2:I:91:THR:HB	2:I:118:THR:HA	1.89	0.55
1:L:39:HIS:HB3	1:L:54:TYR:HA	1.89	0.54
2:H:55:ARG:HH11	2:H:55:ARG:HG3	1.72	0.54
2:I:76:ARG:HG3	2:I:76:ARG:HH11	1.73	0.54
2:H:42:GLU:CD	2:H:42:GLU:H	2.15	0.54
1:M:82:ARG:HH11	1:M:82:ARG:HG3	1.72	0.54
2:I:36:TRP:HE1	2:I:79:LEU:HD22	1.73	0.54
2:H:207:THR:HG23	2:H:221:LYS:C	2.34	0.53
1:L:38:LEU:HD22	1:L:76:PHE:CD2	2.43	0.53
1:M:52:LEU:HD23	1:M:52:LEU:C	2.32	0.53
2:I:42:GLU:O	2:I:43:ARG:HB2	2.07	0.53
1:L:25:SER:O	1:L:74:THR:HB	2.08	0.53
2:H:164:THR:OG1	2:H:211:ALA:HB3	2.09	0.53
1:M:192:GLU:C	1:M:194:HIS:H	2.15	0.53
1:M:8:PRO:CG	1:M:11:LEU:HD13	2.39	0.53
2:H:207:THR:HG23	2:H:221:LYS:O	2.08	0.53
1:M:167:SER:OG	2:I:180:PRO:HD2	2.08	0.53
2:I:48:VAL:O	2:I:49:ALA:HB2	2.09	0.52
2:H:52:THR:CG2	2:H:53:THR:N	2.72	0.52
2:H:205:THR:HB	2:H:222:LYS:HE3	1.91	0.52
1:L:15:LEU:HD21	1:L:111:ILE:HG21	1.91	0.52
1:M:38:LEU:HD22	1:M:76:PHE:CD2	2.44	0.52
1:L:8:PRO:HG2	1:L:10:SER:O	2.10	0.52
1:M:42:LEU:CD1	1:M:44:LYS:HG3	2.39	0.52
2:H:154:LEU:CD2	2:H:156:LYS:HB2	2.40	0.52
2:H:88:SER:O	2:H:91:THR:CG2	2.58	0.52
1:M:123:PHE:HZ	2:I:150:THR:O	1.93	0.51
2:I:71:SER:O	2:I:79:LEU:HD23	2.11	0.51
2:H:205:THR:HA	4:H:342:HOH:O	2.10	0.51
1:M:95:GLN:NE2	1:M:97:THR:H	2.08	0.51
1:L:60:PHE:O	1:L:62:GLY:N	2.43	0.51
1:M:155:ILE:HD12	1:M:160:ARG:HG3	1.91	0.51
2:H:12:VAL:O	2:H:119:VAL:HA	2.10	0.51
2:I:38:ARG:HD3	2:I:48:VAL:HG21	1.92	0.51
2:I:72:ARG:HE	2:I:74:ASN:ND2	2.06	0.51
2:H:150:THR:C	2:H:151:LEU:HD12	2.35	0.51
1:M:120:VAL:HB	1:M:141:LEU:HD13	1.92	0.51
2:H:6:GLU:CD	2:H:114:GLY:H	2.19	0.50
2:H:52:THR:CG2	2:H:55:ARG:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:LEU:HG	1:M:63:PHE:CD2	2.46	0.50
1:M:168:TRP:CD1	1:M:180:MET:HB2	2.46	0.50
2:H:167:TRP:CZ3	2:H:208:CYS:HB3	2.46	0.50
1:M:13:VAL:HG12	1:M:109:LEU:HD11	1.94	0.50
1:L:156:ASP:HA	1:L:196:SER:HB3	1.94	0.50
2:I:6:GLU:CD	2:I:114:GLY:H	2.20	0.50
1:L:88:LEU:HD21	1:L:173:SER:HB3	1.94	0.50
1:M:42:LEU:HD22	1:M:43:GLN:N	2.27	0.50
2:I:83:MET:HE2	2:I:86:LEU:CD2	2.41	0.50
2:I:98:ARG:NH2	2:I:109:ASP:OD2	2.45	0.50
1:L:38:LEU:HG	1:L:39:HIS:N	2.27	0.49
1:L:119:THR:HG22	1:L:119:THR:O	2.12	0.49
2:H:83:MET:HE1	2:H:94:PHE:CE2	2.47	0.49
1:M:48:SER:HB3	2:I:95:TYR:HE2	1.77	0.49
1:M:66:ARG:NH2	1:M:87:ASP:OD1	2.43	0.49
1:L:167:SER:OG	2:H:180:PRO:HD2	2.12	0.49
2:H:60:TYR:HB3	2:H:61:PRO:HD2	1.95	0.49
2:H:151:LEU:CD2	2:H:201:ARG:HD3	2.36	0.49
2:H:38:ARG:HD3	2:H:48:VAL:HG21	1.93	0.49
1:M:180:MET:HG2	1:M:181:SER:N	2.28	0.49
2:I:136:PRO:HG3	2:I:221:LYS:CE	2.42	0.49
2:I:137:LEU:HB2	2:I:152:GLY:CA	2.42	0.48
1:L:27:GLN:HG3	4:I:1319:HOH:O	2.13	0.48
1:M:35:ASN:HB2	1:M:37:TYR:CE2	2.48	0.48
1:M:54:TYR:CD2	1:M:55:LYS:HG3	2.48	0.48
2:I:67:ARG:NH1	2:I:87:ARG:HH21	2.11	0.48
1:M:141:LEU:HD22	1:M:141:LEU:N	2.28	0.48
2:I:134:VAL:HG21	2:I:210:VAL:CG1	2.44	0.48
1:L:85:ALA:O	1:L:88:LEU:HD22	2.14	0.48
2:I:29:PHE:O	2:I:72:ARG:NH2	2.47	0.48
2:H:167:TRP:O	2:H:168:ASN:C	2.56	0.48
1:L:35:ASN:HB2	1:L:37:TYR:CE2	2.48	0.47
1:M:186:LEU:HD13	1:M:191:TYR:HB2	1.96	0.47
2:I:100:GLY:O	2:I:102:LEU:N	2.47	0.47
1:L:118:PRO:HG3	1:L:144:PHE:CB	2.45	0.47
2:H:58:THR:HG21	4:H:332:HOH:O	2.13	0.47
1:L:66:ARG:NH1	1:L:87:ASP:OD2	2.47	0.47
2:I:128:LYS:NZ	2:I:129:THR:HG23	2.30	0.47
1:L:191:TYR:O	1:L:197:TYR:OH	2.28	0.47
2:H:41:PRO:C	2:H:43:ARG:H	2.22	0.47
2:H:91:THR:HB	2:H:118:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:64:VAL:CG1	2:I:68:PHE:HB2	2.44	0.47
1:L:5:THR:HG22	1:L:6:GLN:N	2.29	0.47
1:M:116:ALA:O	1:M:205:THR:HG21	2.15	0.47
2:H:183:LEU:HD12	2:H:187:LEU:O	2.14	0.47
1:M:42:LEU:HD11	1:M:44:LYS:HG3	1.97	0.47
2:I:128:LYS:HZ2	2:I:129:THR:HG23	1.80	0.47
2:I:151:LEU:HG	2:I:223:ILE:HG21	1.96	0.46
1:M:140:PHE:CE2	2:I:193:SER:HB3	2.50	0.46
2:I:137:LEU:HB2	2:I:152:GLY:O	2.14	0.46
2:I:205:THR:CG2	2:I:222:LYS:HE3	2.46	0.46
1:M:200:GLU:HG2	1:M:209:PRO:HB2	1.97	0.46
2:H:104:ASP:O	2:H:105:TYR:O	2.33	0.46
2:H:128:LYS:HD3	2:H:129:THR:H	1.80	0.46
1:M:164:VAL:C	1:M:165:LEU:HD12	2.41	0.46
2:I:11:LEU:HD12	2:I:118:THR:O	2.15	0.46
2:I:167:TRP:HB2	2:I:172:LEU:HB2	1.98	0.46
1:L:81:SER:O	1:L:82:ARG:C	2.58	0.46
1:M:85:ALA:HA	1:M:111:ILE:HD11	1.96	0.46
2:H:149:VAL:HG22	2:H:151:LEU:CD1	2.45	0.46
1:L:180:MET:HG2	1:L:181:SER:N	2.29	0.46
2:I:160:PRO:HD2	2:I:214:ALA:CB	2.46	0.46
2:H:197:PRO:O	2:H:200:SER:HB3	2.16	0.46
2:H:184:GLN:O	2:H:184:GLN:HG2	2.16	0.45
2:H:210:VAL:HG12	2:H:219:VAL:O	2.16	0.45
2:H:134:VAL:HB	2:H:219:VAL:HG11	1.98	0.45
1:M:99:VAL:HA	1:M:100:PRO:C	2.42	0.45
2:I:68:PHE:CZ	2:I:83:MET:HE3	2.51	0.45
2:H:190:LEU:HD12	2:H:191:SER:N	2.31	0.45
1:M:83:VAL:HG12	1:M:84:GLU:N	2.31	0.45
1:M:17:ASP:O	1:M:83:VAL:HG23	2.17	0.45
1:M:44:LYS:HE2	1:M:86:GLU:O	2.16	0.45
1:M:165:LEU:HD23	2:I:182:VAL:CG1	2.47	0.45
1:L:135:ALA:HB3	1:L:186:LEU:HD12	1.98	0.45
2:I:212:HIS:CD2	2:I:215:SER:OG	2.67	0.45
2:I:160:PRO:O	2:I:212:HIS:HE1	2.00	0.45
2:I:190:LEU:C	2:I:190:LEU:CD1	2.89	0.45
2:I:3:MET:N	2:I:3:MET:HE2	2.32	0.45
2:I:76:ARG:HG3	2:I:76:ARG:NH1	2.32	0.45
1:L:13:VAL:HG22	1:L:14:SER:O	2.17	0.44
1:L:110:GLU:HG3	1:L:178:TYR:OH	2.18	0.44
2:H:76:ARG:HH11	2:H:76:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:187:THR:O	1:M:188:LYS:C	2.60	0.44
1:M:188:LYS:HE2	1:M:192:GLU:OE1	2.16	0.44
2:I:104:ASP:O	2:I:105:TYR:O	2.35	0.44
1:L:150:ASN:O	1:L:201:ALA:HA	2.17	0.44
2:H:103:LEU:HD23	2:H:103:LEU:HA	1.78	0.44
1:L:11:LEU:HD22	1:L:21:ILE:HD11	1.99	0.44
1:L:66:ARG:HH22	1:L:87:ASP:CG	2.24	0.44
1:L:160:ARG:NH2	1:L:190:GLU:OE1	2.44	0.44
2:H:135:TYR:HA	2:H:136:PRO:HD3	1.82	0.44
1:M:83:VAL:CG1	1:M:84:GLU:N	2.81	0.44
2:I:83:MET:HE1	2:I:94:PHE:CZ	2.53	0.44
1:M:166:ASN:HB3	1:M:180:MET:HE3	1.99	0.44
1:M:172:ASP:HB3	1:M:175:ASP:OD1	2.16	0.44
1:M:198:THR:HG23	1:M:213:SER:HB3	1.99	0.44
2:I:87:ARG:O	2:I:90:ASP:HB2	2.17	0.44
1:L:12:SER:HA	1:L:110:GLU:O	2.18	0.43
1:M:52:LEU:CD2	1:M:53:ILE:HG13	2.42	0.43
1:M:137:VAL:HG13	1:M:184:LEU:HB3	2.00	0.43
2:I:52:THR:CG2	2:I:53:THR:N	2.81	0.43
2:I:101:LEU:HB2	2:I:104:ASP:O	2.18	0.43
2:I:109:ASP:HB3	2:I:110:TYR:H	1.52	0.43
1:L:156:ASP:OD2	1:L:194:HIS:HB3	2.18	0.43
1:L:189:ASP:OD1	1:L:193:ARG:NH2	2.51	0.43
2:H:55:ARG:HG3	2:H:55:ARG:NH1	2.34	0.43
2:I:167:TRP:HB3	2:I:172:LEU:HD12	2.00	0.43
1:L:57:SER:HB3	1:L:69:GLY:O	2.19	0.43
2:H:11:LEU:HA	2:H:118:THR:O	2.18	0.43
1:M:6:GLN:HA	1:M:22:SER:O	2.19	0.43
1:L:25:SER:HB3	1:L:74:THR:HA	1.99	0.43
1:M:29:LEU:HD12	1:M:76:PHE:CE1	2.53	0.43
1:M:85:ALA:HB1	1:M:173:SER:O	2.19	0.43
1:M:188:LYS:O	1:M:192:GLU:HG3	2.18	0.43
1:M:198:THR:HA	1:M:213:SER:HB3	2.00	0.43
2:I:70:VAL:HG13	2:I:79:LEU:HD21	2.00	0.43
2:I:132:PRO:CB	2:I:158:TYR:HB3	2.45	0.43
2:I:158:TYR:CE1	2:I:188:TYR:HB2	2.53	0.43
1:L:216:ARG:HG2	1:L:216:ARG:HH11	1.82	0.43
1:L:123:PHE:HZ	2:H:150:THR:O	2.02	0.43
1:L:137:VAL:HG12	1:L:184:LEU:HB3	2.00	0.43
1:M:115:ASP:OD2	1:M:204:LYS:HE2	2.19	0.43
1:M:169:THR:HG23	2:I:179:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:32:TYR:CD2	2:I:98:ARG:HD2	2.54	0.43
1:L:41:TYR:OH	2:H:108:MET:HB2	2.19	0.42
1:M:64:PRO:HG2	1:M:66:ARG:HG2	2.01	0.42
1:M:203:HIS:CD2	1:M:205:THR:HG23	2.54	0.42
2:I:60:TYR:CE2	2:I:70:VAL:HG23	2.53	0.42
2:H:11:LEU:HB2	2:H:160:PRO:HG3	2.01	0.42
1:M:95:GLN:NE2	1:M:97:THR:N	2.67	0.42
1:M:88:LEU:HD12	1:M:171:GLN:HB3	2.01	0.42
2:I:6:GLU:HA	2:I:21:SER:O	2.19	0.42
1:L:184:LEU:C	1:L:184:LEU:HD23	2.45	0.42
1:M:35:ASN:HB2	1:M:37:TYR:CZ	2.54	0.42
1:M:62:GLY:O	1:M:63:PHE:C	2.62	0.42
2:I:60:TYR:HB3	2:I:61:PRO:HD2	2.02	0.42
2:I:135:TYR:HA	2:I:136:PRO:HD3	1.77	0.42
1:L:137:VAL:HG13	1:L:184:LEU:HB3	1.99	0.42
2:H:129:THR:HA	2:H:159:PHE:O	2.20	0.42
2:H:134:VAL:HG12	2:H:221:LYS:HG3	2.01	0.42
1:L:42:LEU:HD11	1:L:44:LYS:HG3	2.02	0.42
1:M:192:GLU:C	1:M:194:HIS:N	2.75	0.42
1:L:88:LEU:CD2	1:L:173:SER:HB3	2.50	0.42
2:H:42:GLU:O	2:H:43:ARG:HB2	2.20	0.42
2:H:67:ARG:C	2:H:68:PHE:HD1	2.27	0.42
2:H:52:THR:HG23	2:H:53:THR:N	2.34	0.42
2:I:70:VAL:CG1	2:I:79:LEU:HD21	2.49	0.42
1:L:11:LEU:HD22	1:L:21:ILE:CD1	2.50	0.42
1:L:35:ASN:HB2	1:L:37:TYR:CZ	2.55	0.42
1:M:25:SER:O	1:M:74:THR:HB	2.20	0.42
1:M:63:PHE:HA	1:M:64:PRO:HD2	1.82	0.42
2:H:20:LEU:HG	2:H:115:THR:HG21	2.01	0.42
2:H:68:PHE:N	2:H:68:PHE:CD1	2.88	0.42
1:L:95:GLN:NE2	1:L:98:HIS:H	1.98	0.41
2:H:212:HIS:HD2	2:H:215:SER:CB	2.33	0.41
1:M:160:ARG:NH2	1:M:190:GLU:OE1	2.51	0.41
1:L:13:VAL:HG12	1:L:109:LEU:HD11	2.02	0.41
2:H:48:VAL:O	2:H:49:ALA:HB2	2.20	0.41
2:H:167:TRP:CH2	2:H:208:CYS:HB3	2.55	0.41
2:H:212:HIS:CD2	2:H:215:SER:H	2.38	0.41
2:H:136:PRO:HG3	2:H:221:LYS:HE2	2.02	0.41
2:H:190:LEU:C	2:H:190:LEU:CD1	2.91	0.41
1:M:172:ASP:OD1	1:M:174:LYS:HB2	2.20	0.41
1:L:184:LEU:C	1:L:184:LEU:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:SER:HB3	2:I:95:TYR:CE2	2.55	0.41
2:H:64:VAL:CG1	2:H:68:PHE:HB2	2.50	0.41
2:H:47:TRP:CZ3	2:H:61:PRO:HD3	2.56	0.41
1:L:118:PRO:HG3	1:L:144:PHE:HB3	2.01	0.41
1:L:130:LEU:HD23	1:L:130:LEU:HA	1.93	0.41
1:L:138:VAL:HG12	1:L:139:CYS:N	2.36	0.41
1:L:60:PHE:O	1:L:61:SER:C	2.64	0.41
2:H:71:SER:OG	2:H:80:ASN:HB2	2.21	0.41
1:M:54:TYR:HD2	1:M:55:LYS:HG3	1.86	0.41
1:M:85:ALA:HA	1:M:111:ILE:HD13	2.03	0.40
1:M:120:VAL:HB	1:M:141:LEU:CD1	2.51	0.40
2:I:73:ASP:OD1	2:I:75:ALA:HB3	2.21	0.40
1:L:39:HIS:NE2	1:L:96:SER:OG	2.54	0.40
1:L:83:VAL:HG12	1:L:84:GLU:N	2.37	0.40
1:L:129:GLN:OE1	1:L:136:SER:N	2.47	0.40
1:L:186:LEU:CD1	1:L:191:TYR:HB2	2.51	0.40
1:M:203:HIS:HD2	1:M:205:THR:OG1	2.04	0.40
2:I:17:SER:HB2	2:I:83:MET:O	2.22	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)
1:M:207:THR:OG1	1:M:207:THR:OG1[3_554]	2.02	0.18

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	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	14	41
1	M	211/217 (97%)	192 (91%)	14 (7%)	5 (2%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	209/221 (95%)	191 (91%)	13 (6%)	5 (2%)	4	17
2	I	205/221 (93%)	186 (91%)	15 (7%)	4 (2%)	6	21
All	All	840/876 (96%)	770 (92%)	54 (6%)	16 (2%)	6	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	102	LEU
2	H	105	TYR
1	M	61	SER
2	I	101	LEU
2	I	105	TYR
1	L	61	SER
1	M	62	GLY
1	M	63	PHE
2	I	107	THR
1	L	62	GLY
2	H	107	THR
2	H	185	SER
2	I	109	ASP
1	M	189	ASP
1	M	195	ALA
2	H	160	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	192/192 (100%)	181 (94%)	11 (6%)	18	49
1	M	189/192 (98%)	178 (94%)	11 (6%)	18	49
2	H	186/187 (100%)	166 (89%)	20 (11%)	6	21
2	I	183/187 (98%)	162 (88%)	21 (12%)	5	18
All	All	750/758 (99%)	687 (92%)	63 (8%)	10	32

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	38	LEU
1	L	39	HIS
1	L	42	LEU
1	L	65	ASP
1	L	88	LEU
1	L	95	GLN
1	L	120	VAL
1	L	128	GLU
1	L	160	ARG
1	L	184	LEU
1	L	189	ASP
2	H	20	LEU
2	H	52	THR
2	H	53	THR
2	H	58	THR
2	H	64	VAL
2	H	70	VAL
2	H	79	LEU
2	H	88	SER
2	H	91	THR
2	H	113	GLN
2	H	117	VAL
2	H	129	THR
2	H	151	LEU
2	H	154	LEU
2	H	160	PRO
2	H	190	LEU
2	H	201	ARG
2	H	209	ASN
2	H	210	VAL
2	H	224	VAL
1	M	38	LEU
1	M	39	HIS
1	M	42	LEU
1	M	65	ASP
1	M	88	LEU
1	M	95	GLN
1	M	120	VAL
1	M	128	GLU
1	M	141	LEU
1	M	184	LEU
1	M	186	LEU

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Mol	Chain	Res	Type
2	I	3	MET
2	I	12	VAL
2	I	20	LEU
2	I	52	THR
2	I	53	THR
2	I	58	THR
2	I	64	VAL
2	I	79	LEU
2	I	91	THR
2	I	104	ASP
2	I	117	VAL
2	I	129	THR
2	I	151	LEU
2	I	153	CYS
2	I	154	LEU
2	I	162	PRO
2	I	190	LEU
2	I	201	ARG
2	I	208	CYS
2	I	209	ASN
2	I	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	31	HIS
1	L	35	ASN
1	L	95	GLN
1	L	166	ASN
1	L	171	GLN
1	L	203	HIS
2	H	74	ASN
2	H	212	HIS
1	M	27	GLN
1	M	31	HIS
1	M	95	GLN
1	M	166	ASN
1	M	171	GLN
2	I	74	ASN
2	I	212	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	GA4	I	1300	-	28,28,28	1.28	2 (7%)	46,49,49	1.77	13 (28%)
3	GA4	H	300	-	28,28,28	1.23	2 (7%)	46,49,49	1.76	11 (23%)

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	GA4	I	1300	-	-	0/4/80/80	-
3	GA4	H	300	-	-	0/4/80/80	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1300	GA4	O92-C19	2.76	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	300	GA4	O92-C19	2.75	1.41	1.36
3	I	1300	GA4	C2-C3	2.69	1.56	1.52
3	H	300	GA4	C2-C3	2.64	1.56	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	300	GA4	O92-C10-C1	5.56	110.83	107.36
3	I	1300	GA4	O92-C10-C1	5.24	110.63	107.36
3	H	300	GA4	O92-C19-O91	-3.46	117.17	121.56
3	I	1300	GA4	O72-C7-O71	-3.45	116.24	124.08
3	I	1300	GA4	O92-C19-O91	-3.37	117.27	121.56
3	H	300	GA4	O72-C7-O71	-3.34	116.50	124.08
3	I	1300	GA4	C1-C2-C3	2.97	115.83	111.48
3	I	1300	GA4	O71-C7-C6	2.83	130.35	123.37
3	H	300	GA4	C1-C2-C3	2.83	115.62	111.48
3	H	300	GA4	O71-C7-C6	2.77	130.20	123.37
3	H	300	GA4	O91-C19-C4	2.69	133.81	128.57
3	I	1300	GA4	O91-C19-C4	2.67	133.76	128.57
3	H	300	GA4	C11-C9-C10	-2.56	110.70	118.01
3	I	1300	GA4	C11-C9-C10	-2.51	110.81	118.01
3	I	1300	GA4	C10-C5-C6	2.28	106.41	104.02
3	I	1300	GA4	C11-C12-C13	2.24	115.13	111.18
3	I	1300	GA4	O92-C10-C9	2.21	111.35	108.75
3	H	300	GA4	C10-C5-C6	2.19	106.32	104.02
3	I	1300	GA4	C15-C8-C6	2.17	120.99	116.10
3	I	1300	GA4	C12-C11-C9	2.16	117.26	112.39
3	H	300	GA4	C11-C12-C13	2.14	114.95	111.18
3	H	300	GA4	O92-C10-C9	2.11	111.22	108.75
3	H	300	GA4	C12-C11-C9	2.08	117.08	112.39
3	I	1300	GA4	C11-C9-C8	2.02	115.48	112.97

There are no chirality outliers.

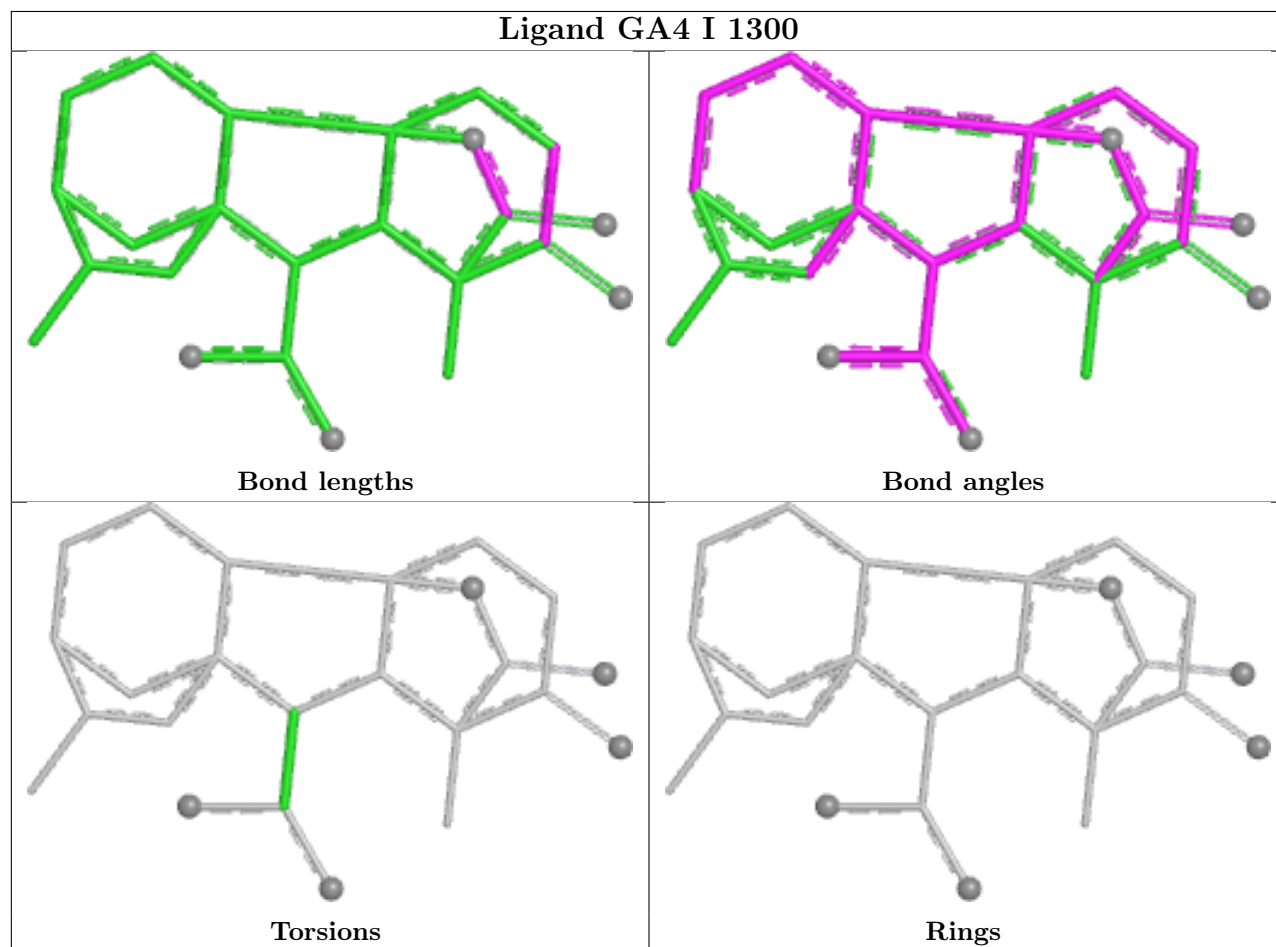
There are no torsion outliers.

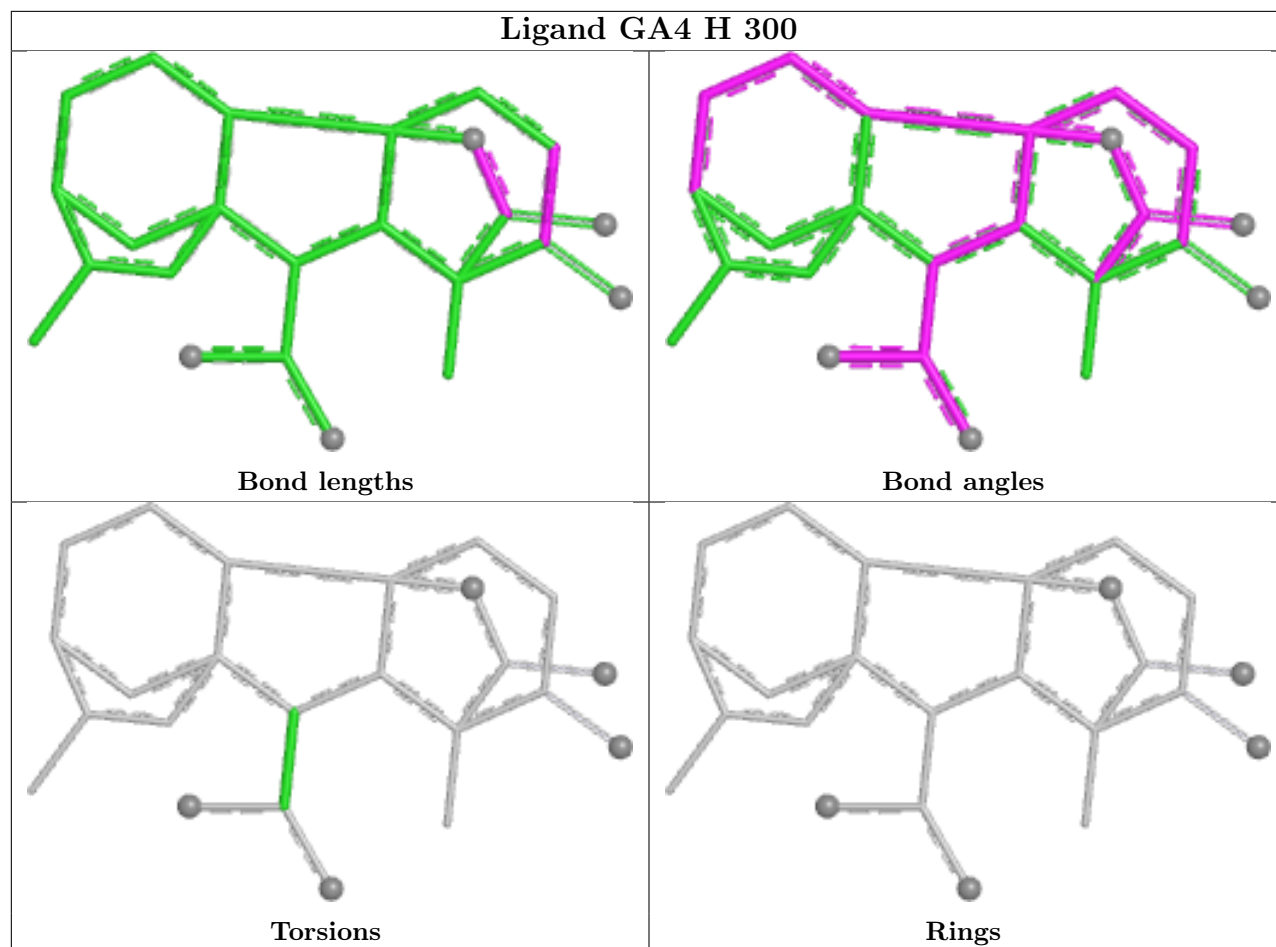
There are no ring outliers.

No monomer is involved in short contacts.

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	217/217 (100%)	0.18	7 (3%)	50	40	11, 39, 66, 122	0
1	M	213/217 (98%)	0.48	12 (5%)	30	23	11, 48, 85, 130	0
2	H	213/221 (96%)	-0.01	5 (2%)	61	51	14, 31, 57, 112	0
2	I	209/221 (94%)	0.12	9 (4%)	40	31	13, 33, 69, 135	0
All	All	852/876 (97%)	0.19	33 (3%)	43	34	11, 37, 76, 135	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	61	SER	4.2
2	H	200	SER	3.9
1	L	217	ALA	3.8
1	L	64	PRO	3.8
1	M	201	ALA	3.6
2	I	3	MET	3.4
2	I	102	LEU	3.4
2	I	128	LYS	3.4
1	L	63	PHE	3.0
1	M	148	ASP	2.8
1	M	195	ALA	2.8
2	I	208	CYS	2.7
2	I	184	GLN	2.6
2	H	102	LEU	2.5
1	L	86	GLU	2.5
1	M	200	GLU	2.5
1	L	150	ASN	2.5
2	I	200	SER	2.4
2	H	136	PRO	2.4
2	I	139	PRO	2.4
1	L	174	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	213	SER	2.3
1	M	111	ILE	2.3
2	H	148	MET	2.3
2	I	205	THR	2.3
1	M	117	GLY	2.3
1	L	112	LYS	2.2
2	I	204	GLU	2.2
1	M	202	ALA	2.2
2	H	104	ASP	2.1
1	M	24	ARG	2.1
1	M	110	GLU	2.1
1	M	86	GLU	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](#)

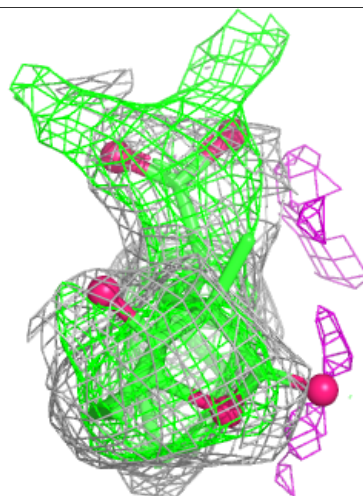
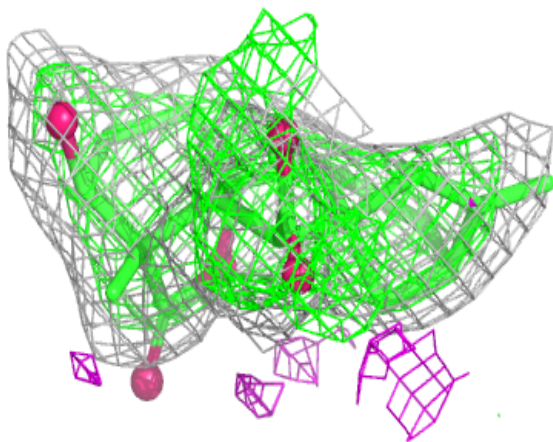
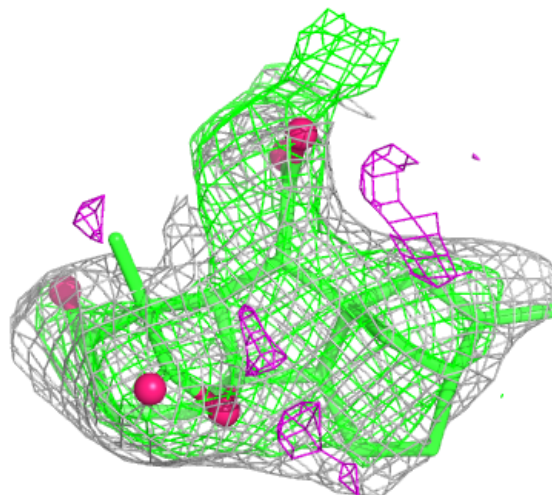
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GA4	H	300	24/24	-	-	2,2,2,2	24
3	GA4	I	1300	24/24	-	-	2,2,2,2	24

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.

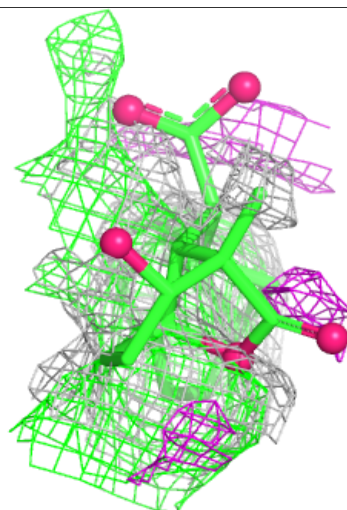
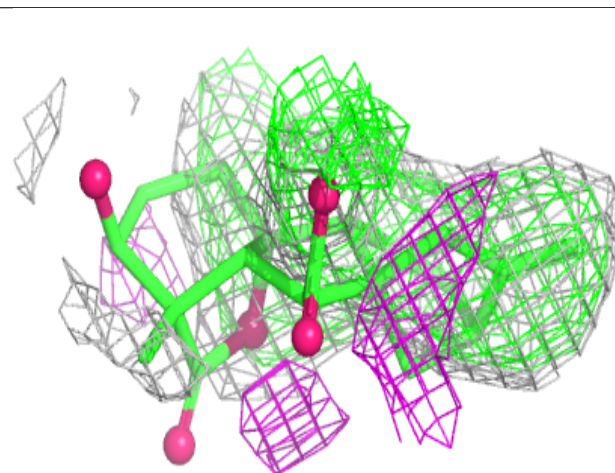
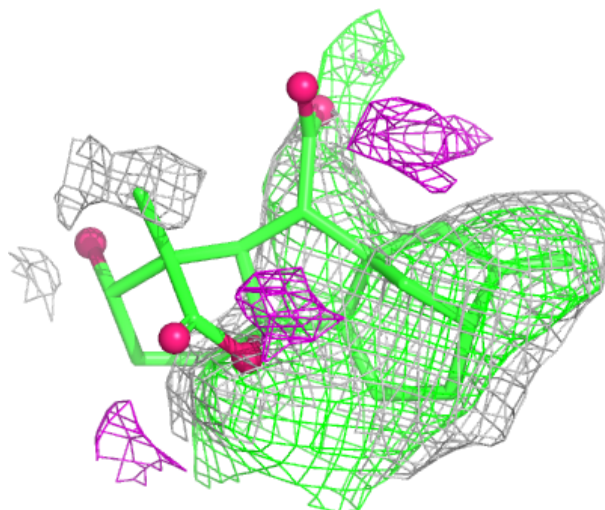
Electron density around GA4 H 300:

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



Electron density around GA4 I 1300:

$2mF_o-DF_c$ (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.