WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:33 am GMT

PDB ID	:	1KFA
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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.
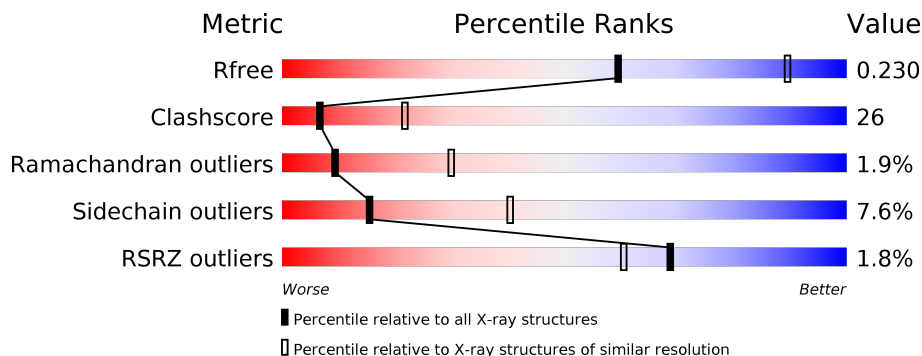
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	217	
1	M	217	
2	H	221	
2	I	221	

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 1671	C 1043	N 284	O 338	S 6	0	0	0
1	M	213	Total 1635	C 1021	N 276	O 332	S 6	0	0	0

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

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

- Molecule 3 is GIBBERELLIN A4 (three-letter code: GA4) (formula: $C_{19}H_{24}O_5$).
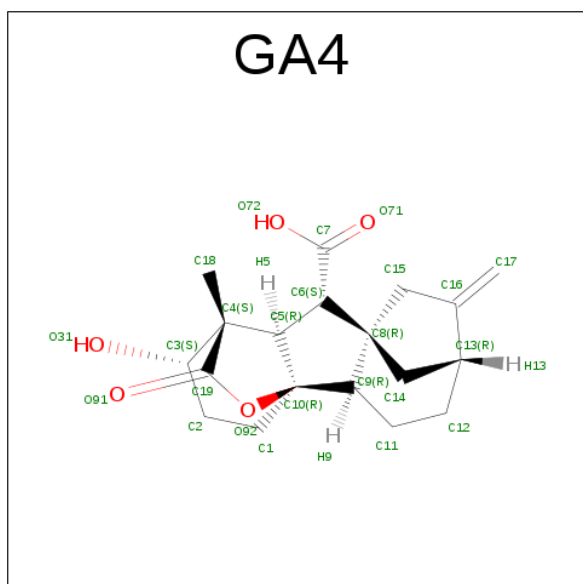
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total 24	C 19	O 5	24	0
3	I	1	Total 24	C 19	O 5	24	0

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

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

• Molecule 1: monoclonal antibody light chain

Chain L:

• Molecule 1: monoclonal antibody light chain

Chain M:

• Molecule 2: monoclonal antibody heavy chain

Chain H:

Q184 S185 D186 L187 L190 S191 S192 P197 S200 R201 P202 T205 V206 T207 C208 N209 V210 A211 H212 S215 V219 D220 K221 K222 D227

• Molecule 2: monoclonal antibody heavy chain

Chain I:

%

53%   35%   6%   • 5%

GLU VAL M3 E6 L11 V12 S17 L20 S21 F29 Y32 W36 V37 R38 E42 R43 V48 A49 T52 T53 R55 T58 F59 Y60 P61 V64 R67 F68 T69 V70 S71 R72 D73 N74 A75 R76 L79 M83 L86 R87 S88 E89 D90 T91

Y95 R98 E99 G100 L101 L102 L103 D104 Y105 F106 T107 M108 D109 Y110 G114 V117 T118 V119 K128 T129 P132 S133 V134 Y135 P136 L137 A138 P139 UNK UNK UNK UNK UNK UNK SER M148 V149 T150 L151 G152 C153 L154 Y158 F159 P160 E161 P162 V163 T164 W167

S171 L172 F179 P180 A181 V182 Y188 T189 L190 S193 P197 S198 R201 P202 S203 E204 T205 V206 T207 C208 N209 V210 A211 H212 P213 A214 S215 K221 K222 I223 V224 P225 ALA ASP

4 Data and refinement statistics (i)

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 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.62-2.80) 100.0 (39.62-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.77 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.313 0.237 , 0.230	Depositor DCC
R_{free} test set	1208 reflections (5.09%)	DCC
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 , 68.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.39	0/1710	0.63	1/2316 (0.0%)
1	M	0.35	0/1673	0.60	0/2268
2	H	0.42	0/1655	0.71	0/2256
2	I	0.39	0/1628	0.70	0/2220
All	All	0.39	0/6666	0.66	1/9060 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	62	GLY	N-CA-C	-6.10	97.84	113.10

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	L	1671	0	1607	79	0
1	M	1635	0	1574	93	1
2	H	1616	0	1589	87	0
2	I	1589	0	1566	87	0
3	H	24	0	24	0	0
3	I	24	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	335	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 26.

All (335) 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:HB3	2:H:201:ARG:HH11	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
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
2:I:49:ALA:HB1	2:I:70:VAL:CG2	2.19	0.72
1:M:189:ASP:HB3	1:M:193:ARG:HH21	1.54	0.72
2:H:72:ARG:HE	2:H:74:ASN:HD21	1.34	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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
2:H:88:SER:O	2:H:91:THR:HG23	1.99	0.63
1:L:120:VAL:HG22	1:L:212:LYS:HG3	1.81	0.63
1:M:155:ILE:CD1	1:M:160:ARG:HG3	2.27	0.62
1:M:66:ARG:HH22	1:M:87:ASP:CG	2.02	0.62
1:L:198:THR:HG23	1:L:213:SER:HB3	1.80	0.62
2:H:68:PHE:CZ	2:H:83:MET:HE2	2.33	0.62
1:L:85:ALA:HA	1:L:111:ILE:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:190:LEU:HD12	2:H:190:LEU:C	2.21	0.61
1:M:127:SER:O	1:M:131:THR:HG23	2.00	0.61
2:H:12:VAL:CG2	2:H:119:VAL:HG22	2.31	0.61
1:L:14:SER:O	1:L:17:ASP:HB2	2.01	0.61
2:I:67:ARG:NH2	2:I:90:ASP:OD2	2.34	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
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:HH11	2:I:43:ARG:HA	1.66	0.60
1:M:156:ASP:OD2	1:M:194:HIS:HB3	2.01	0.59
2:I:137:LEU:HB2	2:I:152:GLY:C	2.21	0.59
2:I:88:SER:O	2:I:91:THR:CG2	2.48	0.59
2:I:164:THR:OG1	2:I:211:ALA:HB3	2.02	0.59
1:M:110:GLU:HG2	1:M:111:ILE:H	1.67	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:110:GLU:HG2	1:L:111:ILE:N	2.17	0.59
1:L:88:LEU:HD12	1:L:171:GLN:HB3	1.83	0.58
2:I:136:PRO:HG3	2:I:221:LYS:HE2	1.85	0.58
1:M:57:SER:HB3	1:M:69:GLY:O	2.03	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
2:I:52:THR:HG22	2:I:55:ARG:N	2.18	0.58
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:I:151:LEU:HD23	2:I:206:VAL:HG11	1.88	0.56
1:M:197:TYR:O	1:M:213:SER:HB2	2.05	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
2:I:134:VAL:HG21	2:I:210:VAL:HG11	1.88	0.56
1:M:120:VAL:HA	1:M:140:PHE:O	2.05	0.56
1:M:140:PHE:C	1:M:141:LEU:HD22	2.25	0.56
1:M:111:ILE:N	1:M:171:GLN:HE22	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.88	0.56
2:I:190:LEU:C	2:I:190:LEU:HD12	2.26	0.55
2:I:128:LYS:HD3	2:I:129:THR:N	2.21	0.55
2:H:177:HIS:O	2:H:192:SER:HA	2.07	0.55
2:I:134:VAL:CG2	2:I:210:VAL:HG11	2.36	0.55
1:L:95:GLN:HE22	1:L:98:HIS:N	1.96	0.55
1:M:189:ASP:HB3	1:M:193:ARG:NH2	2.20	0.55
1:M:13:VAL:CG1	1:M:83:VAL:HG21	2.35	0.55
2:H:201:ARG:CB	2:H:201:ARG:HH11	2.02	0.55
1:L:153:TRP:O	1:L:159:GLU:HA	2.06	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
2:I:91:THR:HB	2:I:118:THR:HA	1.89	0.55
1:L:88:LEU:O	1:L:88:LEU:HD23	2.05	0.55
2:H:55:ARG:HH11	2:H:55:ARG:HG3	1.72	0.54
1:L:39:HIS:HB3	1:L:54:TYR:HA	1.89	0.54
2:I:76:ARG:HG3	2:I:76:ARG:HH11	1.73	0.54
2:I:36:TRP:HE1	2:I:79:LEU:HD22	1.73	0.54
1:M:82:ARG:HG3	1:M:82:ARG:HH11	1.72	0.54
2:I:42:GLU:O	2:I:43:ARG:HB2	2.07	0.53
1:L:38:LEU:HD22	1:L:76:PHE:CD2	2.43	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:9:LEU:C	1:M:107:THR:HG23	2.29	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
2:I:87:ARG:C	2:I:119:VAL:HG11	2.31	0.51
2:I:71:SER:O	2:I:79:LEU:HD23	2.11	0.51
1:M:123:PHE:HZ	2:I:150:THR:O	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:120:VAL:HB	1:M:141:LEU:HD13	1.92	0.51
2:H:52:THR:CG2	2:H:55:ARG:H	2.24	0.50
1:M:168:TRP:CD1	1:M:180:MET:HB2	2.46	0.50
1:M:52:LEU:HG	1:M:63:PHE:CD2	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
2:I:67:ARG:C	2:I:68:PHE:HD1	2.16	0.50
1:L:156:ASP:HA	1:L:196:SER:HB3	1.94	0.50
1:M:192:GLU:C	1:M:194:HIS:H	2.15	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:98:ARG:NH2	2:I:109:ASP:OD2	2.45	0.50
1:M:48:SER:HB3	2:I:95:TYR:HE2	1.77	0.49
1:L:119:THR:HG22	1:L:119:THR:O	2.12	0.49
1:L:38:LEU:HG	1:L:39:HIS:N	2.27	0.49
1:M:66:ARG:NH2	1:M:87:ASP:OD1	2.43	0.49
2:H:42:GLU:H	2:H:42:GLU:CD	2.15	0.49
2:H:60:TYR:HB3	2:H:61:PRO:HD2	1.95	0.49
1:L:167:SER:OG	2:H:180:PRO:HD2	2.12	0.49
2:H:151:LEU:CD2	2:H:201:ARG:HD3	2.36	0.49
2:H:207:THR:HG23	2:H:221:LYS:C	2.34	0.49
2:H:38:ARG:HD3	2:H:48:VAL:HG21	1.93	0.49
2:I:136:PRO:HG3	2:I:221:LYS:CE	2.42	0.49
1:M:180:MET:HG2	1:M:181:SER:N	2.28	0.49
1:M:52:LEU:C	1:M:52:LEU:HD23	2.32	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
2:I:134:VAL:HG21	2:I:210:VAL:CG1	2.44	0.48
1:M:141:LEU:HD22	1:M:141:LEU:N	2.28	0.48
2:I:29:PHE:O	2:I:72:ARG:NH2	2.47	0.48
1:L:85:ALA:O	1:L:88:LEU:HD22	2.14	0.48
2:I:100:GLY:O	2:I:102:LEU:N	2.47	0.47
1:L:35:ASN:HB2	1:L:37:TYR:CE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:186:LEU:HD13	1:M:191:TYR:HB2	1.96	0.47
2:H:58:THR:HG21	4:H:332:HOH:O	2.13	0.47
1:L:118:PRO:HG3	1:L:144:PHE:CB	2.45	0.47
2:I:128:LYS:NZ	2:I:129:THR:HG23	2.30	0.47
1:L:66:ARG:NH1	1:L:87:ASP:OD2	2.47	0.47
2:I:64:VAL:CG1	2:I:68:PHE:HB2	2.44	0.47
2:H:91:THR:HB	2:H:118:THR:HA	1.96	0.47
1:L:191:TYR:O	1:L:197:TYR:OH	2.28	0.47
2:H:150:THR:C	2:H:151:LEU:HD12	2.35	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:151:LEU:HG	2:I:223:ILE:HG21	1.96	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:140:PHE:CE2	2:I:193:SER:HB3	2.50	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
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: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
2:I:160:PRO:HD2	2:I:214:ALA:CB	2.46	0.46
1:L:180:MET:HG2	1:L:181:SER:N	2.29	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
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
2:I:6:GLU:CD	2:I:114:GLY:H	2.20	0.45
1:M:165:LEU:HD23	2:I:182:VAL:CG1	2.47	0.45
1:M:44:LYS:HE2	1:M:86:GLU:O	2.16	0.45
1:M:17:ASP:O	1:M:83:VAL:HG23	2.17	0.45
2:I:212:HIS:CD2	2:I:215:SER:OG	2.67	0.45
1:L:135:ALA:HB3	1:L:186:LEU:HD12	1.98	0.45
2:I:160:PRO:O	2:I:212:HIS:HE1	2.00	0.45
2:I:76:ARG:NH1	2:I:76:ARG:HG3	2.32	0.45
2:I:83:MET:HE2	2:I:86:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:VAL:HG22	1:L:14:SER:O	2.17	0.44
2:H:76:ARG:HG3	2:H:76:ARG:HH11	1.82	0.44
2:I:104:ASP:O	2:I:105:TYR:O	2.35	0.44
1:L:110:GLU:HG3	1:L:178:TYR:OH	2.18	0.44
1:M:188:LYS:HE2	1:M:192:GLU:OE1	2.16	0.44
2:H:103:LEU:HD23	2:H:103:LEU:HA	1.78	0.44
2:H:6:GLU:CD	2:H:114:GLY:H	2.19	0.44
1:L:150:ASN:O	1:L:201:ALA:HA	2.17	0.44
1:L:11:LEU:HD22	1:L:21:ILE:HD11	1.99	0.44
2:H:135:TYR:HA	2:H:136:PRO:HD3	1.82	0.44
1:L:160:ARG:NH2	1:L:190:GLU:OE1	2.44	0.44
1:M:83:VAL:CG1	1:M:84:GLU:N	2.81	0.44
2:I:87:ARG:O	2:I:90:ASP:HB2	2.17	0.44
1:M:166:ASN:HB3	1:M:180:MET:HE2	2.00	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:52:THR:CG2	2:I:53:THR:N	2.81	0.43
1:L:12:SER:HA	1:L:110:GLU:O	2.18	0.43
1:M:137:VAL:HG13	1:M:184:LEU:HB3	2.00	0.43
1:M:52:LEU:CD2	1:M:53:ILE:HG13	2.42	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:167:TRP:O	2:H:168:ASN:C	2.56	0.43
2:H:55:ARG:NH1	2:H:55:ARG:HG3	2.34	0.43
2:I:167:TRP:HB3	2:I:172:LEU:HD12	2.00	0.43
2:H:11:LEU:HA	2:H:118:THR:O	2.18	0.43
1:L:57:SER:HB3	1:L:69:GLY:O	2.19	0.43
1:M:6:GLN:HA	1:M:22:SER:O	2.19	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
2:I:70:VAL:HG13	2:I:79:LEU:HD21	2.00	0.43
1:L:25:SER:HB3	1:L:74:THR:HA	1.99	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
1:M:29:LEU:HD12	1:M:76:PHE:CE1	2.53	0.43
1:L:216:ARG:HH11	1:L:216:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:32:TYR:CD2	2:I:98:ARG:HD2	2.54	0.43
2:I:60:TYR:CE2	2:I:70:VAL:HG23	2.53	0.42
1:L:41:TYR:OH	2:H:108:MET:HB2	2.19	0.42
1:M:203:HIS:CD2	1:M:205:THR:HG23	2.54	0.42
1:M:64:PRO:HG2	1:M:66:ARG:HG2	2.01	0.42
2:H:11:LEU:HB2	2:H:160:PRO:HG3	2.01	0.42
2:I:148:MET:N	2:I:198:SER:HG	2.17	0.42
1:M:95:GLN:NE2	1:M:97:THR:N	2.67	0.42
2:I:6:GLU:HA	2:I:21:SER:O	2.19	0.42
1:M:88:LEU:HD12	1:M:171:GLN:HB3	2.01	0.42
2:H:41:PRO:C	2:H:43:ARG:H	2.22	0.42
2:I:135:TYR:HA	2:I:136:PRO:HD3	1.77	0.42
2:I:60:TYR:HB3	2:I:61:PRO:HD2	2.02	0.42
1:M:35:ASN:HB2	1:M:37:TYR:CZ	2.54	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
2:H:83:MET:HE1	2:H:94:PHE:CZ	2.54	0.42
1:L:137:VAL:HG13	1:L:184:LEU:HB3	1.99	0.42
1:L:42:LEU:HD11	1:L:44:LYS:HG3	2.02	0.42
2:H:42:GLU:O	2:H:43:ARG:HB2	2.20	0.42
1:L:88:LEU:CD2	1:L:173:SER:HB3	2.50	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:63:PHE:HA	1:M:64:PRO:HD2	1.82	0.42
1:M:25:SER:O	1:M:74:THR:HB	2.20	0.42
2:H:20:LEU:HG	2:H:115:THR:HG21	2.01	0.42
2:H:68:PHE:CD1	2:H:68:PHE:N	2.88	0.42
1:M:164:VAL:C	1:M:165:LEU:HD12	2.41	0.42
2:H:212:HIS:HD2	2:H:215:SER:CB	2.33	0.41
2:H:48:VAL:O	2:H:49:ALA:HB2	2.20	0.41
1:L:95:GLN:NE2	1:L:98:HIS:H	1.98	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: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
1:M:172:ASP:OD1	1:M:174:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:SER:O	1:L:82:ARG:C	2.58	0.41
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:HA	1:L:130:LEU:HD23	1.93	0.41
1:L:138:VAL:HG12	1:L:139:CYS:N	2.36	0.41
1:M:99:VAL:HA	1:M:100:PRO:C	2.42	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:120:VAL:HB	1:M:141:LEU:CD1	2.51	0.40
1:M:85:ALA:HA	1:M:111:ILE:HD13	2.03	0.40
2:I:73:ASP:OD1	2:I:75:ALA:HB3	2.21	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:L:83:VAL:HG12	1:L:84:GLU:N	2.37	0.40
2:I:17:SER:HB2	2:I:83:MET:O	2.22	0.40
1:L:198:THR:HG22	1:L:199:CYS:N	2.36	0.40
1:M:203:HIS:HD2	1:M:205:THR:OG1	2.04	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	20	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	211/217 (97%)	192 (91%)	14 (7%)	5 (2%)	7	23
2	H	209/221 (95%)	191 (91%)	13 (6%)	5 (2%)	7	23
2	I	205/221 (93%)	186 (91%)	15 (7%)	4 (2%)	9	28
All	All	840/876 (96%)	770 (92%)	54 (6%)	16 (2%)	9	30

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%)	184 (96%)	8 (4%)	34	68
1	M	189/192 (98%)	181 (96%)	8 (4%)	34	68
2	H	186/187 (100%)	167 (90%)	19 (10%)	8	25
2	I	183/187 (98%)	161 (88%)	22 (12%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	750/758 (99%)	693 (92%)	57 (8%)	15	40

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	38	LEU
1	L	39	HIS
1	L	65	ASP
1	L	88	LEU
1	L	95	GLN
1	L	120	VAL
1	L	160	ARG
1	L	189	ASP
2	H	20	LEU
2	H	52	THR
2	H	53	THR
2	H	58	THR
2	H	60	TYR
2	H	70	VAL
2	H	79	LEU
2	H	88	SER
2	H	91	THR
2	H	105	TYR
2	H	109	ASP
2	H	113	GLN
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
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	184	LEU
1	M	186	LEU
2	I	3	MET
2	I	12	VAL

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Mol	Chain	Res	Type
2	I	20	LEU
2	I	52	THR
2	I	53	THR
2	I	60	TYR
2	I	79	LEU
2	I	91	THR
2	I	104	ASP
2	I	105	TYR
2	I	109	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	43	GLN
1	M	47	GLN
1	M	95	GLN
1	M	166	ASN
1	M	171	GLN
2	I	39	GLN
2	I	74	ASN

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Mol	Chain	Res	Type
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 carbohydrates 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	H	300	-	25,28,28	1.14	2 (8%)	36,49,49	1.81	10 (27%)
3	GA4	I	1300	-	25,28,28	1.19	2 (8%)	36,49,49	1.78	11 (30%)

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	H	300	-	-	0/0/80/80	0/0/5/5
3	GA4	I	1300	-	-	0/0/80/80	0/0/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	300	GA4	O92-C19	2.57	1.41	1.36
3	I	1300	GA4	O92-C19	2.57	1.41	1.36
3	H	300	GA4	C2-C3	2.60	1.56	1.52
3	I	1300	GA4	C2-C3	2.65	1.56	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	300	GA4	O92-C19-O91	-3.26	117.17	121.51
3	I	1300	GA4	O92-C19-O91	-3.18	117.27	121.51
3	H	300	GA4	C11-C9-C10	-2.61	110.70	118.31
3	I	1300	GA4	C11-C9-C10	-2.57	110.81	118.31
3	H	300	GA4	C12-C11-C9	2.01	117.08	112.44
3	H	300	GA4	C11-C9-C8	2.05	115.30	112.88
3	H	300	GA4	C10-C5-C6	2.05	106.32	104.08
3	I	1300	GA4	C15-C8-C6	2.08	120.99	116.01
3	I	1300	GA4	C12-C11-C9	2.09	117.26	112.44
3	I	1300	GA4	C10-C5-C6	2.14	106.41	104.08
3	I	1300	GA4	C11-C9-C8	2.20	115.48	112.88
3	H	300	GA4	C11-C12-C13	2.24	114.95	111.09
3	I	1300	GA4	C11-C12-C13	2.34	115.13	111.09
3	I	1300	GA4	O91-C19-C4	2.48	133.76	128.67
3	H	300	GA4	O91-C19-C4	2.50	133.81	128.67
3	H	300	GA4	C1-C2-C3	2.69	115.62	111.47
3	I	1300	GA4	C1-C2-C3	2.82	115.83	111.47
3	I	1300	GA4	C12-C13-C16	2.90	113.36	110.19
3	H	300	GA4	C12-C13-C16	3.11	113.60	110.19
3	I	1300	GA4	O92-C10-C1	5.32	110.63	107.32
3	H	300	GA4	O92-C10-C1	5.64	110.83	107.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.01	4 (1%)	69	60	11, 39, 66, 122	0
1	M	213/217 (98%)	0.16	8 (3%)	41	30	11, 48, 85, 130	0
2	H	213/221 (96%)	-0.18	0	100	100	14, 31, 57, 112	0
2	I	209/221 (94%)	-0.04	3 (1%)	75	69	13, 33, 69, 135	0
All	All	852/876 (97%)	-0.01	15 (1%)	69	60	11, 37, 76, 135	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	217	ALA	3.8
2	I	197	PRO	3.5
1	M	111	ILE	3.4
2	I	204	GLU	2.9
1	M	158	SER	2.8
1	M	114	ALA	2.8
1	M	193	ARG	2.6
1	M	155	ILE	2.5
1	M	201	ALA	2.4
1	M	196	SER	2.3
1	L	64	PRO	2.3
1	M	191	TYR	2.3
1	L	112	LYS	2.2
2	I	171	SER	2.1
1	L	13	VAL	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GA4	I	1300	24/24	-	-	-	2,2,2,2	24
3	GA4	H	300	24/24	-	-	-	2,2,2,2	24

6.5 Other polymers ⓘ

There are no such residues in this entry.