



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:58 PM UTC

PDB ID : 1A8J / pdb_00001a8j
Title : IMMUNOGLOBULIN LAMBDA LIGHT CHAIN DIMER (MCG) COM-
PLEX WITH ASPARTAME
Authors : Edmundson, A.B.; Manion, C.V.
Deposited on : 1998-03-26
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

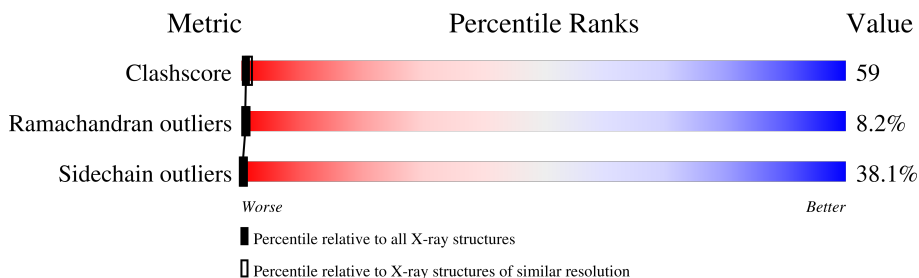
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	216	23% 48% 27% .
1	L	216	24% 46% 26% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PME	H	217	-	-	X	-
2	PME	L	217	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3254 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IMMUNOGLOBULIN LAMBDA LIGHT CHAIN DIMER (MCG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1606	1000	266	335	5			
1	H	216	Total	C	N	O	S	0	0	0
			1606	1000	266	335	5			

There are 44 discrepancies between the modelled and reference sequences:

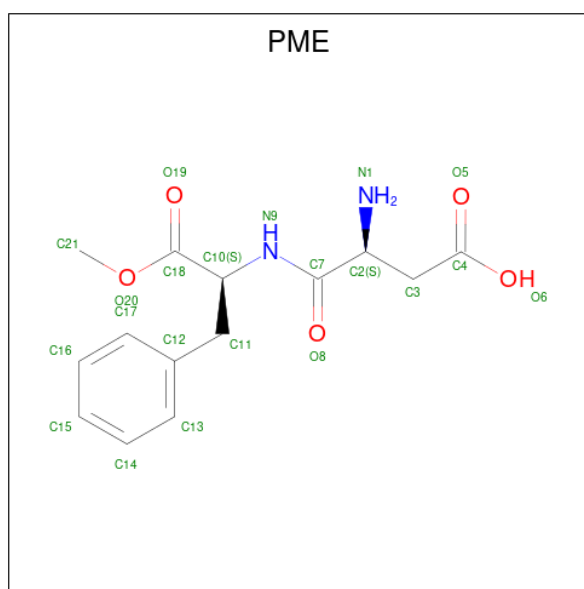
Chain	Residue	Modelled	Actual	Comment	Reference
L	20	ILE	PHE	conflict	UNP P01709
L	23	THR	SER	conflict	UNP P01709
L	29	VAL	ILE	conflict	UNP P01709
L	31	GLY	ASN	conflict	UNP P01709
L	39	GLN	ARG	conflict	UNP P01709
L	42	ALA	PRO	conflict	UNP P01709
L	48	VAL	LEU	conflict	UNP P01709
L	49	ILE	MET	conflict	UNP P01709
L	54	ASN	THR	conflict	UNP P01709
L	62	ASP	ASN	conflict	UNP P01709
L	94	GLU	ALA	conflict	UNP P01709
L	97	ASP	ASN	conflict	UNP P01709
L	98	ASN	SER	conflict	UNP P01709
L	99	PHE	LEU	conflict	UNP P01709
L	100	VAL	ILE	conflict	UNP P01709
L	103	THR	GLY	conflict	UNP P01709
L	106	LYS	ARG	conflict	UNP P01709
L	107	VAL	LEU	conflict	UNP P01709
L	116	ASN	ALA	conflict	UNP P01709
L	118	THR	SER	conflict	UNP P01709
L	156	GLY	SER	conflict	UNP P01709
L	167	LYS	THR	conflict	UNP P01709
H	20	ILE	PHE	conflict	UNP P01709
H	23	THR	SER	conflict	UNP P01709

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	29	VAL	ILE	conflict	UNP P01709
H	31	GLY	ASN	conflict	UNP P01709
H	39	GLN	ARG	conflict	UNP P01709
H	42	ALA	PRO	conflict	UNP P01709
H	48	VAL	LEU	conflict	UNP P01709
H	49	ILE	MET	conflict	UNP P01709
H	54	ASN	THR	conflict	UNP P01709
H	62	ASP	ASN	conflict	UNP P01709
H	94	GLU	ALA	conflict	UNP P01709
H	97	ASP	ASN	conflict	UNP P01709
H	98	ASN	SER	conflict	UNP P01709
H	99	PHE	LEU	conflict	UNP P01709
H	100	VAL	ILE	conflict	UNP P01709
H	103	THR	GLY	conflict	UNP P01709
H	106	LYS	ARG	conflict	UNP P01709
H	107	VAL	LEU	conflict	UNP P01709
H	116	ASN	ALA	conflict	UNP P01709
H	118	THR	SER	conflict	UNP P01709
H	156	GLY	SER	conflict	UNP P01709
H	167	LYS	THR	conflict	UNP P01709

- Molecule 2 is N-L-ALPHA-ASPARTYL L-PHENYLALANINE 1-METHYL ESTER (CCD ID: PME) (formula: C₁₄H₁₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total	C	N	O	0	0
			21	14	2	5		

Continued on next page...

Continued from previous page...

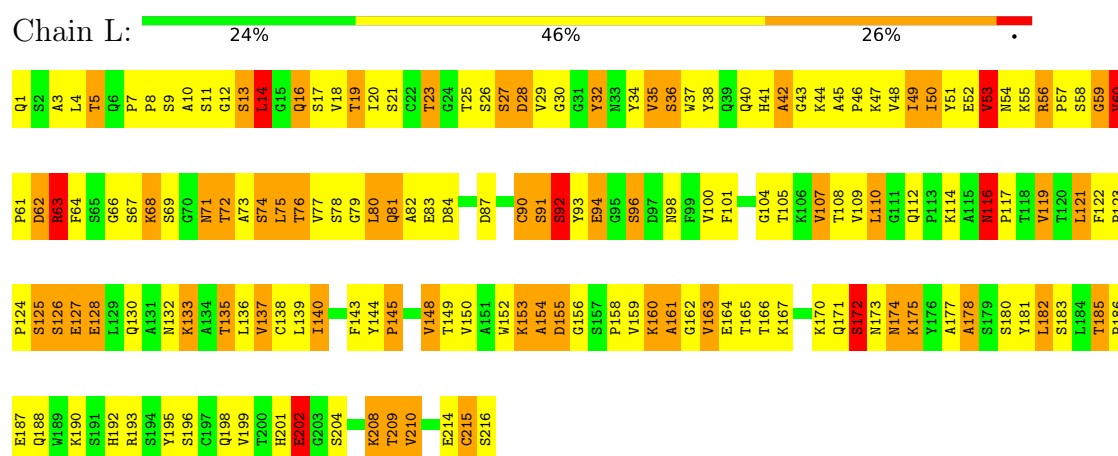
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			21	14	2	5		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: IMMUNOGLOBULIN LAMBDA LIGHT CHAIN DIMER (MCG)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.30 Å 72.30 Å 185.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	62.0 (8.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.220 , 0.380	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3254	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, PME

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	H	0.48	0/1637	0.97	9/2233 (0.4%)
1	L	0.50	0/1637	0.99	10/2233 (0.4%)
All	All	0.49	0/3274	0.98	19/4466 (0.4%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	126	SER	N-CA-C	-8.19	103.27	113.18
1	H	26	SER	N-CA-C	-8.14	102.38	112.47
1	L	71	ASN	N-CA-C	-6.71	104.22	112.88
1	H	129	LEU	N-CA-C	-6.27	105.48	113.01
1	H	97	ASP	N-CA-C	-6.24	104.73	112.72
1	L	116	ASN	N-CA-C	-5.96	102.56	110.07
1	L	63	ARG	N-CA-C	-5.90	106.24	113.50
1	H	29	VAL	N-CA-C	-5.89	105.34	113.00
1	H	143	PHE	N-CA-C	5.87	117.13	108.86
1	L	60	VAL	CA-C-N	5.73	125.71	120.21
1	L	60	VAL	C-N-CA	5.73	125.71	120.21
1	H	142	ASP	N-CA-C	5.67	117.54	110.91
1	H	6	GLN	CA-C-N	5.63	126.18	120.38
1	H	6	GLN	C-N-CA	5.63	126.18	120.38
1	H	202	GLU	N-CA-C	5.54	117.39	110.91
1	L	162	GLY	N-CA-C	-5.26	107.31	115.67
1	L	172	SER	N-CA-C	-5.16	106.84	113.23
1	L	13	SER	N-CA-C	5.14	116.55	107.61
1	L	185	THR	N-CA-C	-5.05	100.04	108.23

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	H	1606	0	1537	175	0
1	L	1606	0	1537	201	0
2	H	21	0	17	16	0
2	L	21	0	17	17	0
All	All	3254	0	3108	375	0

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 59.

All (375) 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)
1:L:127:GLU:HA	1:L:130:GLN:HG3	1.32	1.11
1:H:140:ILE:HG12	1:H:199:VAL:HG11	1.41	1.00
1:H:4:LEU:HD13	1:H:24:GLY:HA3	1.43	0.98
1:L:49:ILE:HA	1:L:60:VAL:HG11	1.45	0.97
1:H:193:ARG:HG3	1:H:194:SER:N	1.80	0.96
1:H:149:THR:HB	1:H:200:THR:HB	1.47	0.95
1:L:16:GLN:HG2	1:L:17:SER:H	1.36	0.88
1:L:11:SER:HB2	1:L:110:LEU:HD11	1.57	0.86
2:L:217:PME:H211	2:H:217:PME:C7	2.06	0.85
1:H:18:VAL:HG22	1:H:77:VAL:HG22	1.57	0.85
1:H:22:CYS:HB3	1:H:73:ALA:HB3	1.58	0.85
1:L:94:GLU:HB3	1:L:98:ASN:HB2	1.57	0.84
1:L:125:SER:HB2	1:L:128:GLU:HB2	1.58	0.84
1:L:171:GLN:HE21	1:L:173:ASN:HD21	1.24	0.83
1:L:121:LEU:HD22	1:L:210:VAL:CG2	2.07	0.83
2:L:217:PME:C21	2:H:217:PME:H2	2.08	0.82
1:L:121:LEU:HD12	1:L:208:LYS:HB2	1.60	0.82
1:H:193:ARG:HG3	1:H:194:SER:H	1.38	0.81
1:H:155:ASP:HA	1:H:193:ARG:HG2	1.62	0.81
1:L:171:GLN:NE2	1:L:173:ASN:HD21	1.79	0.80
2:L:217:PME:H211	2:H:217:PME:H2	1.64	0.80
1:L:51:TYR:CE1	1:L:55:LYS:HB3	2.18	0.78
1:H:9:SER:HB2	1:H:147:ALA:HB3	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:VAL:HG11	1:L:68:LYS:HB2	1.64	0.77
2:L:217:PME:H211	2:H:217:PME:C2	2.14	0.77
1:L:37:TRP:HD1	1:L:50:ILE:HG21	1.49	0.77
1:L:38:TYR:HE1	1:L:91:SER:HB2	1.47	0.77
1:H:40:GLN:HG3	1:H:46:PRO:HG3	1.67	0.76
1:H:94:GLU:HB2	1:H:98:ASN:HB3	1.67	0.76
1:H:186:PRO:O	1:H:190:LYS:HG3	1.85	0.76
1:L:119:VAL:HG22	1:L:208:LYS:HG3	1.68	0.76
1:L:7:PRO:HD3	1:L:21:SER:O	1.85	0.75
2:L:217:PME:H211	2:H:217:PME:O8	1.86	0.75
1:L:4:LEU:HD11	1:L:100:VAL:HG13	1.67	0.75
1:L:48:VAL:HG13	1:L:57:PRO:HG2	1.68	0.75
1:H:187:GLU:HG3	1:H:188:GLN:N	2.03	0.74
1:L:45:ALA:HA	1:H:89:TYR:CE2	2.22	0.74
1:H:198:GLN:HB3	1:H:207:GLU:HG3	1.69	0.74
1:L:154:ALA:N	1:L:159:VAL:HG23	2.03	0.74
1:H:10:ALA:O	1:H:107:VAL:HA	1.87	0.74
1:L:171:GLN:OE1	1:L:177:ALA:HB2	1.87	0.74
1:H:9:SER:CB	1:H:147:ALA:HB3	2.17	0.74
1:L:48:VAL:HG11	1:H:99:PHE:CD2	2.23	0.73
2:H:217:PME:O19	2:H:217:PME:H17	1.89	0.73
1:L:11:SER:HB2	1:L:110:LEU:CD1	2.19	0.73
1:L:16:GLN:HG2	1:L:17:SER:N	2.04	0.73
1:L:37:TRP:H	1:L:50:ILE:HG22	1.53	0.73
1:H:35:VAL:HA	1:H:91:SER:O	1.89	0.72
1:L:10:ALA:HB3	1:L:107:VAL:HG13	1.69	0.72
1:H:155:ASP:CG	1:H:193:ARG:HG2	2.14	0.72
1:H:205:THR:O	1:H:205:THR:HG22	1.89	0.71
1:L:144:TYR:HA	1:L:145:PRO:O	1.92	0.70
1:H:54:ASN:HB3	1:H:66:GLY:O	1.91	0.70
1:L:56:ARG:HH11	1:L:56:ARG:HG3	1.56	0.69
1:L:20:ILE:HD13	1:L:75:LEU:HD23	1.73	0.69
1:L:35:VAL:O	1:L:53:VAL:HA	1.93	0.69
1:L:121:LEU:HD22	1:L:210:VAL:HG22	1.74	0.69
1:L:12:GLY:HA2	1:L:16:GLN:HE22	1.58	0.69
1:L:51:TYR:O	1:L:55:LYS:HB2	1.93	0.68
1:L:81:GLN:O	1:L:109:VAL:HG21	1.93	0.68
1:L:43:GLY:O	1:L:44:LYS:HG3	1.93	0.68
1:L:51:TYR:OH	1:L:55:LYS:HE2	1.94	0.68
1:L:19:THR:HA	1:L:76:THR:HA	1.76	0.67
1:L:52:GLU:C	1:L:53:VAL:HG23	2.18	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:SER:HB3	1:L:209:THR:HG23	1.76	0.67
1:H:29:VAL:HG13	1:H:31:GLY:H	1.58	0.67
1:H:155:ASP:HA	1:H:193:ARG:CG	2.25	0.67
2:H:217:PME:O19	2:H:217:PME:C17	2.42	0.67
1:H:170:LYS:CG	1:H:174:ASN:HA	2.24	0.67
1:L:16:GLN:CG	1:L:17:SER:H	2.02	0.67
1:L:171:GLN:HG2	1:H:164:GLU:HG2	1.75	0.67
1:H:4:LEU:HA	1:H:24:GLY:HA3	1.76	0.66
1:H:125:SER:O	1:H:129:LEU:HD12	1.95	0.66
1:L:121:LEU:HD22	1:L:210:VAL:HG21	1.76	0.66
1:H:18:VAL:HG22	1:H:77:VAL:CG2	2.24	0.66
1:L:171:GLN:HE21	1:L:173:ASN:ND2	1.91	0.65
1:H:170:LYS:HG2	1:H:174:ASN:HA	1.78	0.65
1:L:75:LEU:HG	1:L:76:THR:N	2.12	0.63
1:H:166:THR:HG22	1:H:167:LYS:N	2.12	0.63
1:H:29:VAL:HG13	1:H:31:GLY:N	2.14	0.63
1:L:87:ASP:HA	1:L:105:THR:O	1.99	0.63
1:L:57:PRO:O	1:L:59:GLY:N	2.27	0.62
1:H:34:TYR:O	1:H:92:SER:HA	1.98	0.62
1:L:41:HIS:O	1:L:44:LYS:HB2	1.99	0.62
1:L:52:GLU:O	1:L:53:VAL:HG23	1.99	0.62
1:H:149:THR:O	1:H:199:VAL:HA	1.99	0.62
1:H:22:CYS:O	1:H:24:GLY:N	2.30	0.62
1:H:29:VAL:HG12	1:H:32:TYR:CD2	2.34	0.62
1:L:68:LYS:HA	1:L:73:ALA:HA	1.80	0.62
1:L:45:ALA:HA	1:H:89:TYR:HE2	1.65	0.62
1:L:26:SER:HA	1:L:30:GLY:HA3	1.80	0.61
1:L:34:TYR:CE2	2:L:217:PME:H31	2.34	0.61
1:L:61:PRO:HD2	1:L:64:PHE:CE2	2.34	0.61
1:L:38:TYR:CE1	1:L:91:SER:HB2	2.34	0.61
1:H:25:THR:C	1:H:27:SER:N	2.52	0.61
1:L:56:ARG:HB3	1:L:60:VAL:CG2	2.30	0.61
1:H:155:ASP:CA	1:H:193:ARG:HG2	2.30	0.61
1:H:41:HIS:HB2	1:H:44:LYS:HE2	1.82	0.61
1:L:4:LEU:HD22	1:L:29:VAL:CG2	2.31	0.61
1:H:64:PHE:CE2	1:H:77:VAL:HG12	2.35	0.61
1:H:121:LEU:HD12	1:H:122:PHE:N	2.17	0.60
1:H:110:LEU:HD21	1:H:114:LYS:HE2	1.83	0.60
1:L:17:SER:HA	1:L:77:VAL:O	2.02	0.60
1:L:171:GLN:HG2	1:H:164:GLU:CG	2.32	0.60
1:H:96:SER:C	1:H:99:PHE:HE1	2.09	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:LYS:O	1:L:161:ALA:HB2	2.01	0.59
1:H:166:THR:CG2	1:H:167:LYS:N	2.64	0.59
1:L:150:VAL:HG11	1:L:180:SER:CB	2.33	0.59
1:H:12:GLY:O	1:H:109:VAL:HA	2.03	0.59
1:H:154:ALA:O	1:H:155:ASP:HB2	2.01	0.59
1:L:20:ILE:N	1:L:75:LEU:O	2.34	0.59
2:L:217:PME:H213	2:H:217:PME:H2	1.82	0.59
1:L:37:TRP:N	1:L:50:ILE:HG22	2.18	0.59
1:L:57:PRO:HB3	1:H:97:ASP:O	2.03	0.59
1:L:4:LEU:HD22	1:L:29:VAL:HG23	1.86	0.58
1:H:93:TYR:CE2	2:H:217:PME:H32	2.38	0.58
1:H:121:LEU:HD12	1:H:122:PHE:H	1.69	0.58
1:H:4:LEU:HA	1:H:24:GLY:CA	2.34	0.58
1:H:185:THR:HG22	1:H:186:PRO:HD2	1.86	0.58
1:L:25:THR:O	1:L:30:GLY:N	2.36	0.58
1:L:19:THR:HB	1:L:76:THR:CG2	2.33	0.58
1:L:57:PRO:HA	1:H:97:ASP:OD1	2.04	0.58
1:H:49:ILE:HD13	1:H:60:VAL:HG13	1.86	0.57
1:L:21:SER:HB3	1:L:74:SER:HB2	1.86	0.57
1:H:99:PHE:HD1	1:H:99:PHE:N	2.02	0.57
1:L:30:GLY:HA3	1:L:71:ASN:ND2	2.20	0.57
1:H:47:LYS:O	1:H:47:LYS:HG3	2.04	0.57
1:H:173:ASN:OD1	1:H:175:LYS:HB2	2.05	0.56
1:L:37:TRP:CD1	1:L:50:ILE:HG21	2.35	0.56
1:H:186:PRO:O	1:H:189:TRP:HB3	2.05	0.56
1:L:164:GLU:OE2	1:H:171:GLN:HB3	2.05	0.56
1:H:99:PHE:N	1:H:99:PHE:CD1	2.73	0.56
1:L:93:TYR:HE1	2:L:217:PME:H111	1.71	0.56
1:H:4:LEU:CD1	1:H:24:GLY:HA3	2.27	0.56
1:L:19:THR:HB	1:L:76:THR:HG22	1.88	0.56
1:L:32:TYR:CD1	1:L:32:TYR:N	2.73	0.56
1:H:143:PHE:HE1	1:H:177:ALA:HA	1.71	0.56
1:L:101:PHE:HZ	1:H:38:TYR:HE2	1.53	0.56
1:H:35:VAL:HG11	1:H:73:ALA:CB	2.34	0.56
1:L:46:PRO:HD3	1:H:89:TYR:CE2	2.41	0.55
1:L:73:ALA:O	1:L:74:SER:HB3	2.06	0.55
1:L:4:LEU:CD1	1:L:100:VAL:HG13	2.35	0.55
1:H:155:ASP:CB	1:H:193:ARG:HG2	2.37	0.55
1:L:177:ALA:O	1:L:178:ALA:HB2	2.06	0.55
1:H:124:PRO:O	1:H:129:LEU:HD11	2.06	0.55
1:L:12:GLY:HA2	1:L:16:GLN:NE2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ASN:HA	1:H:68:LYS:NZ	2.22	0.54
1:H:143:PHE:CE1	1:H:177:ALA:HA	2.42	0.54
1:L:48:VAL:HG11	1:H:99:PHE:CG	2.41	0.54
1:H:24:GLY:O	1:H:25:THR:O	2.25	0.54
1:L:56:ARG:HB3	1:L:60:VAL:HG22	1.88	0.54
1:H:189:TRP:NE1	1:H:214:GLU:OE1	2.40	0.54
1:H:25:THR:HG23	1:H:26:SER:H	1.72	0.54
1:H:171:GLN:NE2	1:H:175:LYS:HB3	2.23	0.54
1:H:154:ALA:HB1	1:H:192:HIS:CD2	2.42	0.54
1:H:79:GLY:O	1:H:80:LEU:C	2.51	0.53
1:H:25:THR:OG1	1:H:26:SER:N	2.37	0.53
1:H:193:ARG:CG	1:H:194:SER:N	2.62	0.53
1:L:117:PRO:HA	1:L:143:PHE:HB3	1.88	0.53
1:H:20:ILE:HG12	1:H:105:THR:HG21	1.90	0.53
1:H:56:ARG:HD2	1:H:60:VAL:CG1	2.39	0.53
1:H:9:SER:HB3	1:H:147:ALA:HB3	1.91	0.53
1:H:35:VAL:HG11	1:H:73:ALA:HB1	1.91	0.53
1:L:51:TYR:CZ	1:L:55:LYS:HE2	2.44	0.53
2:L:217:PME:C17	2:L:217:PME:C18	2.86	0.53
1:H:53:VAL:HG12	1:H:67:SER:HA	1.90	0.53
1:L:152:TRP:HZ2	1:L:180:SER:O	1.93	0.52
1:L:159:VAL:CG1	1:L:159:VAL:O	2.57	0.52
1:H:6:GLN:OE1	1:H:90:CYS:SG	2.67	0.52
1:L:34:TYR:CE2	2:L:217:PME:C3	2.93	0.52
1:L:77:VAL:O	1:L:77:VAL:HG23	2.10	0.52
1:H:25:THR:C	1:H:27:SER:H	2.17	0.52
1:L:56:ARG:HG3	1:L:56:ARG:NH1	2.24	0.52
2:L:217:PME:H15	1:H:51:TYR:CD2	2.44	0.52
1:H:82:ALA:C	1:H:84:ASP:H	2.18	0.52
1:H:166:THR:CG2	1:H:167:LYS:H	2.24	0.51
1:L:63:ARG:O	1:L:77:VAL:HA	2.09	0.51
1:H:99:PHE:O	1:H:100:VAL:C	2.52	0.51
1:H:115:ALA:O	1:H:143:PHE:HA	2.10	0.51
1:L:79:GLY:O	1:L:81:GLN:HG2	2.11	0.51
1:H:132:ASN:C	1:H:132:ASN:HD22	2.19	0.51
1:L:18:VAL:O	1:L:76:THR:HA	2.11	0.51
1:L:50:ILE:HA	1:L:55:LYS:O	2.11	0.50
1:L:140:ILE:HD12	1:L:199:VAL:CG2	2.41	0.50
1:L:159:VAL:O	1:L:160:LYS:C	2.54	0.50
1:H:193:ARG:CG	1:H:194:SER:H	2.17	0.50
1:H:62:ASP:OD1	1:H:62:ASP:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:35:VAL:HB	1:L:53:VAL:HG13	1.93	0.50
1:L:56:ARG:NH2	1:L:60:VAL:O	2.44	0.50
1:L:90:CYS:O	1:L:101:PHE:HA	2.11	0.50
1:H:189:TRP:CZ2	1:H:212:PRO:HA	2.47	0.50
1:H:101:PHE:CE2	2:H:217:PME:H14	2.46	0.50
1:L:175:LYS:HD2	1:L:175:LYS:N	2.26	0.50
1:L:144:TYR:HA	1:L:145:PRO:C	2.37	0.50
1:H:148:VAL:HG22	1:H:149:THR:N	2.26	0.50
1:L:50:ILE:HD11	1:L:66:GLY:N	2.27	0.49
1:L:140:ILE:HD12	1:L:199:VAL:HG21	1.94	0.49
1:H:85:GLU:HG3	1:H:108:THR:HA	1.94	0.49
1:L:46:PRO:HD3	1:H:89:TYR:CD2	2.47	0.49
2:L:217:PME:C18	2:L:217:PME:H17	2.42	0.49
1:L:13:SER:O	1:L:14:LEU:C	2.56	0.49
1:L:117:PRO:CA	1:L:143:PHE:HB3	2.43	0.49
1:L:82:ALA:HB3	1:L:174:ASN:HD22	1.78	0.49
1:L:196:SER:CB	1:L:209:THR:HG23	2.42	0.49
1:L:128:GLU:OE1	1:L:135:THR:HG23	2.13	0.49
1:H:24:GLY:O	1:H:25:THR:C	2.55	0.49
1:L:61:PRO:HD2	1:L:64:PHE:CD2	2.46	0.49
1:L:61:PRO:HD2	1:L:64:PHE:HE2	1.77	0.49
1:H:61:PRO:HG2	1:H:64:PHE:CE1	2.48	0.49
1:H:17:SER:OG	1:H:78:SER:HA	2.13	0.49
1:L:56:ARG:HE	1:L:60:VAL:HG23	1.78	0.48
1:H:170:LYS:HE2	1:H:174:ASN:OD1	2.14	0.48
1:L:40:GLN:HB3	1:L:46:PRO:HA	1.95	0.48
1:L:140:ILE:CG2	1:L:199:VAL:HG11	2.44	0.48
1:L:4:LEU:CD1	1:L:92:SER:HB2	2.43	0.48
1:L:148:VAL:CG2	1:L:201:HIS:HB2	2.44	0.48
1:H:52:GLU:O	1:H:54:ASN:N	2.43	0.48
1:L:8:PRO:O	1:L:9:SER:HB3	2.13	0.48
1:L:93:TYR:HE1	2:L:217:PME:C11	2.27	0.48
1:H:155:ASP:OD1	1:H:192:HIS:HB3	2.13	0.48
1:L:93:TYR:CE1	2:L:217:PME:H111	2.48	0.48
1:L:139:LEU:HD22	1:H:137:VAL:HG23	1.95	0.48
1:L:91:SER:HA	1:L:100:VAL:O	2.13	0.48
1:L:125:SER:HB2	1:L:128:GLU:H	1.79	0.48
1:L:148:VAL:HG13	1:L:149:THR:N	2.27	0.48
1:H:128:GLU:HG2	1:H:133:LYS:HG3	1.95	0.48
1:L:17:SER:HB3	1:L:78:SER:HA	1.96	0.48
1:L:30:GLY:CA	1:L:71:ASN:ND2	2.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:52:GLU:C	1:L:53:VAL:CG2	2.86	0.48
1:L:62:ASP:OD1	1:L:62:ASP:N	2.36	0.48
1:L:148:VAL:HG22	1:L:201:HIS:HB2	1.96	0.47
1:L:4:LEU:HD11	1:L:92:SER:HB2	1.95	0.47
1:H:120:THR:OG1	1:H:122:PHE:CE1	2.67	0.47
1:L:119:VAL:HG22	1:L:208:LYS:CG	2.41	0.47
1:L:3:ALA:HB1	1:L:101:PHE:O	2.15	0.47
1:L:54:ASN:O	1:L:55:LYS:HG3	2.14	0.47
1:H:22:CYS:CB	1:H:73:ALA:HB3	2.39	0.47
1:H:93:TYR:CZ	2:H:217:PME:H32	2.50	0.47
1:H:171:GLN:CG	1:H:175:LYS:O	2.62	0.47
1:L:20:ILE:HD13	1:L:75:LEU:CD2	2.41	0.47
2:L:217:PME:C15	2:H:217:PME:H212	2.45	0.47
1:L:4:LEU:CD2	1:L:29:VAL:HG23	2.44	0.47
1:L:16:GLN:CG	1:L:17:SER:N	2.71	0.47
1:H:50:ILE:HD12	1:H:75:LEU:HD12	1.96	0.47
1:L:28:ASP:O	1:L:32:TYR:HD1	1.98	0.47
1:H:133:LYS:HA	1:H:186:PRO:HD3	1.97	0.47
2:H:217:PME:C17	2:H:217:PME:C18	2.92	0.47
1:L:41:HIS:O	1:L:42:ALA:C	2.58	0.46
1:L:7:PRO:O	1:L:104:GLY:O	2.33	0.46
1:L:77:VAL:HG23	1:L:80:LEU:HD13	1.96	0.46
1:H:93:TYR:CG	2:H:217:PME:N1	2.78	0.46
1:H:143:PHE:O	1:H:144:TYR:HB2	2.14	0.46
1:H:34:TYR:OH	2:H:217:PME:H212	2.15	0.46
1:L:29:VAL:HG11	1:L:71:ASN:O	2.15	0.46
1:H:33:ASN:O	1:H:53:VAL:HG23	2.16	0.46
1:H:192:HIS:O	1:H:212:PRO:HG2	2.15	0.46
1:H:8:PRO:O	1:H:147:ALA:HB1	2.16	0.46
1:L:154:ALA:C	1:L:156:GLY:H	2.22	0.46
1:L:185:THR:O	1:L:186:PRO:C	2.58	0.46
1:H:171:GLN:HG3	1:H:175:LYS:O	2.16	0.46
1:L:122:PHE:HA	1:L:123:PRO:HD3	1.80	0.45
1:L:124:PRO:HD3	1:L:136:LEU:HD23	1.98	0.45
1:L:138:CYS:HB2	1:L:152:TRP:CZ2	2.51	0.45
1:L:214:GLU:O	1:L:215:CYS:HB3	2.15	0.45
2:L:217:PME:C17	2:L:217:PME:H212	2.45	0.45
1:H:164:GLU:OE1	1:H:164:GLU:HA	2.16	0.45
1:H:54:ASN:CB	1:H:66:GLY:O	2.62	0.45
1:H:164:GLU:HB3	1:H:181:TYR:CE1	2.52	0.45
1:L:81:GLN:N	1:L:84:ASP:OD2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:SER:HB3	1:H:145:PRO:HG2	1.97	0.45
1:L:7:PRO:O	1:L:105:THR:OG1	2.30	0.45
1:H:63:ARG:NH2	1:H:84:ASP:OD1	2.49	0.45
1:L:4:LEU:HD11	1:L:100:VAL:CG1	2.42	0.45
1:L:125:SER:HB2	1:L:128:GLU:CB	2.37	0.45
1:L:136:LEU:O	1:L:181:TYR:HA	2.17	0.45
1:L:122:PHE:HB2	1:L:137:VAL:HG13	1.98	0.45
1:L:160:LYS:O	1:L:161:ALA:CB	2.64	0.45
1:H:62:ASP:C	1:H:64:PHE:N	2.74	0.45
1:H:93:TYR:CZ	1:H:96:SER:HA	2.51	0.45
1:L:27:SER:O	1:L:32:TYR:HE1	1.98	0.45
1:L:4:LEU:HD22	1:L:29:VAL:HG21	1.99	0.45
1:H:101:PHE:C	1:H:102:GLY:O	2.59	0.45
1:L:201:HIS:O	1:L:202:GLU:C	2.60	0.45
1:L:159:VAL:HG11	1:L:182:LEU:HD21	1.98	0.44
1:H:40:GLN:HG3	1:H:46:PRO:CG	2.43	0.44
1:H:27:SER:O	1:H:28:ASP:O	2.35	0.44
1:H:75:LEU:HG	1:H:76:THR:N	2.32	0.44
1:L:128:GLU:OE1	1:L:135:THR:N	2.50	0.44
1:H:77:VAL:HG23	1:H:77:VAL:O	2.16	0.44
1:L:153:LYS:NZ	1:L:153:LYS:HB3	2.32	0.44
1:H:69:SER:N	1:H:72:THR:O	2.42	0.44
1:L:135:THR:HA	1:L:182:LEU:O	2.18	0.44
1:H:95:GLY:C	1:H:97:ASP:H	2.26	0.44
1:H:198:GLN:HG3	1:H:198:GLN:O	2.18	0.44
1:L:174:ASN:C	1:L:175:LYS:HD2	2.42	0.44
1:H:29:VAL:HG12	1:H:32:TYR:CE2	2.52	0.44
1:L:128:GLU:OE2	1:L:133:LYS:HB3	2.18	0.44
1:L:214:GLU:O	1:L:215:CYS:CB	2.65	0.43
1:H:98:ASN:C	1:H:99:PHE:HD1	2.25	0.43
1:L:40:GLN:HB2	1:L:44:LYS:O	2.18	0.43
1:L:49:ILE:HG22	1:L:60:VAL:CG1	2.47	0.43
1:H:13:SER:OG	1:H:16:GLN:OE1	2.36	0.43
1:H:62:ASP:C	1:H:64:PHE:H	2.25	0.43
1:L:11:SER:CB	1:L:110:LEU:HD11	2.37	0.43
1:H:101:PHE:O	1:H:102:GLY:O	2.37	0.43
1:L:37:TRP:HB2	1:L:50:ILE:HB	2.00	0.43
1:L:56:ARG:CB	1:L:60:VAL:HG22	2.47	0.43
1:L:166:THR:HB	1:H:169:SER:HB3	2.00	0.43
1:L:185:THR:OG1	1:L:188:GLN:CB	2.66	0.43
1:H:22:CYS:HB2	1:H:37:TRP:CZ2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:VAL:CG2	1:H:199:VAL:HB	2.48	0.43
1:L:66:GLY:HA2	1:L:74:SER:O	2.18	0.43
1:L:117:PRO:HD3	1:L:201:HIS:CG	2.53	0.43
1:L:140:ILE:HG21	1:L:199:VAL:HG11	1.99	0.43
1:H:51:TYR:CE1	1:H:55:LYS:HB3	2.53	0.43
1:L:49:ILE:CA	1:L:60:VAL:HG11	2.33	0.43
1:L:155:ASP:OD2	1:L:193:ARG:HB2	2.18	0.43
1:L:159:VAL:O	1:L:159:VAL:HG12	2.19	0.43
1:H:134:ALA:HB3	1:H:184:LEU:HD23	2.00	0.43
1:H:144:TYR:HA	1:H:145:PRO:C	2.44	0.43
1:H:205:THR:O	1:H:205:THR:CG2	2.60	0.43
2:L:217:PME:C15	1:H:51:TYR:CD2	3.02	0.42
1:L:50:ILE:HD11	1:L:66:GLY:H	1.84	0.42
1:H:107:VAL:CG1	1:H:108:THR:N	2.82	0.42
1:L:45:ALA:HA	1:L:46:PRO:HD3	1.86	0.42
1:L:165:THR:HG22	1:L:166:THR:N	2.33	0.42
1:H:22:CYS:HB2	1:H:37:TRP:CH2	2.54	0.42
1:H:91:SER:OG	2:H:217:PME:H15	2.20	0.42
1:L:36:SER:HA	1:L:50:ILE:HG22	2.02	0.42
1:L:161:ALA:H	1:L:163:VAL:CG1	2.32	0.42
1:H:171:GLN:NE2	1:H:175:LYS:O	2.53	0.42
1:L:133:LYS:HB2	1:L:133:LYS:NZ	2.35	0.42
1:L:29:VAL:HG22	1:L:92:SER:OG	2.19	0.42
1:L:42:ALA:O	1:L:44:LYS:HD2	2.20	0.42
1:H:171:GLN:NE2	1:H:173:ASN:OD1	2.47	0.42
1:L:23:THR:HA	1:L:72:THR:HB	2.02	0.42
1:L:10:ALA:HB1	1:L:18:VAL:HG21	2.01	0.41
1:L:56:ARG:HB3	1:L:60:VAL:HG21	2.01	0.41
1:L:66:GLY:HA2	1:L:75:LEU:HA	2.02	0.41
1:H:41:HIS:CB	1:H:44:LYS:HE2	2.48	0.41
1:H:25:THR:O	1:H:26:SER:C	2.61	0.41
1:H:213:THR:O	1:H:214:GLU:O	2.39	0.41
1:H:61:PRO:HG2	1:H:64:PHE:HE1	1.85	0.41
1:L:154:ALA:C	1:L:156:GLY:N	2.78	0.41
1:H:119:VAL:HA	1:H:139:LEU:O	2.20	0.41
1:L:63:ARG:HB3	1:L:78:SER:O	2.21	0.41
1:H:99:PHE:O	1:H:100:VAL:O	2.39	0.41
1:H:165:THR:HG22	1:H:166:THR:O	2.20	0.41
1:L:116:ASN:ND2	1:L:204:SER:OG	2.45	0.41
1:L:171:GLN:HB3	1:L:172:SER:H	1.66	0.41
1:H:118:THR:O	1:H:118:THR:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:HIS:O	1:H:202:GLU:HB2	2.21	0.41
1:L:21:SER:CB	1:L:74:SER:HB2	2.49	0.41
1:L:148:VAL:CG1	1:L:149:THR:N	2.83	0.41
1:H:20:ILE:CG1	1:H:105:THR:HG21	2.50	0.41
1:H:110:LEU:HD12	1:H:110:LEU:HA	1.82	0.41
1:H:50:ILE:HD12	1:H:75:LEU:CD1	2.50	0.41
1:H:94:GLU:N	1:H:98:ASN:O	2.52	0.41
1:H:211:ALA:HA	1:H:212:PRO:HD3	1.89	0.41
1:H:206:VAL:O	1:H:206:VAL:HG13	2.21	0.40
1:L:7:PRO:CD	1:L:21:SER:O	2.63	0.40
1:L:192:HIS:CD2	1:L:195:TYR:OH	2.74	0.40
1:L:170:LYS:HA	1:L:175:LYS:O	2.20	0.40
1:H:82:ALA:O	1:H:84:ASP:N	2.52	0.40
1:H:122:PHE:CD1	1:H:137:VAL:HG12	2.56	0.40
1:H:167:LYS:HB2	1:H:167:LYS:HE2	1.66	0.40
1:L:18:VAL:CG1	1:L:77:VAL:HG22	2.51	0.40
1:L:54:ASN:CG	1:L:66:GLY:O	2.65	0.40
1:L:155:ASP:OD1	1:L:193:ARG:N	2.52	0.40
1:H:69:SER:O	1:H:71:ASN:N	2.49	0.40
1:H:109:VAL:O	1:H:110:LEU:C	2.65	0.40
1:L:51:TYR:CD1	1:L:55:LYS:HB3	2.56	0.40
1:L:154:ALA:HB2	1:L:159:VAL:CG2	2.52	0.40
1:H:117:PRO:HB3	1:H:140:ILE:CG2	2.52	0.40
1:H:119:VAL:HG22	1:H:208:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

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	H	214/216 (99%)	164 (77%)	34 (16%)	16 (8%)	1 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	214/216 (99%)	167 (78%)	28 (13%)	19 (9%)	0	0
All	All	428/432 (99%)	331 (77%)	62 (14%)	35 (8%)	0	1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	58	SER
1	L	96	SER
1	L	161	ALA
1	L	215	CYS
1	H	16	GLN
1	H	23	THR
1	H	25	THR
1	H	100	VAL
1	H	214	GLU
1	L	14	LEU
1	L	16	GLN
1	L	42	ALA
1	H	28	ASP
1	H	83	GLU
1	L	158	PRO
1	L	178	ALA
1	H	80	LEU
1	L	59	GLY
1	L	74	SER
1	L	92	SER
1	L	154	ALA
1	L	160	LYS
1	L	202	GLU
1	H	7	PRO
1	H	27	SER
1	H	46	PRO
1	H	48	VAL
1	H	71	ASN
1	H	189	TRP
1	H	201	HIS
1	L	5	THR
1	L	125	SER
1	H	102	GLY
1	L	53	VAL
1	L	145	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	H	180/180 (100%)	108 (60%)	72 (40%)	0	0
1	L	180/180 (100%)	115 (64%)	65 (36%)	0	0
All	All	360/360 (100%)	223 (62%)	137 (38%)	0	0

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	14	LEU
1	L	19	THR
1	L	23	THR
1	L	27	SER
1	L	28	ASP
1	L	32	TYR
1	L	35	VAL
1	L	36	SER
1	L	47	LYS
1	L	49	ILE
1	L	50	ILE
1	L	53	VAL
1	L	56	ARG
1	L	60	VAL
1	L	62	ASP
1	L	63	ARG
1	L	67	SER
1	L	68	LYS
1	L	69	SER
1	L	72	THR
1	L	75	LEU
1	L	76	THR
1	L	80	LEU
1	L	81	GLN
1	L	83	GLU
1	L	90	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	91	SER
1	L	92	SER
1	L	94	GLU
1	L	96	SER
1	L	107	VAL
1	L	108	THR
1	L	110	LEU
1	L	112	GLN
1	L	114	LYS
1	L	116	ASN
1	L	119	VAL
1	L	121	LEU
1	L	126	SER
1	L	127	GLU
1	L	128	GLU
1	L	132	ASN
1	L	133	LYS
1	L	135	THR
1	L	137	VAL
1	L	140	ILE
1	L	148	VAL
1	L	153	LYS
1	L	155	ASP
1	L	163	VAL
1	L	167	LYS
1	L	172	SER
1	L	174	ASN
1	L	175	LYS
1	L	182	LEU
1	L	183	SER
1	L	187	GLU
1	L	190	LYS
1	L	198	GLN
1	L	202	GLU
1	L	208	LYS
1	L	209	THR
1	L	210	VAL
1	L	216	SER
1	H	2	SER
1	H	5	THR
1	H	9	SER
1	H	13	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	14	LEU
1	H	16	GLN
1	H	18	VAL
1	H	21	SER
1	H	23	THR
1	H	25	THR
1	H	28	ASP
1	H	36	SER
1	H	40	GLN
1	H	47	LYS
1	H	49	ILE
1	H	50	ILE
1	H	55	LYS
1	H	56	ARG
1	H	62	ASP
1	H	63	ARG
1	H	65	SER
1	H	67	SER
1	H	68	LYS
1	H	69	SER
1	H	71	ASN
1	H	75	LEU
1	H	76	THR
1	H	78	SER
1	H	80	LEU
1	H	83	GLU
1	H	91	SER
1	H	92	SER
1	H	98	ASN
1	H	99	PHE
1	H	101	PHE
1	H	103	THR
1	H	106	LYS
1	H	108	THR
1	H	109	VAL
1	H	110	LEU
1	H	112	GLN
1	H	114	LYS
1	H	119	VAL
1	H	120	THR
1	H	121	LEU
1	H	126	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	127	GLU
1	H	133	LYS
1	H	136	LEU
1	H	137	VAL
1	H	141	SER
1	H	149	THR
1	H	153	LYS
1	H	157	SER
1	H	160	LYS
1	H	167	LYS
1	H	170	LYS
1	H	175	LYS
1	H	182	LEU
1	H	184	LEU
1	H	187	GLU
1	H	188	GLN
1	H	190	LYS
1	H	198	GLN
1	H	199	VAL
1	H	204	SER
1	H	208	LYS
1	H	209	THR
1	H	210	VAL
1	H	213	THR
1	H	214	GLU
1	H	215	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	16	GLN
1	L	71	ASN
1	L	98	ASN
1	L	171	GLN
1	L	174	ASN
1	L	188	GLN
1	L	192	HIS
1	H	41	HIS
1	H	98	ASN
1	H	130	GLN
1	H	132	ASN
1	H	188	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	201	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	L	1	1	7,8,9	1.12	1 (14%)	9,10,12	0.94	0
1	PCA	H	1	1	7,8,9	1.22	1 (14%)	9,10,12	0.95	0

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
1	PCA	L	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	PCA	CA-N	2.87	1.49	1.46
1	L	1	PCA	CA-N	2.66	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	PME	L	217	-	21,21,21	1.89	1 (4%)	27,27,27	1.41	3 (11%)
2	PME	H	217	-	21,21,21	1.46	1 (4%)	27,27,27	1.33	3 (11%)

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
2	PME	L	217	-	-	15/22/22/22	0/1/1/1
2	PME	H	217	-	-	6/22/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	217	PME	O20-C18	7.63	1.52	1.33
2	H	217	PME	O20-C18	5.80	1.47	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	217	PME	C21-O20-C18	-4.34	106.07	115.92
2	L	217	PME	O20-C18-C10	4.29	122.41	111.49
2	H	217	PME	O20-C18-C10	3.82	121.21	111.49
2	H	217	PME	C21-O20-C18	-3.77	107.36	115.92
2	H	217	PME	O20-C18-O19	-2.91	118.18	123.85
2	L	217	PME	O20-C18-O19	-2.35	119.27	123.85

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	217	PME	C7-C2-C3-C4
2	L	217	PME	N1-C2-C7-N9
2	L	217	PME	C3-C2-C7-O8
2	L	217	PME	C3-C2-C7-N9
2	H	217	PME	N1-C2-C3-C4
2	H	217	PME	C7-C2-C3-C4
2	H	217	PME	C10-C18-O20-C21
2	H	217	PME	O19-C18-O20-C21
2	L	217	PME	C10-C18-O20-C21
2	L	217	PME	O19-C18-O20-C21
2	L	217	PME	N1-C2-C3-C4
2	L	217	PME	C10-C11-C12-C17
2	L	217	PME	C10-C11-C12-C13
2	L	217	PME	N1-C2-C7-O8
2	H	217	PME	C10-C11-C12-C17
2	L	217	PME	N9-C10-C18-O20
2	H	217	PME	C10-C11-C12-C13
2	L	217	PME	N9-C10-C18-O19
2	L	217	PME	C11-C10-N9-C7
2	L	217	PME	C11-C10-C18-O20
2	L	217	PME	C11-C10-C18-O19

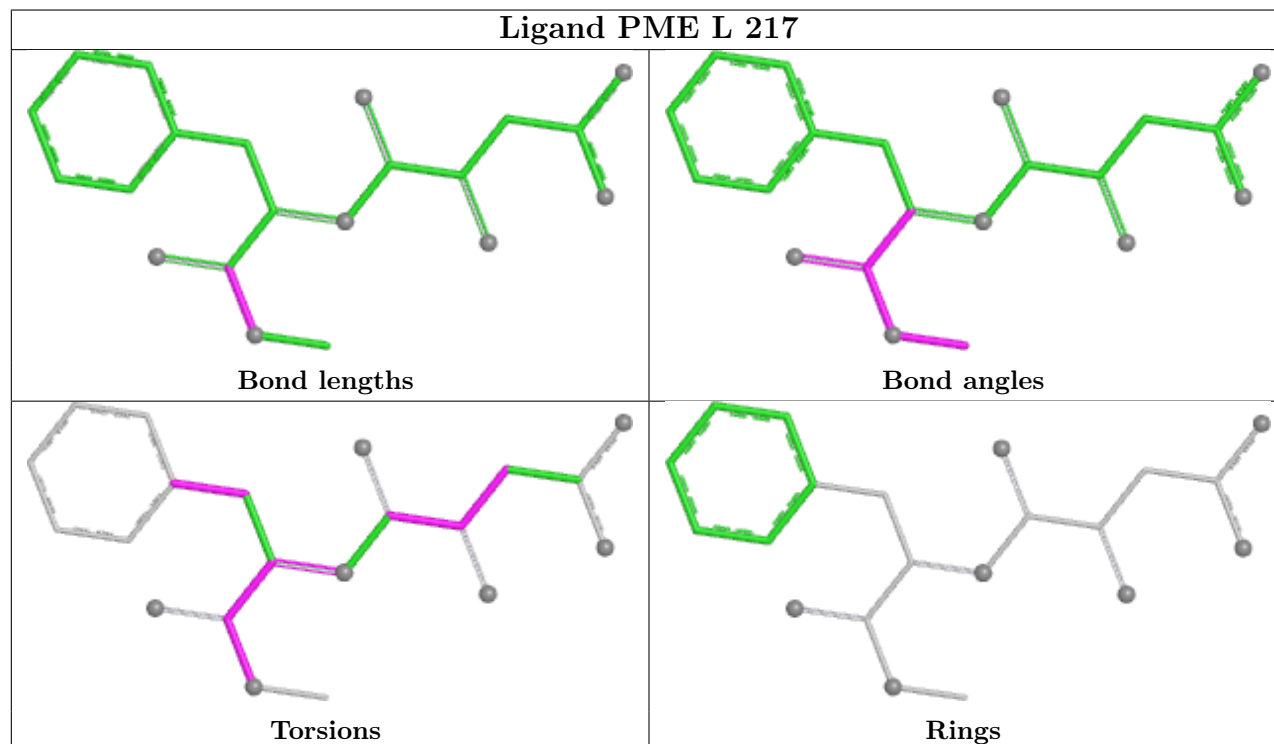
There are no ring outliers.

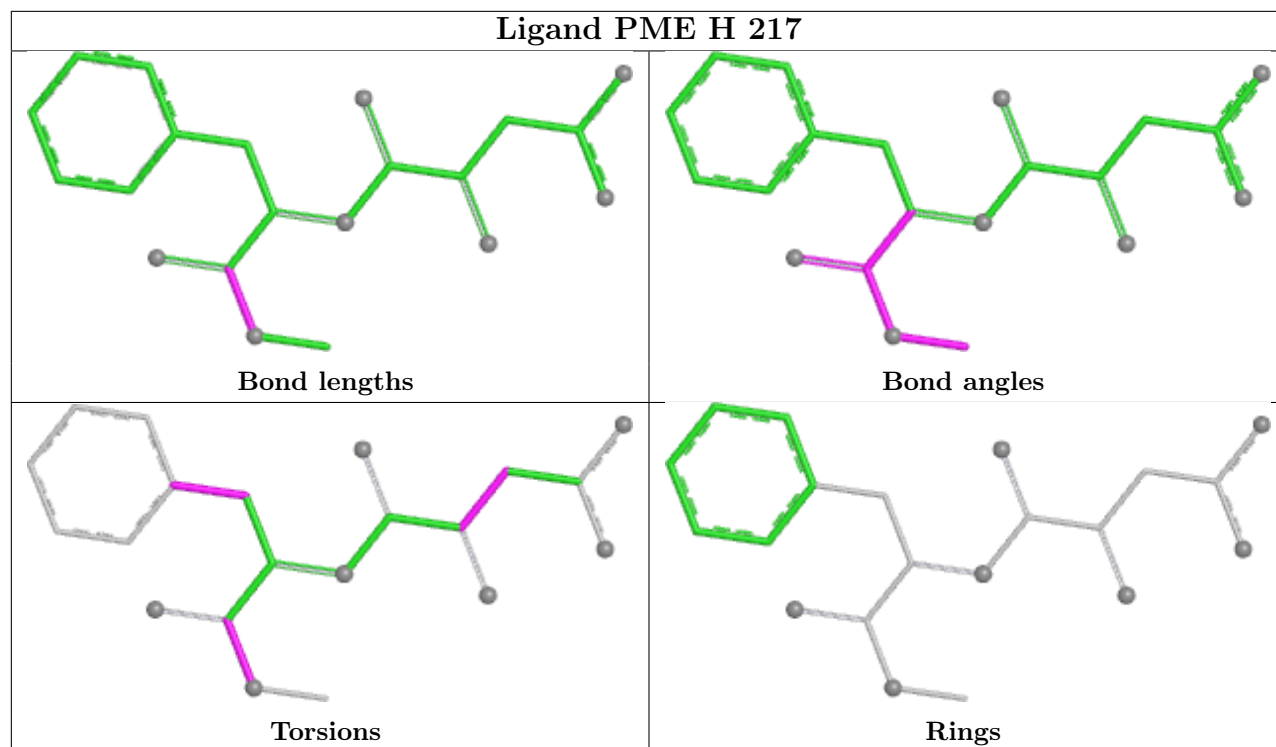
2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	217	PME	17	0
2	H	217	PME	16	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.