



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 AM UTC

PDB ID : 3LB6 / pdb_00003lb6
Title : The structure of IL-13 in complex with IL-13Ralpha2
Authors : Lupardus, P.J.; Garcia, K.C.; Birnbaum, M.E.
Deposited on : 2010-01-07
Resolution : 3.05 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
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

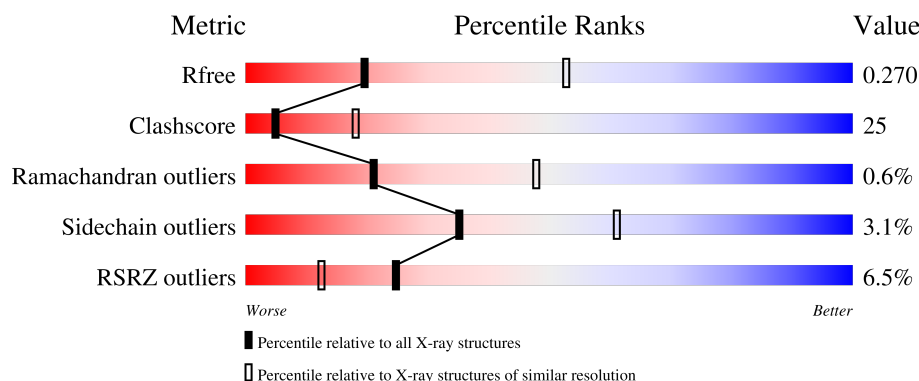
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	132	5% 49% 30% • 17%
2	C	380	6% 35% 28% • 34%
3	B	132	5% 59% 17% 6% 17%
4	D	380	3% 43% 30% • 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6088 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 Interleukin-13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			830	526	145	152	7			

- Molecule 2 is a protein called Interleukin-13 receptor subunit alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	252	Total	C	N	O	S	0	0	0
			2047	1343	315	379	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	151	GLN	ARG	engineered mutation	UNP A8K7E2

- Molecule 3 is a protein called Interleukin-13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	109	Total	C	N	O	S	0	0	0
			840	533	147	153	7			

- Molecule 4 is a protein called Interleukin-13 receptor subunit alpha-2.

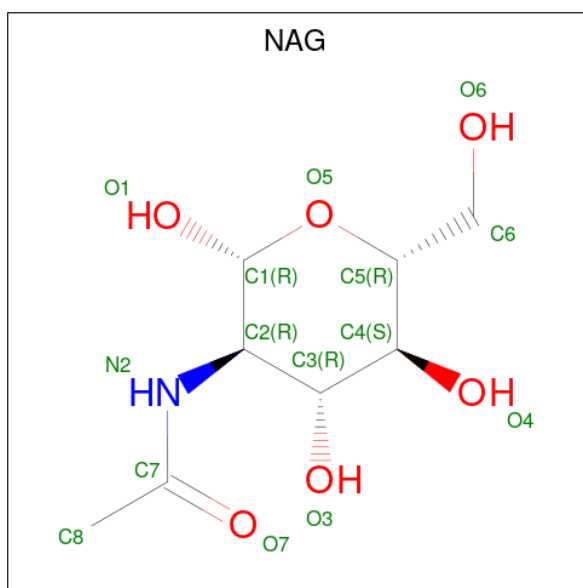
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	286	Total	C	N	O	S	5	0	0
			2310	1501	362	435	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLN	ARG	engineered mutation	UNP A8K7E2

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

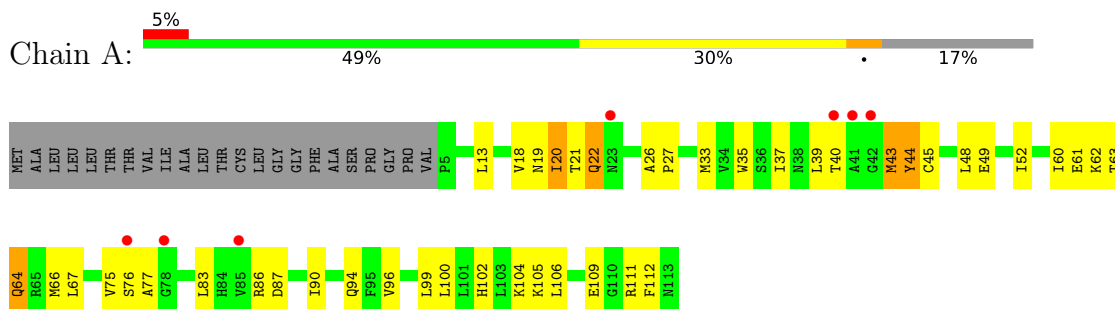
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	O	0	0
			7	7		
7	C	4	Total	O	0	0
			4	4		
7	B	4	Total	O	0	0
			4	4		
7	D	16	Total	O	0	0
			16	16		

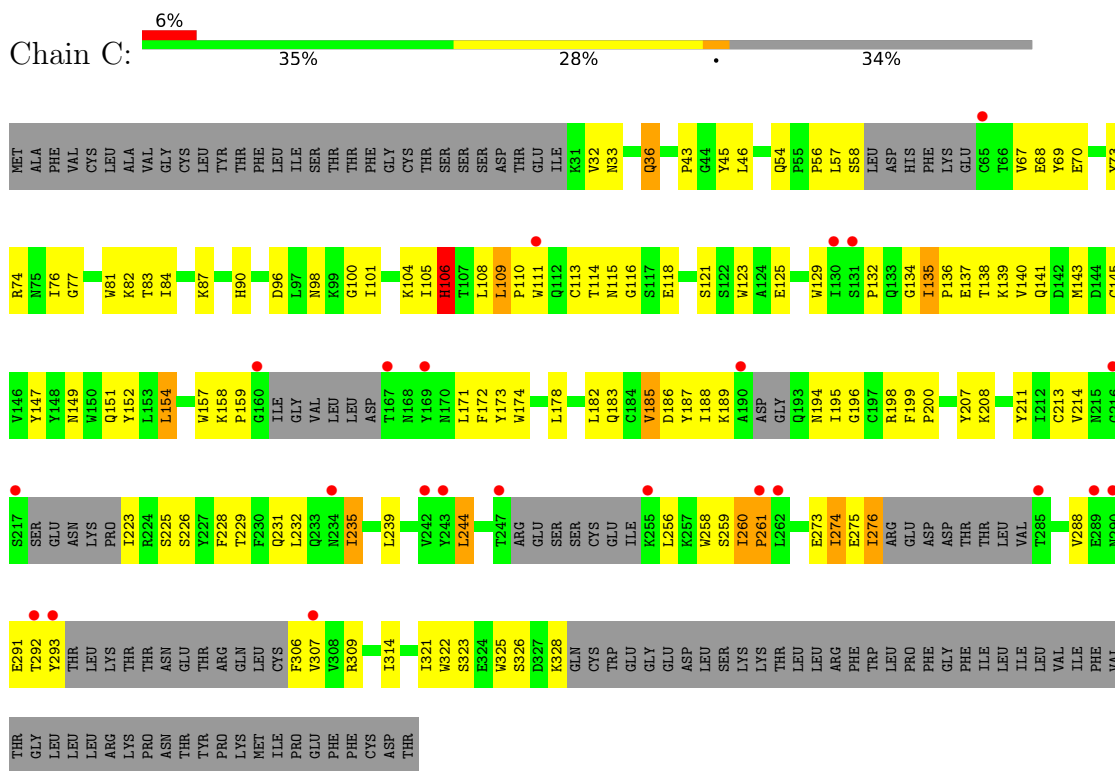
3 Residue-property plots

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

• Molecule 1: Interleukin-13



• Molecule 2: Interleukin-13 receptor subunit alpha-2

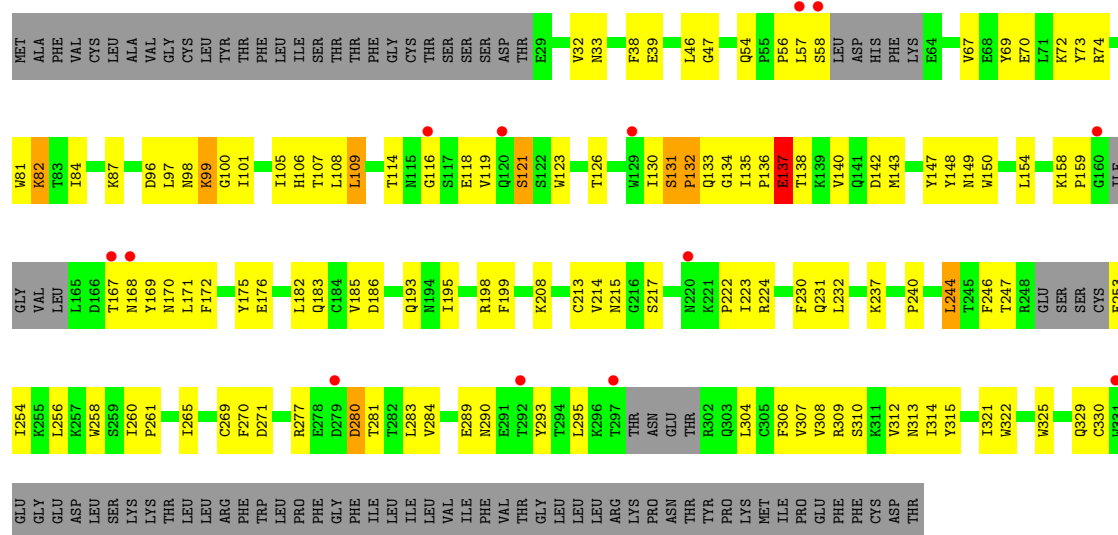
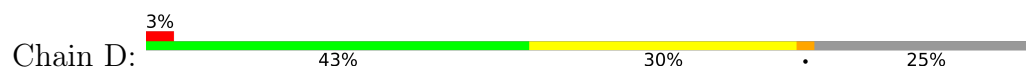


• Molecule 3: Interleukin-13





- Molecule 4: Interleukin-13 receptor subunit alpha-2



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.37Å 86.57Å 166.79Å 90.00° 96.77° 90.00°	Depositor
Resolution (Å)	82.80 – 3.05 82.80 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.2 (82.80-3.05) 100.0 (82.80-3.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.219 , 0.269 0.221 , 0.270	Depositor DCC
R_{free} test set	1020 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6088	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: MLY, NAG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	3/844 (0.4%)	1.09	7/1140 (0.6%)
2	C	0.61	5/2090 (0.2%)	0.99	14/2858 (0.5%)
3	B	0.79	4/843 (0.5%)	1.08	7/1138 (0.6%)
4	D	0.76	1/2357 (0.0%)	1.03	9/3225 (0.3%)
All	All	0.71	13/6134 (0.2%)	1.03	37/8361 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	261	PRO	N-CD	6.28	1.56	1.47
1	A	102	HIS	ND1-CE1	5.63	1.38	1.32
3	B	102	HIS	ND1-CE1	5.43	1.38	1.32
3	B	84	HIS	ND1-CE1	5.42	1.38	1.32
2	C	90	HIS	ND1-CE1	5.32	1.37	1.32
2	C	106	HIS	ND1-CE1	5.27	1.37	1.32
2	C	36	GLN	CD-OE1	5.26	1.33	1.23
1	A	22	GLN	CD-OE1	5.23	1.33	1.23
3	B	22	GLN	CD-OE1	5.22	1.33	1.23
3	B	38	ASN	CG-OD1	5.21	1.33	1.23
1	A	64	GLN	CD-OE1	5.15	1.33	1.23
2	C	54	GLN	CD-OE1	5.06	1.33	1.23
4	D	54	GLN	CD-NE2	-5.05	1.22	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	N-CA-C	9.55	121.48	108.11
2	C	260	ILE	N-CA-C	7.97	116.43	109.02
1	A	22	GLN	N-CA-C	-7.67	104.45	113.88
3	B	44	TYR	N-CA-C	-7.12	102.72	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	A	44	TYR	N-CA-C	-6.59	104.10	111.28
2	C	90	HIS	CB-CG-CD2	-6.56	122.67	131.20
3	B	102	HIS	CB-CG-CD2	-6.55	122.68	131.20
2	C	106	HIS	CB-CG-CD2	-6.54	122.70	131.20
3	B	84	HIS	CB-CG-CD2	-6.47	122.79	131.20
3	B	75	VAL	N-CA-C	6.46	117.15	108.11
2	C	274	ILE	N-CA-C	6.36	118.18	107.18
4	D	315	TYR	N-CA-C	-6.33	105.72	113.50
4	D	277	ARG	N-CA-C	6.31	119.47	109.50
1	A	39	LEU	N-CA-CB	-6.21	101.63	110.58
2	C	200	PRO	CB-CA-C	-6.18	101.37	111.56
1	A	43	MET	CB-CA-C	-5.91	99.09	109.02
4	D	280	ASP	N-CA-C	5.89	119.83	110.70
4	D	199	PHE	CA-C-N	5.87	127.18	119.84
4	D	199	PHE	C-N-CA	5.87	127.18	119.84
1	A	102	HIS	CB-CG-ND1	5.86	131.49	122.70
3	B	40	THR	CB-CA-C	-5.85	101.81	113.80
2	C	259	SER	N-CA-C	5.78	117.01	108.86
4	D	137	GLU	N-CA-C	-5.73	104.83	113.89
3	B	102	HIS	CB-CG-ND1	5.72	131.28	122.70
2	C	90	HIS	CB-CG-ND1	5.65	131.17	122.70
3	B	84	HIS	CB-CG-ND1	5.63	131.15	122.70
2	C	106	HIS	CB-CG-ND1	5.63	131.15	122.70
4	D	67	VAL	O-C-N	-5.59	117.00	122.93
4	D	121	SER	N-CA-C	5.58	118.50	109.79
2	C	135	ILE	CB-CA-C	5.51	117.11	110.78
2	C	288	VAL	N-CA-C	5.44	115.47	107.75
2	C	199	PHE	CA-C-N	5.32	126.49	119.84
2	C	199	PHE	C-N-CA	5.32	126.49	119.84
2	C	185	VAL	CB-CA-C	-5.28	107.22	111.71
4	D	39	GLU	N-CA-C	5.15	117.64	109.50
2	C	77	GLY	N-CA-C	-5.06	108.45	114.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	830	0	832	31	1
2	C	2047	0	1874	128	1
3	B	840	0	851	23	0
4	D	2310	0	2140	123	1
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	7	0	0	2	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
7	D	16	0	0	2	0
All	All	6088	0	5723	297	2

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 25.

All (297) 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)
4:D:167:THR:HG23	4:D:217:SER:O	1.21	1.30
2:C:140:VAL:HG21	2:C:157:TRP:CD1	1.77	1.19
2:C:292:THR:HG22	2:C:293:TYR:H	1.26	1.00
4:D:134:GLY:O	4:D:224:ARG:NH2	1.94	1.00
4:D:167:THR:CG2	4:D:217:SER:O	2.08	0.99
4:D:280:ASP:O	4:D:281:THR:HG22	1.67	0.93
3:B:43:MET:HG3	3:B:44:TYR:N	1.84	0.93
4:D:169:TYR:HE2	4:D:193:GLN:HE21	1.17	0.92
4:D:148:TYR:CE2	4:D:154:LEU:HD12	2.05	0.91
3:B:60:ILE:O	3:B:64:GLN:HG3	1.71	0.90
1:A:62:LYS:HD3	1:A:66:MET:HE3	1.54	0.88
2:C:140:VAL:HG21	2:C:157:TRP:HD1	1.41	0.86
2:C:292:THR:HG22	2:C:293:TYR:N	1.84	0.83
4:D:247:THR:O	4:D:254:ILE:HG13	1.79	0.83
4:D:140:VAL:CG1	4:D:169:TYR:CE1	2.63	0.81
4:D:169:TYR:HE2	4:D:193:GLN:NE2	1.79	0.80
4:D:97:LEU:HD13	4:D:130:ILE:HD11	1.63	0.80
4:D:290:ASN:OD1	7:D:397:HOH:O	1.99	0.80
2:C:76:ILE:HD12	2:C:100:GLY:HA3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:244:LEU:HB3	2:C:306:PHE:CZ	2.17	0.80
2:C:276:ILE:HG22	2:C:306:PHE:HA	1.64	0.80
2:C:135:ILE:O	2:C:138:THR:HG22	1.82	0.79
2:C:69:TYR:HB3	2:C:105:ILE:HD11	1.66	0.78
3:B:87:ASP:HB3	4:D:87:LYS:HE2	1.67	0.77
2:C:275:GLU:O	2:C:275:GLU:HG2	1.82	0.77
4:D:96:ASP:OD2	4:D:98:ASN:HB2	1.84	0.76
2:C:140:VAL:CG2	2:C:157:TRP:CD1	2.64	0.76
2:C:140:VAL:HG23	2:C:158:LYS:O	1.86	0.76
2:C:292:THR:CG2	2:C:293:TYR:H	1.99	0.75
2:C:260:ILE:HD12	2:C:261:PRO:O	1.87	0.75
4:D:280:ASP:O	4:D:281:THR:CG2	2.35	0.75
4:D:280:ASP:C	4:D:281:THR:CG2	2.60	0.74
1:A:112:PHE:HB3	7:A:119:HOH:O	1.88	0.74
4:D:74:ARG:HH11	4:D:81:TRP:NE1	1.86	0.74
1:A:94:GLN:NE2	7:A:120:HOH:O	2.19	0.74
2:C:185:VAL:HG23	2:C:186:ASP:N	2.01	0.73
2:C:137:GLU:H	2:C:139:MLY:CG	2.01	0.73
3:B:43:MET:CG	3:B:44:TYR:N	2.52	0.73
2:C:174:TRP:HA	2:C:178:LEU:HD12	1.72	0.72
2:C:185:VAL:HG23	2:C:186:ASP:H	1.55	0.71
4:D:97:LEU:HB3	4:D:130:ILE:HD12	1.72	0.71
2:C:137:GLU:H	2:C:139:MLY:HG3	1.56	0.70
2:C:273:GLU:OE1	2:C:309:ARG:NH2	2.24	0.69
4:D:131:SER:O	4:D:132:PRO:C	2.33	0.69
4:D:309:ARG:HD3	4:D:325:TRP:CE2	2.28	0.69
4:D:38:PHE:CE2	4:D:126:THR:HG22	2.28	0.69
2:C:293:TYR:HD2	2:C:293:TYR:O	1.76	0.67
4:D:170:ASN:HB3	4:D:172:PHE:HE1	1.58	0.67
3:B:102:HIS:NE2	3:B:106:LEU:HD11	2.09	0.67
2:C:32:VAL:HG13	2:C:121:SER:HB3	1.77	0.67
4:D:154:LEU:CD2	4:D:198:ARG:HG2	2.24	0.66
2:C:226:SER:HB3	2:C:228:PHE:CE1	2.31	0.66
2:C:276:ILE:HG21	2:C:306:PHE:HB2	1.76	0.66
4:D:254:ILE:CG2	4:D:295:LEU:HB3	2.26	0.65
1:A:43:MET:HG3	1:A:44:TYR:N	2.10	0.65
2:C:110:PRO:HD2	2:C:113:CYS:SG	2.37	0.65
4:D:74:ARG:NH1	4:D:81:TRP:NE1	2.44	0.65
2:C:57:LEU:O	2:C:58:SER:HB2	1.95	0.65
2:C:68:GLU:HB2	2:C:108:LEU:HB3	1.79	0.64
2:C:140:VAL:CG2	2:C:157:TRP:HD1	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:140:VAL:CG2	2:C:158:LYS:O	2.46	0.64
4:D:100:GLY:C	4:D:101:ILE:HD12	2.22	0.64
2:C:256:LEU:C	2:C:256:LEU:HD12	2.23	0.64
4:D:289:GLU:O	7:D:397:HOH:O	2.15	0.64
1:A:109:GLU:OE1	1:A:111:ARG:HD2	1.98	0.64
2:C:106:HIS:O	2:C:106:HIS:ND1	2.30	0.63
4:D:32:VAL:HG13	4:D:121:SER:HB3	1.80	0.63
1:A:35:TRP:CD2	1:A:86:ARG:HG2	2.35	0.62
2:C:309:ARG:HD2	2:C:323:SER:O	1.99	0.62
1:A:37:ILE:HG22	1:A:83:LEU:HD13	1.81	0.62
4:D:253:GLU:HA	4:D:295:LEU:O	1.99	0.62
4:D:140:VAL:HG12	4:D:169:TYR:CE1	2.34	0.62
4:D:131:SER:O	4:D:132:PRO:O	2.18	0.61
4:D:280:ASP:C	4:D:281:THR:HG23	2.23	0.61
2:C:134:GLY:HA3	2:C:223:ILE:HA	1.81	0.61
2:C:275:GLU:O	2:C:275:GLU:CG	2.49	0.61
2:C:45:TYR:O	2:C:46:LEU:HB2	2.01	0.61
4:D:32:VAL:HG22	4:D:33:ASN:N	2.14	0.61
3:B:18:VAL:HG21	4:D:314:ILE:HD12	1.83	0.61
2:C:171:LEU:C	2:C:171:LEU:HD23	2.26	0.60
2:C:171:LEU:HD23	2:C:172:PHE:N	2.16	0.60
1:A:87:ASP:HB3	2:C:87:LYS:HE2	1.83	0.60
2:C:137:GLU:N	2:C:139:MLY:HG3	2.18	0.59
4:D:246:PHE:CE1	4:D:256:LEU:HD12	2.37	0.59
2:C:309:ARG:HG3	2:C:323:SER:O	2.02	0.59
2:C:109:LEU:O	2:C:118:GLU:HG3	2.03	0.59
4:D:101:ILE:HD12	4:D:101:ILE:N	2.17	0.59
4:D:167:THR:HG22	4:D:168:ASN:N	2.17	0.59
2:C:274:ILE:HG23	2:C:274:ILE:O	2.03	0.58
2:C:135:ILE:O	2:C:138:THR:CG2	2.52	0.58
1:A:13:LEU:HD12	1:A:13:LEU:O	2.04	0.57
2:C:185:VAL:CG2	2:C:186:ASP:H	2.18	0.57
4:D:133:GLN:O	4:D:133:GLN:HG3	2.04	0.57
2:C:232:LEU:O	2:C:235:ILE:HG22	2.05	0.57
3:B:13:LEU:HD12	3:B:13:LEU:O	2.04	0.57
2:C:76:ILE:HD12	2:C:100:GLY:CA	2.33	0.57
4:D:172:PHE:CE2	4:D:183:GLN:HB2	2.40	0.57
2:C:188:ILE:HB	2:C:196:GLY:HA3	1.87	0.56
4:D:46:LEU:HD23	4:D:213:CYS:N	2.19	0.56
1:A:18:VAL:O	1:A:22:GLN:HG2	2.05	0.56
3:B:37:ILE:HG22	3:B:83:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:PRO:HG2	4:D:107:THR:HG21	1.85	0.56
2:C:185:VAL:CG2	2:C:186:ASP:N	2.68	0.56
2:C:309:ARG:CG	2:C:323:SER:O	2.54	0.56
2:C:32:VAL:HG22	2:C:33:ASN:N	2.19	0.56
4:D:271:ASP:OD2	4:D:313:ASN:HB3	2.06	0.56
4:D:140:VAL:HG11	4:D:169:TYR:CD1	2.41	0.56
4:D:106:HIS:CE1	4:D:123:TRP:CH2	2.94	0.56
4:D:72:LYS:HA	4:D:82:MLY:O	2.06	0.55
4:D:171:LEU:HD23	4:D:171:LEU:C	2.30	0.55
4:D:256:LEU:HD21	4:D:306:PHE:CD1	2.41	0.55
4:D:185:VAL:HG23	4:D:186:ASP:H	1.70	0.55
2:C:74:ARG:HH11	2:C:81:TRP:NE1	2.05	0.55
2:C:256:LEU:HD13	2:C:306:PHE:CZ	2.42	0.55
3:B:18:VAL:O	3:B:22:GLN:HG2	2.07	0.55
2:C:83:THR:O	2:C:84:ILE:CG2	2.55	0.54
2:C:276:ILE:CG2	2:C:306:PHE:HA	2.35	0.54
2:C:292:THR:CG2	2:C:293:TYR:N	2.55	0.54
2:C:293:TYR:O	2:C:293:TYR:CD2	2.60	0.54
1:A:62:LYS:HD3	1:A:66:MET:CE	2.34	0.54
4:D:244:LEU:HB3	4:D:306:PHE:CZ	2.43	0.54
4:D:114:THR:C	4:D:116:GLY:H	2.16	0.53
1:A:40:THR:O	1:A:43:MET:HB3	2.08	0.53
1:A:62:LYS:O	1:A:63:THR:C	2.51	0.53
4:D:244:LEU:HD22	4:D:258:TRP:HB2	1.91	0.53
2:C:256:LEU:O	2:C:292:THR:HA	2.09	0.53
3:B:24:GLN:O	3:B:24:GLN:HG3	2.09	0.53
4:D:148:TYR:CD2	4:D:154:LEU:HD12	2.44	0.53
2:C:70:GLU:HB3	2:C:106:HIS:CE1	2.44	0.52
2:C:195:ILE:C	2:C:195:ILE:HD12	2.34	0.52
2:C:187:TYR:HB2	2:C:189:LYS:HE3	1.90	0.52
2:C:256:LEU:HD12	2:C:256:LEU:O	2.10	0.52
1:A:45:CYS:O	1:A:49:GLU:HG3	2.09	0.52
4:D:131:SER:C	4:D:132:PRO:O	2.52	0.52
2:C:36:GLN:OE1	2:C:57:LEU:HD11	2.09	0.52
2:C:106:HIS:CD2	2:C:123:TRP:CZ2	2.98	0.52
4:D:135:ILE:HB	4:D:136:PRO:HD2	1.91	0.52
4:D:170:ASN:HB3	4:D:172:PHE:CE1	2.43	0.52
2:C:145:CYS:C	2:C:235:ILE:HD11	2.35	0.51
3:B:40:THR:O	3:B:43:MET:HB3	2.11	0.51
4:D:171:LEU:HD23	4:D:172:PHE:N	2.25	0.51
4:D:135:ILE:C	4:D:137:GLU:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:VAL:CG1	4:D:169:TYR:CD1	2.94	0.51
2:C:140:VAL:HG22	2:C:141:GLN:N	2.26	0.51
1:A:104:LYS:HE2	2:C:314:ILE:O	2.11	0.51
4:D:307:VAL:HG12	4:D:308:VAL:N	2.27	0.50
2:C:96:ASP:OD2	2:C:98:ASN:HB2	2.11	0.50
2:C:309:ARG:CD	2:C:323:SER:O	2.60	0.50
4:D:142:ASP:OD2	4:D:158:LYS:HD2	2.11	0.50
4:D:260:ILE:HB	4:D:261:PRO:HD2	1.93	0.50
1:A:48:LEU:HD13	1:A:67:LEU:HB2	1.94	0.50
2:C:84:ILE:HD12	2:C:84:ILE:C	2.37	0.50
2:C:226:SER:HB3	2:C:228:PHE:CZ	2.47	0.50
4:D:271:ASP:CG	4:D:313:ASN:HB3	2.37	0.50
2:C:189:LYS:HD3	2:C:194:ASN:OD1	2.12	0.49
2:C:106:HIS:CD2	2:C:123:TRP:CH2	3.00	0.49
3:B:73:HIS:CE1	3:B:75:VAL:HG22	2.48	0.49
4:D:304:LEU:O	4:D:330:CYS:HA	2.12	0.49
4:D:154:LEU:HD21	4:D:198:ARG:HG2	1.94	0.49
4:D:170:ASN:HB2	4:D:215:ASN:HB2	1.94	0.49
4:D:283:LEU:HD21	4:D:295:LEU:HD11	1.95	0.49
2:C:139:MLY:HD2	2:C:139:MLY:HH22	1.58	0.48
2:C:101:ILE:N	2:C:101:ILE:HD12	2.28	0.48
4:D:246:PHE:HE2	4:D:329:GLN:C	2.21	0.48
2:C:73:TYR:HE2	2:C:82:LYS:HD3	1.77	0.48
2:C:154:LEU:HD11	2:C:198:ARG:HG2	1.95	0.48
4:D:185:VAL:HG23	4:D:186:ASP:N	2.29	0.48
2:C:73:TYR:CE2	2:C:82:LYS:HB2	2.48	0.48
2:C:258:TRP:CZ2	2:C:291:GLU:HA	2.49	0.48
1:A:60:ILE:O	1:A:64:GLN:HG3	2.12	0.48
3:B:80:PHE:CD1	3:B:86:ARG:HD2	2.49	0.48
4:D:138:THR:HB	4:D:223:ILE:HB	1.96	0.47
1:A:37:ILE:HG22	1:A:83:LEU:CD1	2.44	0.47
2:C:83:THR:C	2:C:84:ILE:HG23	2.38	0.47
4:D:254:ILE:HG22	4:D:295:LEU:HB3	1.95	0.47
4:D:167:THR:CG2	4:D:168:ASN:N	2.78	0.47
2:C:145:CYS:CB	2:C:235:ILE:HD11	2.45	0.47
4:D:217:SER:HA	4:D:222:PRO:HA	1.96	0.47
2:C:276:ILE:HG21	2:C:306:PHE:CB	2.42	0.46
3:B:40:THR:HB	3:B:41:ALA:H	1.55	0.46
3:B:87:ASP:CB	4:D:87:LYS:HE2	2.43	0.46
2:C:273:GLU:HB2	2:C:322:TRP:CH2	2.49	0.46
4:D:138:THR:CB	4:D:223:ILE:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:TRP:O	2:C:115:ASN:N	2.49	0.46
2:C:43:PRO:HB2	2:C:45:TYR:CD1	2.51	0.46
2:C:136:PRO:HA	2:C:139:MLY:HG3	1.98	0.46
4:D:32:VAL:CG2	4:D:33:ASN:N	2.78	0.46
4:D:57:LEU:O	4:D:58:SER:CB	2.64	0.46
4:D:97:LEU:HB3	4:D:130:ILE:CD1	2.42	0.46
2:C:276:ILE:CG2	2:C:306:PHE:HB2	2.45	0.45
4:D:132:PRO:O	4:D:132:PRO:HG2	2.17	0.45
2:C:145:CYS:HB3	2:C:235:ILE:HD11	1.98	0.45
2:C:244:LEU:HD11	2:C:326:SER:OG	2.16	0.45
4:D:99:MLY:HD3	4:D:99:MLY:HH22	1.74	0.45
2:C:45:TYR:HB3	2:C:174:TRP:CE3	2.51	0.45
4:D:69:TYR:HB3	4:D:105:ILE:HD11	1.98	0.45
2:C:83:THR:O	2:C:84:ILE:HG22	2.16	0.45
2:C:244:LEU:HD22	2:C:258:TRP:HB2	1.99	0.45
1:A:33:MET:HE1	2:C:84:ILE:HA	1.99	0.45
2:C:147:TYR:HB2	2:C:235:ILE:HG23	1.99	0.45
2:C:314:ILE:O	2:C:314:ILE:HG13	2.17	0.45
4:D:244:LEU:HD22	4:D:258:TRP:CB	2.46	0.45
2:C:174:TRP:CD1	2:C:178:LEU:HB2	2.52	0.44
2:C:143:MET:HG2	2:C:228:PHE:CE2	2.52	0.44
2:C:274:ILE:HG13	2:C:307:VAL:O	2.17	0.44
4:D:310:SER:O	4:D:322:TRP:HE3	2.00	0.44
1:A:52:ILE:HG23	1:A:77:ALA:HA	1.99	0.44
2:C:129:TRP:CH2	2:C:132:PRO:CG	3.01	0.44
2:C:244:LEU:HB3	2:C:306:PHE:HZ	1.79	0.44
1:A:43:MET:CG	1:A:44:TYR:N	2.78	0.44
4:D:240:PRO:O	4:D:261:PRO:HB3	2.16	0.44
4:D:269:CYS:O	4:D:312:VAL:HA	2.18	0.44
4:D:284:VAL:HG11	4:D:293:TYR:OH	2.18	0.44
4:D:310:SER:O	4:D:322:TRP:CE3	2.71	0.44
4:D:82:MLY:HH22	4:D:82:MLY:HD3	1.74	0.44
4:D:109:LEU:HB2	4:D:119:VAL:HG13	2.00	0.44
4:D:154:LEU:CD2	4:D:198:ARG:CG	2.95	0.44
1:A:20:ILE:O	1:A:20:ILE:HG13	2.18	0.43
1:A:99:LEU:O	1:A:100:LEU:C	2.60	0.43
2:C:100:GLY:HA2	2:C:129:TRP:HD1	1.83	0.43
4:D:138:THR:HG1	4:D:224:ARG:H	1.61	0.43
2:C:244:LEU:N	2:C:244:LEU:HD23	2.33	0.43
2:C:307:VAL:HG12	2:C:328:LYS:HA	1.99	0.43
4:D:246:PHE:HE2	4:D:329:GLN:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLU:O	1:A:62:LYS:C	2.59	0.43
2:C:83:THR:C	2:C:84:ILE:CG2	2.92	0.43
2:C:228:PHE:CD1	2:C:228:PHE:N	2.86	0.43
2:C:275:GLU:HB3	2:C:325:TRP:CH2	2.54	0.43
4:D:134:GLY:H	4:D:224:ARG:HE	1.64	0.43
1:A:106:LEU:HD22	1:A:111:ARG:HD3	2.00	0.43
2:C:33:ASN:O	2:C:56:PRO:HB3	2.18	0.43
3:B:43:MET:O	3:B:44:TYR:C	2.60	0.43
2:C:136:PRO:O	2:C:137:GLU:CB	2.66	0.43
4:D:307:VAL:HG12	4:D:325:TRP:HE3	1.84	0.43
3:B:13:LEU:HD12	3:B:13:LEU:C	2.43	0.43
2:C:114:THR:C	2:C:116:GLY:H	2.26	0.43
2:C:235:ILE:HG12	2:C:235:ILE:O	2.18	0.43
4:D:147:TYR:CD2	4:D:232:LEU:HB3	2.54	0.43
2:C:129:TRP:CZ2	2:C:132:PRO:HG3	2.54	0.42
2:C:151:GLN:HG2	2:C:152:TYR:CE1	2.54	0.42
2:C:158:LYS:HA	2:C:159:PRO:HD3	1.80	0.42
1:A:19:ASN:C	1:A:21:THR:H	2.27	0.42
3:B:17:LEU:HA	3:B:17:LEU:HD23	1.79	0.42
4:D:105:ILE:O	4:D:105:ILE:HG23	2.19	0.42
2:C:76:ILE:H	2:C:76:ILE:HG13	1.67	0.42
2:C:172:PHE:HA	2:C:182:LEU:O	2.19	0.42
4:D:260:ILE:HD12	4:D:261:PRO:O	2.19	0.42
4:D:96:ASP:OD2	4:D:98:ASN:N	2.45	0.42
4:D:175:TYR:O	4:D:176:GLU:C	2.61	0.42
2:C:229:THR:O	2:C:229:THR:HG23	2.20	0.42
3:B:48:LEU:O	3:B:52:ILE:HB	2.20	0.42
3:B:74:LYS:HG3	3:B:75:VAL:N	2.34	0.42
4:D:130:ILE:O	4:D:132:PRO:N	2.53	0.42
4:D:140:VAL:HG21	4:D:214:VAL:HG11	2.01	0.42
2:C:173:TYR:HA	2:C:211:TYR:O	2.19	0.42
3:B:5:PRO:HB2	3:B:8:THR:HG23	2.01	0.42
2:C:114:THR:C	2:C:116:GLY:N	2.77	0.42
4:D:47:GLY:HA2	4:D:97:LEU:HG	2.02	0.42
4:D:172:PHE:HA	4:D:182:LEU:O	2.20	0.42
4:D:154:LEU:HD23	4:D:198:ARG:HA	2.01	0.41
3:B:89:MLY:HH23	3:B:89:MLY:HD2	1.73	0.41
4:D:73:TYR:CE2	4:D:82:MLY:HD3	2.55	0.41
4:D:74:ARG:HD3	4:D:81:TRP:CD2	2.55	0.41
4:D:265:ILE:CG2	4:D:270:PHE:CE1	3.03	0.41
1:A:62:LYS:CD	1:A:66:MET:HE3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:ILE:HB	2:C:196:GLY:CA	2.50	0.41
4:D:158:LYS:HA	4:D:159:PRO:HD3	1.87	0.41
4:D:208:LYS:O	4:D:231:GLN:HG2	2.20	0.41
1:A:13:LEU:HD12	1:A:13:LEU:C	2.45	0.41
2:C:291:GLU:O	2:C:292:THR:OG1	2.33	0.41
4:D:142:ASP:O	4:D:143:MET:C	2.62	0.41
1:A:105:LYS:HG3	2:C:207:TYR:CG	2.55	0.41
4:D:149:ASN:O	4:D:150:TRP:C	2.62	0.41
4:D:244:LEU:HD13	4:D:306:PHE:CE1	2.55	0.41
4:D:170:ASN:O	4:D:214:VAL:HA	2.21	0.41
2:C:140:VAL:HG11	2:C:214:VAL:HG11	2.02	0.41
4:D:237:LYS:HG3	4:D:322:TRP:O	2.20	0.41
1:A:26:ALA:HB1	1:A:27:PRO:HD2	2.03	0.41
1:A:33:MET:HE3	1:A:33:MET:HB3	1.92	0.41
2:C:138:THR:O	2:C:223:ILE:HD13	2.21	0.41
2:C:149:ASN:ND2	2:C:239:LEU:HD12	2.36	0.41
2:C:208:LYS:C	2:C:231:GLN:NE2	2.79	0.41
4:D:74:ARG:HH11	4:D:81:TRP:CD1	2.38	0.41
4:D:195:ILE:C	4:D:195:ILE:HD12	2.46	0.41
2:C:32:VAL:CG2	2:C:33:ASN:N	2.84	0.41
2:C:172:PHE:CE2	2:C:183:GLN:HB2	2.56	0.41
4:D:70:GLU:HB3	4:D:106:HIS:NE2	2.37	0.41
4:D:138:THR:OG1	4:D:224:ARG:N	2.47	0.41
4:D:283:LEU:HG	4:D:284:VAL:HG23	2.03	0.41
4:D:106:HIS:ND1	4:D:123:TRP:CH2	2.89	0.40
4:D:246:PHE:CZ	4:D:306:PHE:HD2	2.38	0.40
2:C:46:LEU:HD23	2:C:213:CYS:N	2.36	0.40
4:D:230:PHE:HE1	4:D:232:LEU:HD23	1.86	0.40
4:D:254:ILE:HG23	4:D:295:LEU:HB3	2.02	0.40
3:B:90:ILE:HG22	4:D:84:ILE:HG22	2.03	0.40
4:D:246:PHE:CE2	4:D:329:GLN:O	2.74	0.40
2:C:74:ARG:NH1	2:C:81:TRP:NE1	2.69	0.40

All (2) 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:A:76:SER:OG	4:D:118:GLU:OE1[4_555]	1.96	0.24
2:C:198:ARG:NH2	2:C:260:ILE:CD1[2_655]	2.11	0.09

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	A	107/132 (81%)	94 (88%)	12 (11%)	1 (1%)	14	39
2	C	234/380 (62%)	204 (87%)	30 (13%)	0	100	100
3	B	106/132 (80%)	94 (89%)	11 (10%)	1 (1%)	14	39
4	D	274/380 (72%)	240 (88%)	32 (12%)	2 (1%)	18	45
All	All	721/1024 (70%)	632 (88%)	85 (12%)	4 (1%)	21	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	131	SER
4	D	132	PRO
1	A	20	ILE
3	B	6	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	A	91/112 (81%)	89 (98%)	2 (2%)	45	67
2	C	215/349 (62%)	205 (95%)	10 (5%)	23	51
3	B	92/111 (83%)	89 (97%)	3 (3%)	33	60
4	D	246/349 (70%)	241 (98%)	5 (2%)	48	69
All	All	644/921 (70%)	624 (97%)	20 (3%)	35	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ILE
1	A	96	VAL
2	C	67	VAL
2	C	106	HIS
2	C	109	LEU
2	C	125	GLU
2	C	154	LEU
2	C	225	SER
2	C	235	ILE
2	C	244	LEU
2	C	276	ILE
2	C	321	ILE
3	B	74	LYS
3	B	90	ILE
3	B	113	ASN
4	D	108	LEU
4	D	109	LEU
4	D	137	GLU
4	D	244	LEU
4	D	321	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
2	C	115	ASN
3	B	79	GLN
4	D	183	GLN
4	D	329	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	$\# Z > 2$
4	MLY	D	99	4	9,10,11	0.65	0	6,11,13	1.43	1 (16%)
3	MLY	B	89	3	9,10,11	0.53	0	6,11,13	1.54	1 (16%)
2	MLY	C	139	2	9,10,11	0.59	0	6,11,13	0.77	0
2	MLY	C	104	2	9,10,11	0.54	0	6,11,13	1.11	1 (16%)
4	MLY	D	82	4	9,10,11	0.58	0	6,11,13	1.50	1 (16%)

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
4	MLY	D	99	4	-	0/8/9/11	-
3	MLY	B	89	3	-	1/8/9/11	-
2	MLY	C	139	2	-	4/8/9/11	-
2	MLY	C	104	2	-	1/8/9/11	-
4	MLY	D	82	4	-	0/8/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	99	MLY	CD-CE-NZ	-2.95	106.09	113.71
3	B	89	MLY	CD-CE-NZ	-2.80	106.47	113.71
4	D	82	MLY	CD-CE-NZ	-2.65	106.86	113.71
2	C	104	MLY	CD-CE-NZ	-2.17	108.09	113.71

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	104	MLY	O-C-CA-CB
2	C	139	MLY	CE-CD-CG-CB
2	C	139	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
2	C	139	MLY	N-CA-CB-CG
2	C	139	MLY	CD-CE-NZ-CH2
3	B	89	MLY	CD-CE-NZ-CH2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	99	MLY	1	0
3	B	89	MLY	1	0
2	C	139	MLY	5	0
4	D	82	MLY	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
5	NAG	D	501	4	14,14,15	0.55	0	17,19,21	1.15	3 (17%)
5	NAG	C	501	2	14,14,15	0.58	0	17,19,21	1.21	3 (17%)

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
5	NAG	D	501	4	-	2/6/23/26	0/1/1/1
5	NAG	C	501	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	NAG	C2-N2-C7	-2.49	119.56	122.90
5	C	501	NAG	C1-C2-N2	-2.30	106.81	110.43
5	C	501	NAG	C4-C3-C2	2.14	114.15	111.02
5	D	501	NAG	C1-C2-N2	-2.08	107.16	110.43
5	D	501	NAG	O5-C1-C2	2.05	114.47	111.29
5	C	501	NAG	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	501	NAG	C8-C7-N2-C2
5	D	501	NAG	O7-C7-N2-C2

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	A	109/132 (82%)	0.09	7 (6%) 25 13	17, 52, 107, 169	0
2	C	250/380 (65%)	0.46	23 (9%) 14 8	25, 59, 125, 204	0
3	B	108/132 (81%)	0.10	6 (5%) 30 15	20, 48, 93, 145	0
4	D	284/380 (74%)	0.05	13 (4%) 37 19	18, 44, 90, 143	1 (0%)
All	All	751/1024 (73%)	0.20	49 (6%) 25 12	17, 51, 111, 204	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	262	LEU	5.6
2	C	217	SER	5.2
2	C	160	GLY	4.4
2	C	247	THR	4.2
4	D	279	ASP	3.6
2	C	65	CYS	3.6
1	A	85	VAL	3.5
2	C	216	GLY	3.4
1	A	76	SER	3.3
2	C	190	ALA	3.2
2	C	131	SER	3.1
4	D	297	THR	3.0
4	D	116	GLY	3.0
1	A	23	ASN	2.9
4	D	57	LEU	2.9
2	C	290	ASN	2.9
2	C	293	TYR	2.8
1	A	40	THR	2.7
1	A	42	GLY	2.7
2	C	130	ILE	2.7
1	A	41	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	B	31	GLY	2.6
4	D	129	TRP	2.5
2	C	242	VAL	2.5
2	C	285	THR	2.5
4	D	58	SER	2.5
4	D	220	ASN	2.5
2	C	307	VAL	2.5
3	B	55	SER	2.4
2	C	167	THR	2.4
3	B	23	ASN	2.4
2	C	289	GLU	2.4
2	C	243	TYR	2.4
4	D	292	THR	2.3
2	C	169	TYR	2.3
4	D	160	GLY	2.3
4	D	167	THR	2.3
4	D	331	TRP	2.2
2	C	261	PRO	2.2
3	B	76	SER	2.2
2	C	292	THR	2.2
4	D	168	ASN	2.2
1	A	78	GLY	2.2
2	C	255	LYS	2.1
2	C	111	TRP	2.0
3	B	24	GLN	2.0
2	C	234	ASN	2.0
3	B	79	GLN	2.0
4	D	120	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	MLY	C	139	11/12	0.75	0.19	66,89,95,97	0
4	MLY	D	99	11/12	0.90	0.13	33,35,47,51	0
4	MLY	D	82	11/12	0.94	0.10	33,36,40,40	0
2	MLY	C	104	11/12	0.95	0.09	29,33,54,64	0
3	MLY	B	89	11/12	0.97	0.08	24,35,45,46	0

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
5	NAG	D	501	14/15	0.80	0.16	78,80,83,84	0
5	NAG	C	501	14/15	0.84	0.11	67,69,71,72	0
6	CA	D	381	1/1	0.87	0.19	70,70,70,70	0
6	CA	C	381	1/1	0.91	0.13	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.