



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:03 PM UTC

PDB ID : 3D85 / pdb_00003d85
Title : Crystal structure of IL-23 in complex with neutralizing FAB
Authors : Beyer, B.M.; Ingram, R.; Ramanathan, L.; Reichert, P.; Le, H.; Madison, V.
Deposited on : 2008-05-22
Resolution : 1.90 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

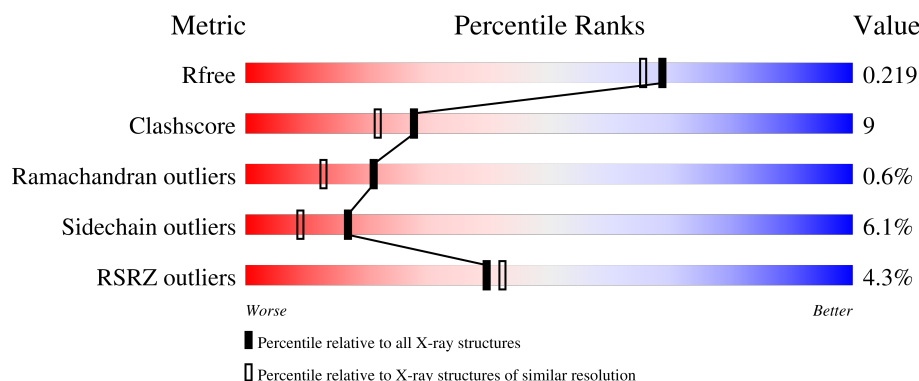
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	214	
2	B	223	
3	C	178	
4	D	306	

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
6	MPD	B	501	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7509 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 FAB of antibody 7G10, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	1	0
			1643	1025	279	334	5			

- Molecule 2 is a protein called FAB of antibody 7G10, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	3	0
			1632	1034	266	325	7			

- Molecule 3 is a protein called Interleukin-23 subunit p19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	133	Total	C	N	O	S	0	0	0
			1031	662	183	181	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	171	GLY	-	expression tag	UNP Q9NPF7
C	172	SER	-	expression tag	UNP Q9NPF7
C	173	HIS	-	expression tag	UNP Q9NPF7
C	174	HIS	-	expression tag	UNP Q9NPF7
C	175	HIS	-	expression tag	UNP Q9NPF7
C	176	HIS	-	expression tag	UNP Q9NPF7
C	177	HIS	-	expression tag	UNP Q9NPF7
C	178	HIS	-	expression tag	UNP Q9NPF7

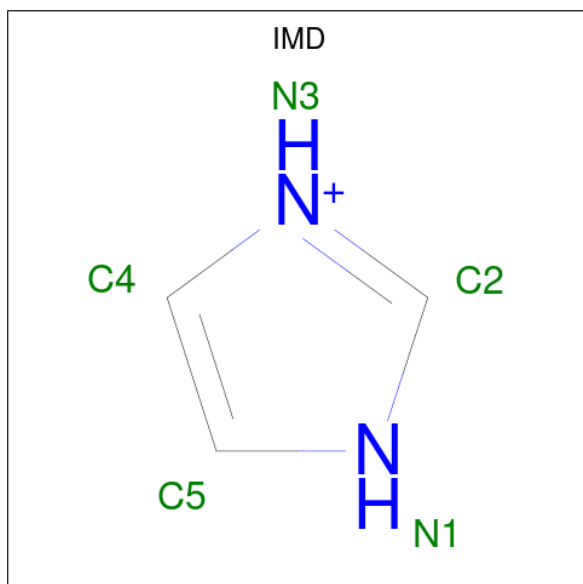
- Molecule 4 is a protein called Interleukin-12 subunit p40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	290	Total	C	N	O	S	0	0	0
			2276	1445	364	455	12			

There is a discrepancy between the modelled and reference sequences:

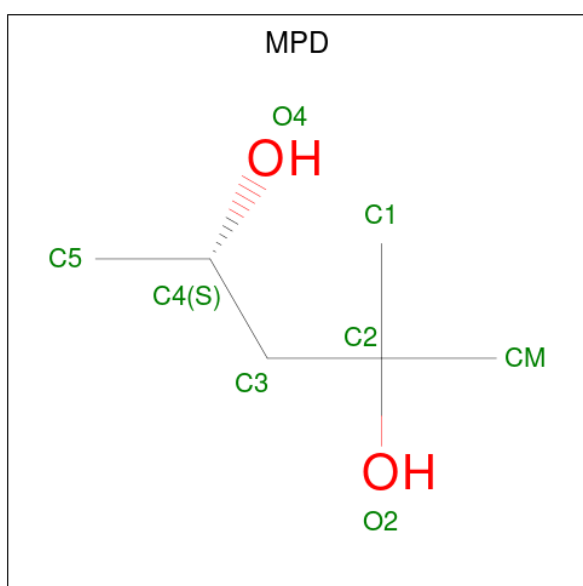
Chain	Residue	Modelled	Actual	Comment	Reference
D	200	GLN	ASN	engineered mutation	UNP P29460

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

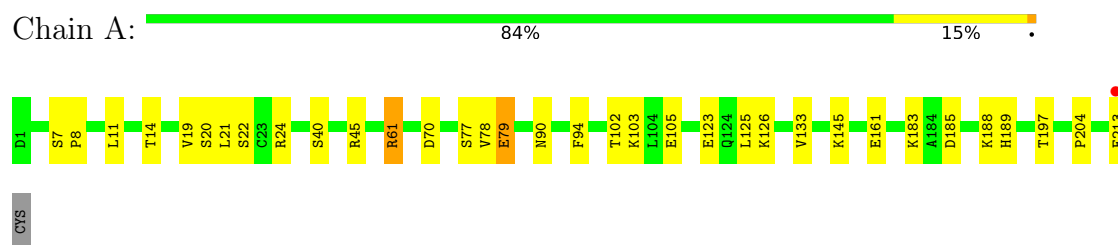
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	256	Total	O	0	0
			256	256		
7	B	281	Total	O	0	0
			281	281		
7	C	101	Total	O	0	0
			101	101		
7	D	268	Total	O	0	0
			268	268		

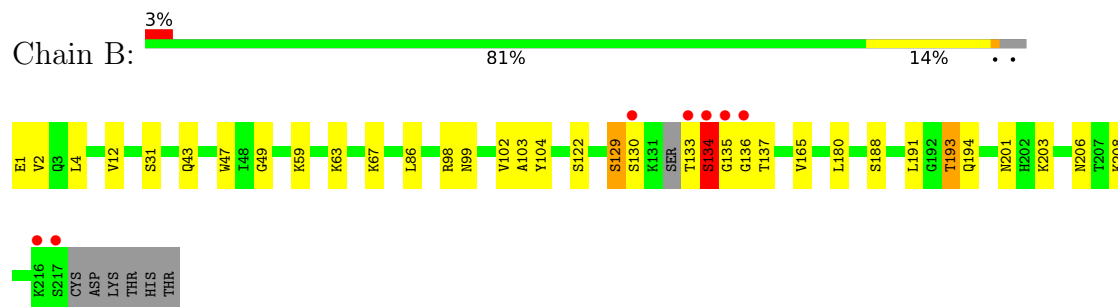
3 Residue-property plots

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.

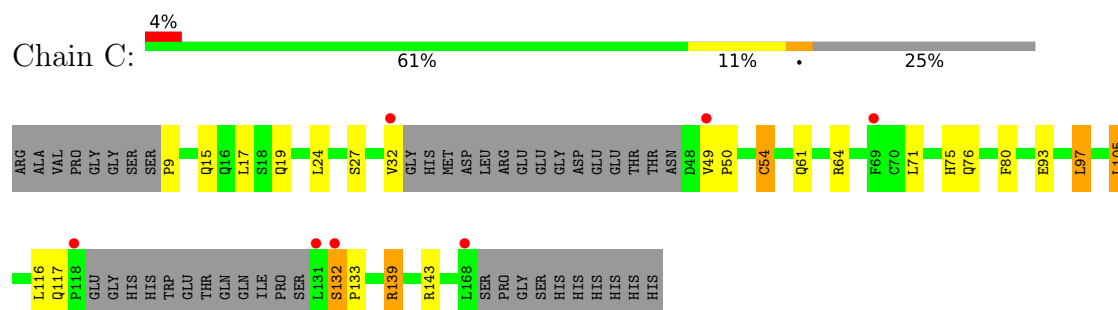
- Molecule 1: FAB of antibody 7G10, light chain



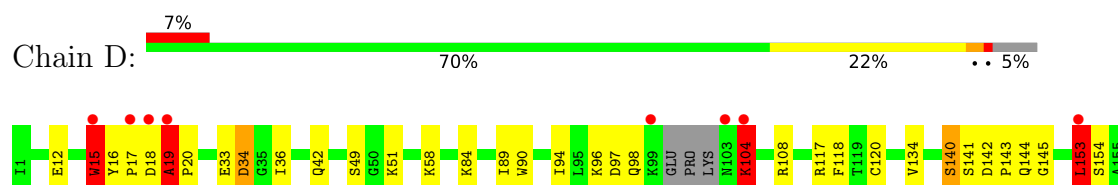
- Molecule 2: FAB of antibody 7G10, heavy chain

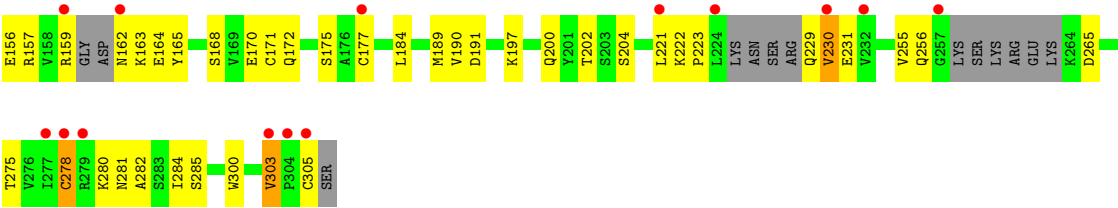


- Molecule 3: Interleukin-23 subunit p19



- Molecule 4: Interleukin-12 subunit p40





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.39Å 62.09Å 107.26Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	106.60 – 1.90 106.36 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (106.60-1.90) 99.3 (106.36-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.91Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.171 , 0.214 0.171 , 0.219	Depositor DCC
R_{free} test set	1541 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7509	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.85	0/1685	1.02	3/2285 (0.1%)
2	B	0.97	1/1683 (0.1%)	1.09	8/2290 (0.3%)
3	C	0.70	0/1056	1.02	6/1435 (0.4%)
4	D	0.66	0/2330	1.02	10/3169 (0.3%)
All	All	0.80	1/6754 (0.0%)	1.04	27/9179 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	VAL	CA-CB	6.05	1.62	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	19	ALA	C-N-CD	-8.73	101.39	120.60
4	D	19	ALA	CA-C-N	8.22	146.73	127.00
4	D	19	ALA	C-N-CA	8.22	146.73	127.00
2	B	67	LYS	N-CA-C	-8.22	103.19	113.55
4	D	16	TYR	CA-C-N	7.67	129.43	119.84
4	D	16	TYR	C-N-CA	7.67	129.43	119.84
3	C	97	LEU	CA-C-N	-7.25	112.72	119.82
3	C	97	LEU	C-N-CA	-7.25	112.72	119.82
4	D	94	ILE	N-CA-C	7.16	117.25	110.53
2	B	191	LEU	N-CA-C	7.10	119.93	111.33
4	D	184	LEU	CA-C-N	-6.63	113.95	120.52
4	D	184	LEU	C-N-CA	-6.63	113.95	120.52
3	C	49	VAL	CA-C-N	-6.42	112.88	120.13
3	C	49	VAL	C-N-CA	-6.42	112.88	120.13
2	B	203	LYS	CA-C-N	-6.15	113.29	119.56
2	B	203	LYS	C-N-CA	-6.15	113.29	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	ALA	N-CA-C	5.74	119.55	111.52
4	D	153	LEU	N-CA-C	-5.70	102.59	110.35
1	A	133	VAL	N-CA-C	5.57	115.96	108.17
2	B	122	SER	N-CA-C	-5.55	100.65	109.76
3	C	27	SER	N-CA-C	5.34	117.85	111.71
1	A	14	THR	CA-C-N	-5.31	114.31	119.78
1	A	14	THR	C-N-CA	-5.31	114.31	119.78
4	D	15	TRP	N-CA-C	5.19	116.77	108.41
3	C	139	ARG	N-CA-C	5.13	116.95	111.36
2	B	134	SER	CA-C-N	5.12	130.91	121.70
2	B	134	SER	C-N-CA	5.12	130.91	121.70

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	1643	0	1587	24	0
2	B	1632	0	1606	27	0
3	C	1031	0	1036	18	0
4	D	2276	0	2148	49	0
5	A	5	0	5	0	0
6	A	8	0	14	1	0
6	B	8	0	14	3	0
7	A	256	0	0	4	0
7	B	281	0	0	3	0
7	C	101	0	0	6	0
7	D	268	0	0	5	0
All	All	7509	0	6410	117	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 9.

All (117) 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:104:LYS:HE3	4:D:104:LYS:H	1.13	1.07
4:D:189:MET:HE3	4:D:200:GLN:HG3	1.39	1.04
2:B:134:SER:HB3	2:B:135:GLY:C	1.91	0.96
1:A:61:ARG:HH21	1:A:61:ARG:HG3	1.32	0.95
2:B:31:SER:HA	6:B:501:MPD:H52	1.49	0.94
4:D:189:MET:HE3	4:D:200:GLN:CG	2.02	0.88
2:B:12:VAL:HG11	2:B:86:LEU:HD12	1.57	0.87
2:B:12:VAL:HG11	2:B:86:LEU:CD1	2.06	0.86
4:D:19:ALA:HB2	4:D:58:LYS:HD2	1.58	0.85
4:D:104:LYS:HE3	4:D:104:LYS:N	1.92	0.83
2:B:134:SER:HB2	2:B:137:THR:H	1.44	0.82
2:B:134:SER:CB	2:B:137:THR:H	1.95	0.79
4:D:282:ALA:O	4:D:305:CYS:HB2	1.85	0.76
4:D:104:LYS:H	4:D:104:LYS:CE	1.97	0.75
4:D:19:ALA:CB	4:D:58:LYS:HD2	2.17	0.74
1:A:19:VAL:CG2	1:A:78:VAL:HG21	2.18	0.74
6:B:501:MPD:O2	6:B:501:MPD:H53	1.86	0.74
4:D:230:VAL:CG2	4:D:278:CYS:HB2	2.18	0.73
4:D:278:CYS:SG	4:D:284:ILE:HD11	2.29	0.73
2:B:134:SER:HB3	2:B:135:GLY:CA	2.18	0.72
1:A:61:ARG:HD3	1:A:77:SER:O	1.89	0.70
1:A:79:GLU:HG2	7:A:727:HOH:O	1.93	0.69
2:B:133:THR:N	7:B:631:HOH:O	2.26	0.68
3:C:132:SER:CB	3:C:133:PRO:HD2	2.25	0.67
3:C:9:PRO:HD3	3:C:71:LEU:CD1	2.26	0.66
1:A:19:VAL:HG21	1:A:78:VAL:HG21	1.76	0.65
2:B:31:SER:HA	6:B:501:MPD:C5	2.24	0.65
3:C:19:GLN:NE2	7:C:1269:HOH:O	2.31	0.64
4:D:156:GLU:OE1	4:D:163:LYS:HD3	1.99	0.62
2:B:134:SER:HB3	2:B:136:GLY:N	2.15	0.61
4:D:19:ALA:HB1	4:D:20:PRO:C	2.26	0.61
4:D:19:ALA:HB1	4:D:20:PRO:CA	2.31	0.61
2:B:201[B]:ASN:OD1	2:B:208:LYS:HG2	2.01	0.61
4:D:189:MET:HE3	4:D:200:GLN:CD	2.25	0.60
1:A:19:VAL:HG23	1:A:78:VAL:HG21	1.84	0.59
1:A:61:ARG:HG3	1:A:61:ARG:NH2	2.11	0.58
3:C:132:SER:HB2	3:C:133:PRO:HD2	1.84	0.58
4:D:42:GLN:HG3	7:D:1244:HOH:O	2.04	0.57
4:D:222:LYS:C	4:D:230:VAL:HG12	2.30	0.57
1:A:94:PHE:CD1	2:B:59:LYS:HE2	2.41	0.56
2:B:129:SER:HB2	7:B:1220:HOH:O	2.06	0.56
1:A:24:ARG:HG2	1:A:70:ASP:OD1	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:280:LYS:O	4:D:281:ASN:HB2	2.05	0.55
2:B:134:SER:HB3	2:B:137:THR:H	1.72	0.54
2:B:134:SER:CB	2:B:135:GLY:CA	2.85	0.54
2:B:134:SER:HB2	2:B:137:THR:N	2.18	0.54
4:D:223:PRO:CA	4:D:230:VAL:HG13	2.38	0.54
4:D:33:GLU:HG2	7:D:1300:HOH:O	2.07	0.53
2:B:201[B]:ASN:ND2	7:B:662:HOH:O	2.40	0.53
4:D:223:PRO:N	4:D:230:VAL:HG12	2.24	0.52
1:A:19:VAL:HG23	1:A:78:VAL:CG2	2.40	0.52
3:C:15:GLN:NE2	7:C:1262:HOH:O	2.35	0.52
4:D:223:PRO:HA	4:D:230:VAL:HG13	1.92	0.52
2:B:12:VAL:HG11	2:B:86:LEU:HD13	1.91	0.51
3:C:54:CYS:HB3	4:D:177:CYS:SG	2.52	0.50
3:C:24:LEU:HB3	3:C:105:LEU:HD13	1.92	0.50
3:C:75:HIS:HD2	7:C:928:HOH:O	1.94	0.50
1:A:8:PRO:HG3	1:A:11:LEU:HD13	1.94	0.49
2:B:180:LEU:C	2:B:180:LEU:HD12	2.37	0.49
1:A:188:LYS:NZ	7:A:744:HOH:O	2.45	0.49
3:C:32:VAL:HG13	3:C:32:VAL:O	2.12	0.49
4:D:98:GLN:HE22	4:D:108:ARG:HB2	1.78	0.49
4:D:159:ARG:N	4:D:162:ASN:O	2.38	0.48
4:D:34:ASP:HB3	7:D:1296:HOH:O	2.12	0.48
4:D:221:LEU:HG	4:D:303:VAL:HG11	1.94	0.48
4:D:19:ALA:CB	4:D:20:PRO:CA	2.92	0.48
1:A:19:VAL:CG2	1:A:78:VAL:CG2	2.91	0.48
3:C:97:LEU:HD12	7:C:1397:HOH:O	2.14	0.46
3:C:139:ARG:O	3:C:143:ARG:HG3	2.15	0.46
4:D:189:MET:HE2	4:D:191:ASP:OD1	2.16	0.46
3:C:116:LEU:O	3:C:117:GLN:HG2	2.16	0.46
4:D:145:GLY:HA2	7:D:778:HOH:O	2.16	0.46
1:A:21:LEU:HD22	1:A:102:THR:HG21	1.98	0.46
4:D:157:ARG:HD2	4:D:164:GLU:OE1	2.16	0.45
2:B:193:THR:HG22	2:B:194:GLN:N	2.31	0.45
4:D:118:PHE:CZ	4:D:171:CYS:HB2	2.51	0.45
3:C:50:PRO:HD2	3:C:80:PHE:CD2	2.52	0.45
4:D:223:PRO:N	4:D:230:VAL:CG1	2.80	0.45
4:D:285:SER:HB3	4:D:300:TRP:CE3	2.52	0.45
4:D:15:TRP:CD1	4:D:84:LYS:HG2	2.53	0.44
4:D:153:LEU:HD11	4:D:165:TYR:HB3	2.00	0.44
4:D:117:ARG:HB2	4:D:172:GLN:OE1	2.18	0.44
2:B:99:ASN:O	2:B:102:VAL:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:HIS:HE1	7:C:1195:HOH:O	2.01	0.43
3:C:9:PRO:HD3	3:C:71:LEU:HD13	2.00	0.43
4:D:255:VAL:HG12	4:D:284:ILE:HG12	2.00	0.43
1:A:103:LYS:HG2	7:A:576:HOH:O	2.17	0.43
4:D:142:ASP:N	4:D:143:PRO:CD	2.81	0.43
2:B:12:VAL:CG1	2:B:86:LEU:HD12	2.39	0.43
4:D:140:SER:O	4:D:143:PRO:HD3	2.18	0.43
1:A:123:GLU:HA	1:A:126:LYS:HE3	2.00	0.43
4:D:189:MET:HG3	4:D:202:THR:HG22	1.99	0.43
4:D:282:ALA:C	4:D:305:CYS:HB2	2.44	0.43
4:D:197:LYS:NZ	7:D:816:HOH:O	2.40	0.43
4:D:36:ILE:O	4:D:49:SER:HA	2.19	0.42
1:A:189:HIS:CE1	6:A:502:MPD:H52	2.54	0.42
1:A:125:LEU:O	1:A:183:LYS:HD2	2.20	0.42
1:A:61:ARG:NH2	1:A:61:ARG:CG	2.79	0.42
3:C:15:GLN:HG2	7:C:685:HOH:O	2.19	0.42
4:D:15:TRP:CD2	4:D:84:LYS:HD2	2.54	0.42
4:D:157:ARG:HG2	4:D:164:GLU:HG3	2.01	0.42
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.54	0.42
3:C:93:GLU:O	3:C:139:ARG:HD2	2.20	0.42
1:A:161:GLU:HG3	7:A:537:HOH:O	2.20	0.42
1:A:197:THR:HG22	1:A:204:PRO:HG3	2.01	0.41
1:A:185:ASP:O	1:A:189:HIS:HD2	2.03	0.41
1:A:145:LYS:HB3	1:A:197:THR:OG1	2.21	0.41
4:D:12:GLU:OE2	4:D:90:TRP:CH2	2.73	0.41
4:D:97:ASP:OD2	4:D:104:LYS:HA	2.21	0.41
2:B:2:VAL:HB	2:B:104:TYR:CE2	2.56	0.41
4:D:120:CYS:O	4:D:168:SER:HA	2.21	0.41
2:B:4:LEU:HD11	2:B:98:ARG:HG3	2.02	0.41
4:D:134:VAL:HG22	4:D:190:VAL:HG22	2.01	0.41
2:B:134:SER:CB	2:B:135:GLY:HA3	2.51	0.40
1:A:11:LEU:HD22	1:A:21:LEU:CD2	2.51	0.40
3:C:61:GLN:O	3:C:64:ARG:HB3	2.21	0.40

There are no symmetry-related clashes.

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	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
2	B	215/223 (96%)	208 (97%)	6 (3%)	1 (0%)	24	16
3	C	127/178 (71%)	125 (98%)	2 (2%)	0	100	100
4	D	280/306 (92%)	265 (95%)	11 (4%)	4 (1%)	9	3
All	All	834/921 (91%)	804 (96%)	25 (3%)	5 (1%)	21	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	SER
4	D	19	ALA
4	D	104	LYS
4	D	18	ASP
4	D	17	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	191/191 (100%)	181 (95%)	10 (5%)	21	13
2	B	186/191 (97%)	178 (96%)	8 (4%)	26	18
3	C	113/151 (75%)	108 (96%)	5 (4%)	25	17
4	D	253/277 (91%)	231 (91%)	22 (9%)	9	4
All	All	743/810 (92%)	698 (94%)	45 (6%)	17	9

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	20	SER
1	A	22	SER
1	A	40	SER
1	A	45	ARG
1	A	61	ARG
1	A	79	GLU
1	A	90	ASN
1	A	105	GLU
1	A	213	GLU
2	B	1	GLU
2	B	43	GLN
2	B	129	SER
2	B	130	SER
2	B	134	SER
2	B	188	SER
2	B	193	THR
2	B	206	ASN
3	C	17	LEU
3	C	54	CYS
3	C	76	GLN
3	C	105	LEU
3	C	132	SER
4	D	15	TRP
4	D	34	ASP
4	D	51	LYS
4	D	89	ILE
4	D	96	LYS
4	D	104	LYS
4	D	140	SER
4	D	141	SER
4	D	144	GLN
4	D	153	LEU
4	D	154	SER
4	D	170	GLU
4	D	175	SER
4	D	204	SER
4	D	229	GLN
4	D	230	VAL
4	D	231	GLU
4	D	256	GLN
4	D	265	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	275	THR
4	D	278	CYS
4	D	303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	189	HIS
2	B	166	HIS
3	C	19	GLN
3	C	29	HIS
3	C	66	ASN
3	C	72	GLN
3	C	75	HIS
3	C	76	GLN
4	D	98	GLN
4	D	194	HIS
4	D	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
6	MPD	B	501	-	7,7,7	0.64	0	9,10,10	1.45	1 (11%)
6	MPD	A	502	-	7,7,7	1.10	0	9,10,10	1.05	0
5	IMD	A	503	-	5,5,5	0.54	0	5,5,5	0.56	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
6	MPD	B	501	-	1/1/2/2	1/5/5/5	-
5	IMD	A	503	-	-	-	0/1/1/1
6	MPD	A	502	-	-	0/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	MPD	CM-C2-C1	2.23	115.61	110.63

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	501	MPD	C4

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	MPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	MPD	3	0
6	A	502	MPD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	213/214 (99%)	-0.18	1 (0%) 87 89	17, 30, 49, 77	1 (0%)
2	B	216/223 (96%)	-0.24	7 (3%) 50 54	13, 25, 50, 91	3 (1%)
3	C	133/178 (74%)	0.22	7 (5%) 32 34	22, 36, 68, 80	0
4	D	290/306 (94%)	0.38	22 (7%) 20 21	25, 40, 77, 101	0
All	All	852/921 (92%)	0.06	37 (4%) 40 42	13, 33, 67, 101	4 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	134	SER	5.7
4	D	103	ASN	4.6
3	C	168	LEU	4.5
4	D	257	GLY	4.0
2	B	133	THR	3.9
2	B	135	GLY	3.6
3	C	118	PRO	3.5
4	D	17	PRO	3.5
4	D	177	CYS	3.3
2	B	136	GLY	3.3
4	D	303	VAL	3.2
3	C	131	LEU	3.1
4	D	224	LEU	3.1
3	C	69	PHE	3.1
4	D	159	ARG	3.0
4	D	278	CYS	3.0
2	B	217	SER	2.9
3	C	32	VAL	2.8
3	C	49	VAL	2.8
4	D	18	ASP	2.6
4	D	15	TRP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	104	LYS	2.6
4	D	19	ALA	2.5
4	D	230	VAL	2.5
3	C	132	SER	2.4
4	D	221	LEU	2.3
4	D	232	VAL	2.3
4	D	99	LYS	2.2
4	D	304	PRO	2.1
4	D	305	CYS	2.1
4	D	153	LEU	2.1
2	B	130	SER	2.1
2	B	216	LYS	2.1
4	D	279	ARG	2.1
4	D	277	ILE	2.0
1	A	213	GLU	2.0
4	D	162	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IMD	A	503	5/5	0.58	0.20	77,78,78,79	0
6	MPD	B	501	8/8	0.89	0.10	43,45,47,49	0
6	MPD	A	502	8/8	0.92	0.10	37,37,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.