



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:58 PM UTC

PDB ID : 1MCF / pdb_00001mcf
Title : PRINCIPLES AND PITFALLS IN DESIGNING SITE DIRECTED PEP-
TIDE LIGANDS
Authors : Edmundson, A.B.; Harris, D.L.; Fan, Z.-C.; Guddat, L.W.
Deposited on : 1993-02-25
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
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

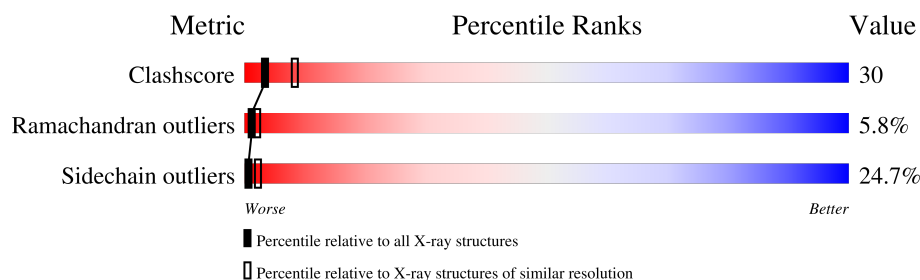
1 Overall quality at a glance

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	A	216	34% 47% 16% .
1	B	216	40% 44% 12% .
2	P	7	57% 43%

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	DPR	P	4	-	-	X	-
2	BAL	P	5	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BAL	P	6	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3261 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-1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1605	1000	266	334	5			
1	B	216	Total	C	N	O	S	0	0	0
			1605	1000	266	334	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP P0DOX8
B	1	PRO	-	expression tag	UNP P0DOX8

- Molecule 2 is a protein called PEPTIDE N-ACETYL-L-GLN-D-PHE-L-HIS-D-PRO-B-AL A-B-ALA-OH.

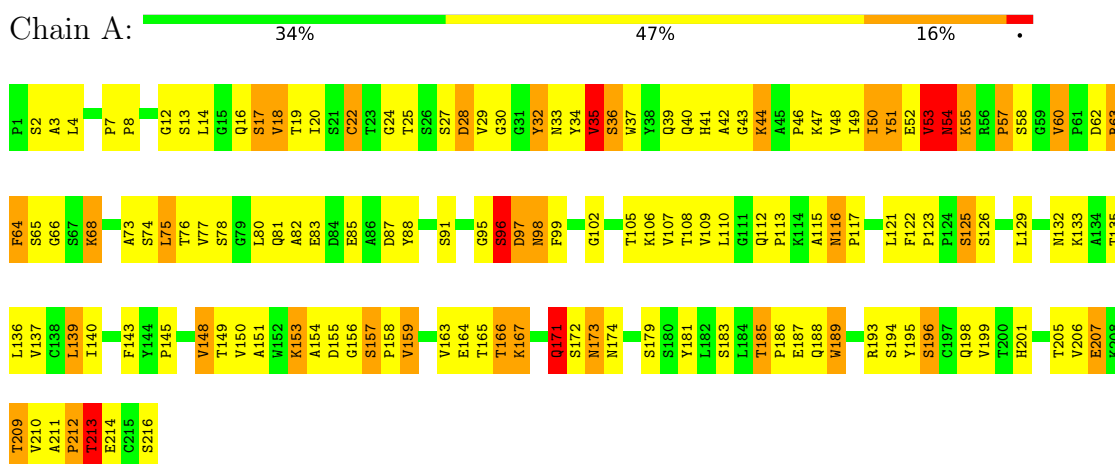
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			51	33	9	9			

3 Residue-property plots

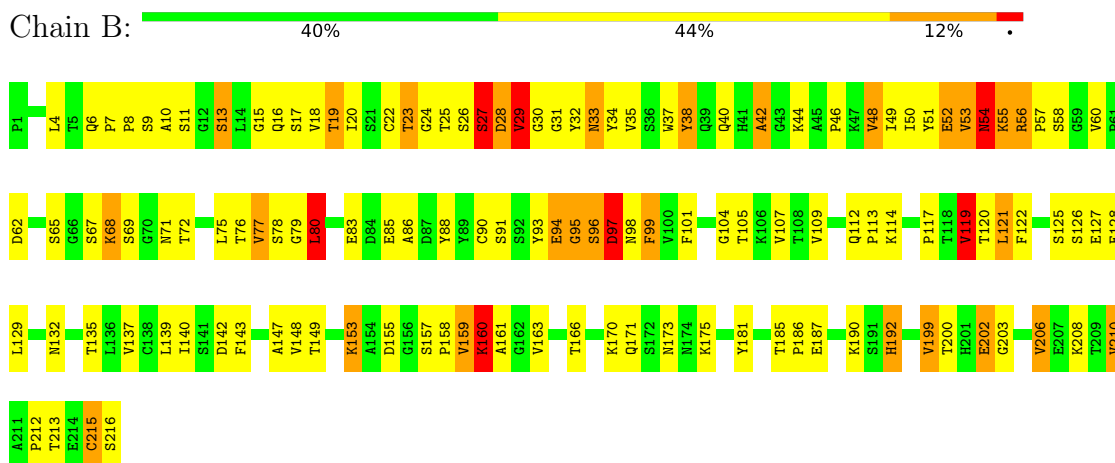
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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-1 light chain



• Molecule 1: Immunoglobulin lambda-1 light chain



• Molecule 2: PEPTIDE N-ACETYL-L-GLN-D-PHE-L-HIS-D-PRO-B-ALA-B-ALA-OH



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)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3261	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: DPN, ACE, BAL, DPR

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	1.05	1/1644 (0.1%)	1.66	25/2241 (1.1%)
1	B	1.04	1/1644 (0.1%)	1.79	26/2241 (1.2%)
2	P	0.56	0/19	1.17	0/23
All	All	1.04	2/3307 (0.1%)	1.72	51/4505 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	VAL	N-CA	6.17	1.54	1.46
1	A	18	VAL	N-CA	6.00	1.53	1.46

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ASP	CA-CB-CG	17.12	129.72	112.60
1	A	28	ASP	CA-CB-CG	8.77	121.37	112.60
1	B	76	THR	CA-C-N	-8.61	111.65	123.10
1	B	76	THR	C-N-CA	-8.61	111.65	123.10
1	B	122	PHE	CA-CB-CG	8.61	122.41	113.80
1	B	192	HIS	CA-CB-CG	-7.04	106.76	113.80
1	B	202	GLU	CA-CB-CG	6.69	127.48	114.10
1	B	80	LEU	CB-CA-C	6.67	120.56	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	THR	O-C-N	6.66	131.40	123.27
1	A	30	GLY	N-CA-C	-6.60	103.72	112.82
1	A	64	PHE	N-CA-CB	6.17	122.23	110.82
1	A	96	SER	CA-C-N	5.94	132.89	121.54
1	A	96	SER	C-N-CA	5.94	132.89	121.54
1	B	54	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	116	ASN	CA-CB-CG	5.82	118.42	112.60
1	B	203	GLY	CA-C-N	-5.80	113.81	122.39
1	B	203	GLY	C-N-CA	-5.80	113.81	122.39
1	B	159	VAL	N-CA-C	5.75	116.58	108.36
1	B	33	ASN	CA-CB-CG	5.70	118.30	112.60
1	B	187	GLU	CA-CB-CG	5.69	125.49	114.10
1	B	95	GLY	CA-C-N	5.68	132.39	121.54
1	B	95	GLY	C-N-CA	5.68	132.39	121.54
1	B	77	VAL	O-C-N	5.68	129.22	123.20
1	A	64	PHE	O-C-N	5.61	131.91	122.93
1	B	119	VAL	CB-CA-C	5.61	118.89	110.98
1	A	171	GLN	CA-CB-CG	5.54	125.19	114.10
1	B	143	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	159	VAL	CA-C-O	5.51	126.47	120.57
1	B	19	THR	N-CA-CB	5.47	119.85	110.77
1	B	104	GLY	CA-C-O	-5.46	118.46	122.23
1	A	17	SER	O-C-N	5.44	128.31	123.41
1	B	27	SER	N-CA-C	5.42	122.34	110.80
1	A	22	CYS	CB-CA-C	5.40	119.13	110.16
1	A	17	SER	CA-C-N	-5.38	114.61	122.58
1	A	17	SER	C-N-CA	-5.38	114.61	122.58
1	A	22	CYS	CA-CB-SG	5.32	126.62	114.40
1	A	35	VAL	O-C-N	5.30	129.41	122.94
1	B	52	GLU	CA-CB-CG	5.28	124.66	114.10
1	A	195	TYR	CA-C-N	-5.27	113.67	122.21
1	A	195	TYR	C-N-CA	-5.27	113.67	122.21
1	A	17	SER	N-CA-C	5.27	116.45	108.07
1	A	122	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	143	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	213	THR	CA-CB-CG2	5.20	119.34	110.50
1	A	153	LYS	O-C-N	5.11	129.20	123.27
1	A	54	ASN	N-CA-CB	5.11	118.76	110.43
1	B	28	ASP	N-CA-C	5.09	119.48	113.12
1	A	157	SER	O-C-N	5.08	125.82	121.30
1	B	72	THR	N-CA-C	5.06	117.65	108.69
1	A	206	VAL	N-CA-C	-5.04	101.38	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	53	VAL	CB-CA-C	5.01	119.50	111.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	5	BAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1605	0	1540	101	0
1	B	1605	0	1540	88	0
2	P	51	0	41	25	0
All	All	3261	0	3121	193	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 30.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:4:DPR:HA	2:P:6:BAL:HA1	1.22	1.16
1:B:215:CYS:SG	1:B:216:SER:N	2.46	0.89
2:P:4:DPR:CA	2:P:6:BAL:HA1	2.06	0.85
1:B:126:SER:HB3	1:B:215:CYS:SG	2.20	0.82
1:A:54:ASN:HB2	1:A:66:GLY:O	1.80	0.81
1:A:35:VAL:HA	1:A:91:SER:O	1.83	0.77
1:B:9:SER:HB3	1:B:147:ALA:HB3	1.67	0.75
2:P:4:DPR:HA	2:P:6:BAL:CA	2.10	0.75
1:A:68:LYS:HZ3	1:A:68:LYS:HB3	1.51	0.74
1:A:123:PRO:HA	1:A:136:LEU:HD23	1.71	0.71
1:B:121:LEU:HD13	1:B:210:VAL:HB	1.73	0.71
1:B:29:VAL:HG13	1:B:30:GLY:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:1:GLN:HB3	2:P:3:HIS:HB2	1.72	0.69
1:A:51:TYR:HB2	2:P:3:HIS:CE1	2.27	0.69
2:P:3:HIS:C	2:P:5:BAL:N	2.51	0.69
1:A:55:LYS:O	1:A:57:PRO:HD3	1.93	0.68
1:B:37:TRP:HB2	1:B:50:ILE:HB	1.75	0.68
1:B:94:GLU:O	1:B:96:SER:N	2.22	0.67
1:B:101:PHE:HE1	2:P:0:ACE:H3	1.60	0.66
1:B:10:ALA:O	1:B:107:VAL:HA	1.95	0.66
1:A:41:HIS:O	1:A:44:LYS:HB2	1.95	0.66
1:A:62:ASP:CG	1:A:63:ARG:H	2.05	0.65
1:A:85:GLU:HG3	1:A:108:THR:HA	1.78	0.65
2:P:3:HIS:O	2:P:5:BAL:N	2.31	0.64
1:A:51:TYR:CD1	1:A:55:LYS:HB3	2.33	0.64
1:B:160:LYS:HE2	1:B:161:ALA:H	1.63	0.63
1:A:105:THR:HG22	1:A:107:VAL:HG23	1.81	0.63
2:P:4:DPR:C	2:P:6:BAL:H	2.10	0.63
1:B:4:LEU:HD13	1:B:90:CYS:SG	2.40	0.62
1:B:51:TYR:O	1:B:55:LYS:HB2	2.01	0.61
1:A:132:ASN:HD22	1:A:186:PRO:HG2	1.65	0.61
1:A:82:ALA:HB1	1:A:112:GLN:OE1	2.01	0.61
1:A:48:VAL:HG21	1:B:99:PHE:CD1	2.35	0.60
1:A:17:SER:HA	1:A:80:LEU:HG	1.83	0.60
1:B:173:ASN:HD22	1:B:175:LYS:NZ	1.99	0.60
1:B:126:SER:HA	1:B:129:LEU:HD12	1.82	0.60
1:A:155:ASP:O	1:A:157:SER:N	2.35	0.60
1:B:119:VAL:HA	1:B:139:LEU:O	2.03	0.59
1:A:68:LYS:HA	1:A:73:ALA:HA	1.85	0.59
1:A:132:ASN:C	1:A:133:LYS:HD2	2.27	0.59
1:A:95:GLY:O	1:A:96:SER:C	2.45	0.58
1:A:4:LEU:O	1:A:102:GLY:HA2	2.04	0.57
1:A:148:VAL:HG22	1:A:201:HIS:HB2	1.86	0.57
1:B:173:ASN:HD21	1:B:175:LYS:HB2	1.69	0.57
2:P:1:GLN:HB3	2:P:3:HIS:CB	2.35	0.57
1:A:123:PRO:HA	1:A:136:LEU:CD2	2.35	0.57
1:B:25:THR:O	1:B:27:SER:N	2.38	0.57
1:A:48:VAL:HG11	2:P:0:ACE:H2	1.86	0.56
1:A:36:SER:HB3	1:A:51:TYR:HA	1.87	0.56
1:B:56:ARG:HG3	1:B:60:VAL:CG1	2.35	0.56
1:B:29:VAL:HG13	1:B:30:GLY:H	1.70	0.56
1:A:63:ARG:CB	1:A:78:SER:HB2	2.35	0.56
1:B:48:VAL:HG11	2:P:2:DPN:CZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:CG2	1:A:80:LEU:HD21	2.37	0.55
1:B:15:GLY:C	1:B:79:GLY:HA2	2.32	0.55
1:B:48:VAL:HG11	2:P:2:DPN:HZ	1.89	0.55
1:B:28:ASP:O	1:B:29:VAL:HG12	2.07	0.55
1:A:4:LEU:HD23	1:A:22:CYS:SG	2.47	0.55
1:A:63:ARG:HG3	1:A:78:SER:O	2.07	0.55
1:B:192:HIS:O	1:B:212:PRO:HG2	2.07	0.55
1:B:101:PHE:CE1	2:P:0:ACE:H3	2.42	0.55
1:A:53:VAL:HG11	1:A:68:LYS:NZ	2.22	0.54
1:A:62:ASP:CG	1:A:63:ARG:N	2.64	0.54
1:B:17:SER:HA	1:B:77:VAL:O	2.08	0.54
1:B:6:GLN:HB3	1:B:105:THR:OG1	2.07	0.54
1:A:46:PRO:HG2	1:B:101:PHE:CE2	2.42	0.53
1:A:53:VAL:HG11	1:A:68:LYS:HZ2	1.73	0.53
1:A:121:LEU:HD21	1:A:210:VAL:HG12	1.91	0.53
2:P:4:DPR:C	2:P:6:BAL:N	2.71	0.53
1:B:117:PRO:HB2	1:B:140:ILE:HG23	1.91	0.53
1:A:27:SER:O	1:A:32:TYR:HE1	1.92	0.53
1:A:99:PHE:CE1	2:P:5:BAL:HB2	2.44	0.52
1:B:16:GLN:O	1:B:80:LEU:HB3	2.09	0.52
1:B:125:SER:O	1:B:128:GLU:HB2	2.09	0.52
1:A:116:ASN:HA	1:A:201:HIS:CD2	2.45	0.52
1:A:51:TYR:CE1	1:A:55:LYS:HB3	2.45	0.52
1:A:185:THR:O	1:A:188:GLN:HB2	2.10	0.52
1:B:53:VAL:HG21	1:B:68:LYS:HG2	1.91	0.51
1:A:153:LYS:C	1:A:159:VAL:HG12	2.35	0.51
1:A:196:SER:HB3	1:A:209:THR:HG23	1.92	0.51
1:A:2:SER:O	1:A:3:ALA:HB3	2.11	0.51
1:A:133:LYS:HD2	1:A:133:LYS:N	2.26	0.51
1:B:11:SER:OG	1:B:114:LYS:HE2	2.11	0.51
1:A:65:SER:O	1:A:75:LEU:HA	2.11	0.50
1:A:48:VAL:CG2	1:B:99:PHE:HD1	2.22	0.50
1:A:52:GLU:HG3	2:P:3:HIS:CE1	2.47	0.50
1:A:125:SER:O	1:A:129:LEU:HD12	2.11	0.50
1:B:57:PRO:HD2	1:B:60:VAL:HG21	1.92	0.50
1:B:163:VAL:HA	1:B:181:TYR:O	2.12	0.50
1:A:139:LEU:HD11	1:B:181:TYR:CD2	2.47	0.49
1:B:4:LEU:HD23	1:B:24:GLY:HA2	1.95	0.49
1:A:48:VAL:HG21	1:B:99:PHE:HD1	1.75	0.49
1:A:189:TRP:CH2	1:A:212:PRO:HA	2.47	0.49
1:B:38:TYR:OH	2:P:0:ACE:H1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:CE1	1:A:77:VAL:HG12	2.48	0.49
1:B:38:TYR:O	1:B:88:TYR:HA	2.13	0.49
1:B:54:ASN:C	1:B:54:ASN:HD22	2.20	0.49
1:A:171:GLN:O	1:A:173:ASN:N	2.44	0.49
1:A:164:GLU:HB2	1:A:181:TYR:CZ	2.48	0.49
1:B:173:ASN:HD22	1:B:175:LYS:HZ2	1.59	0.48
1:B:38:TYR:HE1	1:B:91:SER:HB2	1.78	0.48
1:B:96:SER:O	1:B:97:ASP:HB3	2.13	0.48
1:A:19:THR:HG23	1:A:76:THR:OG1	2.12	0.48
1:A:63:ARG:HB2	1:A:78:SER:HB2	1.96	0.48
1:A:145:PRO:O	1:A:201:HIS:HE1	1.97	0.47
1:B:112:GLN:HB2	1:B:113:PRO:CD	2.44	0.47
2:P:1:GLN:NE2	2:P:1:GLN:HA	2.28	0.47
1:B:6:GLN:HG2	1:B:22:CYS:SG	2.54	0.47
1:A:132:ASN:ND2	1:A:186:PRO:HG2	2.31	0.46
1:B:40:GLN:OE1	1:B:46:PRO:HG3	2.15	0.46
1:B:23:THR:HA	1:B:71:ASN:O	2.15	0.46
1:A:151:ALA:HB3	1:A:198:GLN:HB3	1.98	0.46
1:A:115:ALA:O	1:A:201:HIS:NE2	2.48	0.46
1:B:28:ASP:O	1:B:31:GLY:HA3	2.15	0.46
1:A:116:ASN:HD22	1:A:201:HIS:HD2	1.64	0.46
1:B:85:GLU:HG3	1:B:109:VAL:HG23	1.98	0.46
1:A:95:GLY:O	1:A:97:ASP:N	2.48	0.46
1:A:112:GLN:HA	1:A:113:PRO:HD3	1.80	0.46
1:A:137:VAL:HG11	1:B:137:VAL:HG11	1.98	0.46
1:B:49:ILE:O	1:B:50:ILE:HG12	2.15	0.45
1:A:2:SER:O	1:A:3:ALA:CB	2.64	0.45
1:A:34:TYR:HD1	2:P:3:HIS:CG	2.35	0.45
1:A:37:TRP:HD1	1:A:50:ILE:HG21	1.79	0.45
1:B:13:SER:O	1:B:16:GLN:HB2	2.17	0.45
1:B:42:ALA:O	1:B:44:LYS:NZ	2.49	0.45
1:A:37:TRP:H	1:A:50:ILE:HG22	1.81	0.45
1:B:56:ARG:HG3	1:B:60:VAL:HG12	1.99	0.45
1:A:20:ILE:O	1:A:74:SER:HA	2.17	0.45
1:A:77:VAL:HG23	1:A:80:LEU:HD21	1.99	0.45
1:A:155:ASP:OD1	1:A:193:ARG:HB3	2.17	0.45
1:A:77:VAL:HG23	1:A:77:VAL:O	2.17	0.44
1:B:119:VAL:HG22	1:B:208:LYS:HG2	1.99	0.44
1:B:171:GLN:HB2	1:B:173:ASN:OD1	2.17	0.44
1:A:51:TYR:HB2	2:P:3:HIS:HE1	1.79	0.44
1:A:85:GLU:HA	1:A:107:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ALA:O	1:A:213:THR:N	2.50	0.44
1:B:8:PRO:HG3	1:B:200:THR:HG22	2.00	0.44
2:P:1:GLN:O	2:P:2:DPN:CD1	2.65	0.44
1:A:34:TYR:HD1	2:P:3:HIS:ND1	2.16	0.44
1:B:40:GLN:O	1:B:86:ALA:HB1	2.18	0.44
1:A:181:TYR:CD2	1:B:139:LEU:HD11	2.53	0.44
1:B:160:LYS:HD3	1:B:160:LYS:H	1.83	0.44
1:B:157:SER:HA	1:B:158:PRO:HD2	1.83	0.44
1:A:40:GLN:NE2	1:A:44:LYS:O	2.50	0.43
1:A:97:ASP:OD1	2:P:5:BAL:O	2.36	0.43
1:A:17:SER:OG	1:A:18:VAL:N	2.51	0.43
1:A:37:TRP:N	1:A:50:ILE:HG22	2.34	0.43
1:B:153:LYS:HA	1:B:157:SER:O	2.19	0.43
1:A:18:VAL:H	1:A:77:VAL:HG23	1.83	0.43
1:A:20:ILE:HD12	1:A:75:LEU:HD23	2.00	0.43
1:A:214:GLU:HB3	1:A:216:SER:OG	2.18	0.43
1:B:29:VAL:HG23	1:B:71:ASN:OD1	2.18	0.43
1:B:55:LYS:O	1:B:56:ARG:HB3	2.17	0.43
1:B:119:VAL:HG13	1:B:206:VAL:HG11	2.01	0.43
1:A:24:GLY:HA3	1:A:29:VAL:CG2	2.48	0.43
1:B:68:LYS:HD2	1:B:69:SER:N	2.34	0.43
1:A:7:PRO:HA	1:A:8:PRO:HD3	1.82	0.43
1:A:12:GLY:HA3	1:A:80:LEU:CD1	2.48	0.43
1:A:88:TYR:CE1	1:A:107:VAL:HB	2.54	0.43
1:B:112:GLN:HB2	1:B:113:PRO:HD2	2.01	0.43
1:B:119:VAL:HG22	1:B:208:LYS:CG	2.48	0.43
1:B:173:ASN:ND2	1:B:175:LYS:NZ	2.65	0.43
1:A:196:SER:HB2	1:A:207:GLU:OE1	2.19	0.43
1:A:117:PRO:CB	1:A:140:ILE:HG22	2.49	0.43
1:B:155:ASP:C	1:B:157:SER:H	2.27	0.43
1:A:48:VAL:CG2	1:B:99:PHE:CD1	2.99	0.42
1:A:140:ILE:HG23	1:A:199:VAL:HG11	2.02	0.42
1:B:29:VAL:O	1:B:32:TYR:N	2.52	0.42
1:A:153:LYS:HA	1:A:158:PRO:HA	2.01	0.42
1:B:93:TYR:OH	1:B:96:SER:HB3	2.20	0.42
1:B:149:THR:O	1:B:199:VAL:HA	2.20	0.42
1:B:29:VAL:CG1	1:B:30:GLY:N	2.74	0.42
1:B:15:GLY:O	1:B:79:GLY:HA2	2.19	0.42
1:B:20:ILE:HG12	1:B:105:THR:HG21	2.01	0.42
1:A:49:ILE:HG22	1:A:60:VAL:HG13	2.02	0.42
1:A:116:ASN:HB3	1:A:117:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:SER:HB3	1:A:216:SER:HB3	2.02	0.41
1:A:54:ASN:ND2	1:A:55:LYS:N	2.69	0.41
1:B:186:PRO:O	1:B:190:LYS:HB2	2.20	0.41
1:B:35:VAL:HB	1:B:53:VAL:CG2	2.51	0.41
1:B:51:TYR:CE1	1:B:55:LYS:HB3	2.55	0.41
1:A:213:THR:O	1:A:213:THR:CG2	2.68	0.41
1:B:18:VAL:CG1	1:B:19:THR:N	2.84	0.41
1:B:29:VAL:C	1:B:31:GLY:N	2.79	0.41
1:B:52:GLU:O	1:B:53:VAL:HB	2.21	0.41
1:B:185:THR:HA	1:B:186:PRO:HD3	1.91	0.41
1:A:82:ALA:HA	1:A:109:VAL:HG21	2.02	0.41
1:A:95:GLY:O	1:A:98:ASN:N	2.53	0.40
1:A:166:THR:HG23	1:A:167:LYS:O	2.21	0.40
1:B:51:TYR:CZ	1:B:55:LYS:HD2	2.56	0.40
1:A:18:VAL:HG13	1:A:77:VAL:CG2	2.50	0.40
1:A:24:GLY:HA3	1:A:29:VAL:HG21	2.03	0.40
2:P:1:GLN:HB3	2:P:3:HIS:CG	2.56	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	214/216 (99%)	175 (82%)	27 (13%)	12 (6%)		
1	B	214/216 (99%)	177 (83%)	24 (11%)	13 (6%)		
2	P	2/7 (29%)	2 (100%)	0	0		
All	All	430/439 (98%)	354 (82%)	51 (12%)	25 (6%)		

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	97	ASP
1	A	172	SER
1	A	173	ASN
1	B	26	SER
1	B	95	GLY
1	B	96	SER
1	A	16	GLN
1	A	53	VAL
1	A	154	ALA
1	A	156	GLY
1	A	212	PRO
1	B	27	SER
1	B	29	VAL
1	B	42	ALA
1	B	160	LYS
1	A	42	ALA
1	B	94	GLU
1	B	97	ASP
1	B	202	GLU
1	B	56	ARG
1	B	83	GLU
1	B	55	LYS
1	A	43	GLY
1	A	57	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	181/181 (100%)	131 (72%)	50 (28%)	0	1
1	B	181/181 (100%)	142 (78%)	39 (22%)	1	3
2	P	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	364/364 (100%)	274 (75%)	90 (25%)	1	2

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	14	LEU
1	A	25	THR
1	A	28	ASP
1	A	32	TYR
1	A	33	ASN
1	A	35	VAL
1	A	36	SER
1	A	39	GLN
1	A	44	LYS
1	A	47	LYS
1	A	50	ILE
1	A	51	TYR
1	A	54	ASN
1	A	55	LYS
1	A	58	SER
1	A	60	VAL
1	A	63	ARG
1	A	68	LYS
1	A	75	LEU
1	A	81	GLN
1	A	83	GLU
1	A	87	ASP
1	A	98	ASN
1	A	106	LYS
1	A	110	LEU
1	A	125	SER
1	A	135	THR
1	A	139	LEU
1	A	148	VAL
1	A	149	THR
1	A	150	VAL
1	A	159	VAL
1	A	163	VAL
1	A	165	THR
1	A	166	THR
1	A	167	LYS
1	A	171	GLN
1	A	174	ASN
1	A	179	SER
1	A	183	SER
1	A	185	THR
1	A	187	GLU

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Mol	Chain	Res	Type
1	A	189	TRP
1	A	194	SER
1	A	196	SER
1	A	205	THR
1	A	207	GLU
1	A	209	THR
1	A	213	THR
1	B	7	PRO
1	B	13	SER
1	B	23	THR
1	B	29	VAL
1	B	33	ASN
1	B	34	TYR
1	B	38	TYR
1	B	48	VAL
1	B	53	VAL
1	B	54	ASN
1	B	58	SER
1	B	62	ASP
1	B	65	SER
1	B	67	SER
1	B	68	LYS
1	B	75	LEU
1	B	78	SER
1	B	80	LEU
1	B	97	ASP
1	B	98	ASN
1	B	99	PHE
1	B	119	VAL
1	B	120	THR
1	B	121	LEU
1	B	127	GLU
1	B	132	ASN
1	B	135	THR
1	B	142	ASP
1	B	148	VAL
1	B	153	LYS
1	B	159	VAL
1	B	160	LYS
1	B	166	THR
1	B	170	LYS
1	B	199	VAL

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Mol	Chain	Res	Type
1	B	206	VAL
1	B	210	VAL
1	B	213	THR
1	B	215	CYS
2	P	3	HIS

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

Mol	Chain	Res	Type
1	A	33	ASN
1	A	40	GLN
1	A	41	HIS
1	A	81	GLN
1	A	98	ASN
1	A	116	ASN
1	A	132	ASN
1	A	198	GLN
1	B	40	GLN
1	B	54	ASN
1	B	98	ASN
1	B	130	GLN
1	B	132	ASN
1	B	173	ASN
2	P	1	GLN
2	P	3	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
2	BAL	P	6	2	5,5,5	0.97	0	5,5,5	1.42	1 (20%)
2	BAL	P	5	2	3,4,5	0.41	0	3,3,5	1.06	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
2	BAL	P	6	2	-	3/3/3/3	-
2	BAL	P	5	2	-	1/1/2/3	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	6	BAL	CB-CA-C	2.59	118.58	112.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	6	BAL	C-CA-CB-N
2	P	6	BAL	OXT-C-CA-CB
2	P	6	BAL	O-C-CA-CB
2	P	5	BAL	C-CA-CB-N

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	6	BAL	5	0
2	P	5	BAL	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.