



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:11 AM UTC

PDB ID : 1MCD / pdb\_00001mcd  
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 : Not provided

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](mailto: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>.

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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)  
Xtrriage (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

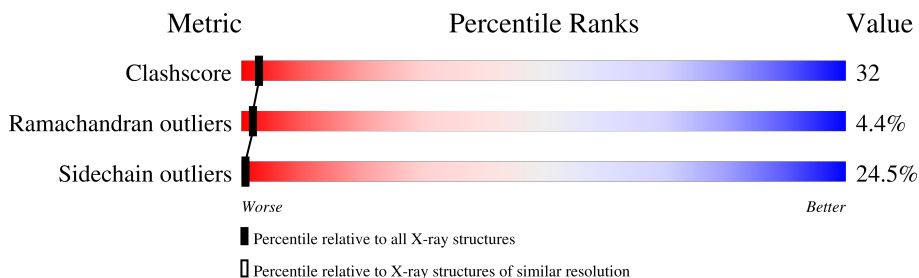
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is unknown.

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	-
Ramachandran outliers	187476	-
Sidechain outliers	187428	-

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  $\geq 3$ , 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	
1	B	216	
2	P	6	

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 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3247 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
			Total	C	N	O	S			
1	A	216	1605	1000	266	334	5	0	0	0
1	B	216	1605	1000	266	334	5	0	0	0

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-D-PHE-B-ALA-L-HIS-D-PRO-NH2.

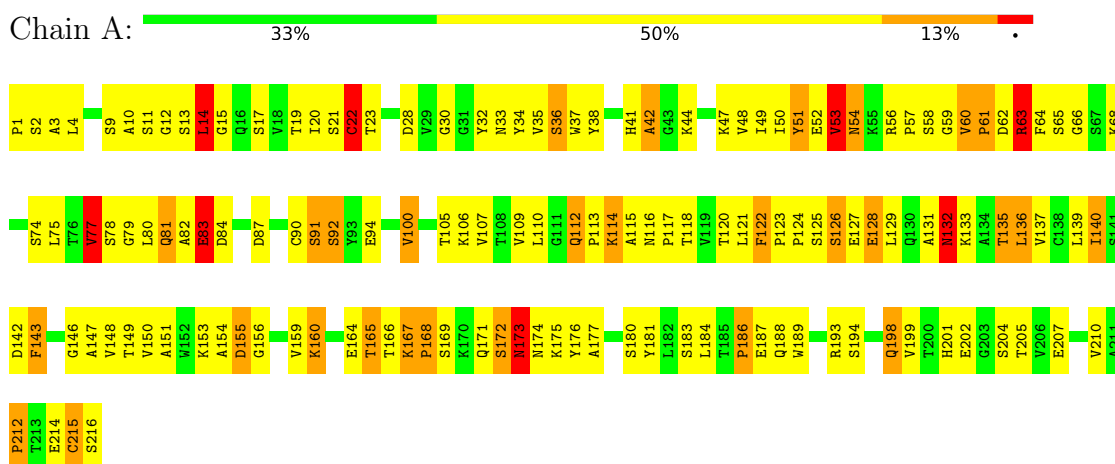
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	6	37	25	7	5	0	0	1

### 3 Residue-property plots

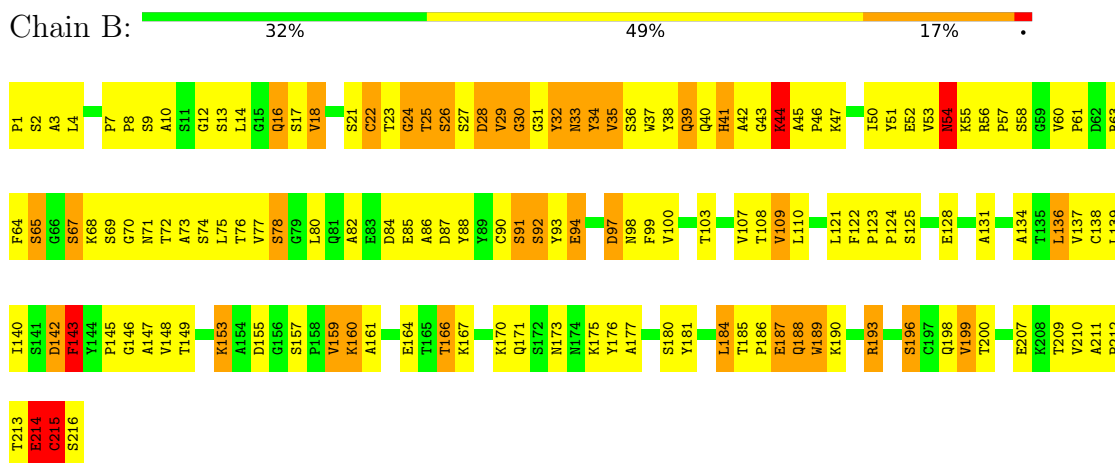
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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-D-PHE-B-ALA-L-HIS-D-PRO-NH2



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	72.30Å 72.30Å 185.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – (Not available)	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-(Not available))	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3247	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DPR, BAL, DPN, NH2, ACE

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	1.03	2/1644 (0.1%)	1.76	31/2241 (1.4%)
1	B	1.10	2/1644 (0.1%)	1.79	26/2241 (1.2%)
2	P	1.05	0/10	1.60	0/12
All	All	1.07	4/3298 (0.1%)	1.77	57/4494 (1.3%)

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
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	THR	CA-CB	5.77	1.60	1.53
1	B	44	LYS	N-CA	5.76	1.52	1.46
1	A	12	GLY	N-CA	5.60	1.50	1.45
1	B	18	VAL	N-CA	5.19	1.52	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	PHE	CA-CB-CG	16.48	130.28	113.80
1	B	29	VAL	N-CA-C	10.03	123.57	108.23
1	B	215	CYS	CA-CB-SG	9.51	136.27	114.40
1	A	2	SER	N-CA-C	9.18	124.36	109.85
1	A	122	PHE	CA-CB-CG	9.16	122.96	113.80
1	B	54	ASN	CA-CB-CG	8.67	121.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	PHE	CA-CB-CG	8.47	122.27	113.80
1	B	159	VAL	CB-CA-C	8.34	120.65	110.73
1	B	34	TYR	CA-CB-CG	8.25	128.75	113.90
1	B	87	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	214	GLU	CA-CB-CG	7.34	128.78	114.10
1	A	83	GLU	CB-CG-CD	7.08	124.64	112.60
1	A	51	TYR	CA-CB-CG	6.95	126.42	113.90
1	A	143	PHE	CA-CB-CG	6.91	120.71	113.80
1	A	122	PHE	CA-C-N	6.83	124.64	119.66
1	A	122	PHE	C-N-CA	6.83	124.64	119.66
1	B	110	LEU	N-CA-C	6.70	122.35	111.37
1	A	202	GLU	CA-CB-CG	6.46	127.02	114.10
1	B	32	TYR	CA-CB-CG	-6.44	102.30	113.90
1	B	31	GLY	N-CA-C	-6.27	98.31	113.18
1	A	168	PRO	N-CA-C	6.16	125.16	112.47
1	A	2	SER	CA-C-O	6.11	128.61	121.46
1	A	22	CYS	CA-CB-SG	6.06	128.33	114.40
1	A	215	CYS	CA-CB-SG	5.94	128.06	114.40
1	B	142	ASP	CA-CB-CG	-5.94	106.66	112.60
1	B	189	TRP	CA-CB-CG	5.92	124.84	113.60
1	A	83	GLU	CA-CB-CG	5.83	125.77	114.10
1	B	30	GLY	N-CA-C	-5.81	99.40	113.18
1	A	79	GLY	N-CA-C	-5.75	106.52	115.67
1	B	16	GLN	N-CA-C	-5.69	103.19	110.53
1	A	215	CYS	N-CA-CB	5.66	120.05	110.49
1	A	54	ASN	N-CA-CB	5.65	119.72	110.90
1	A	60	VAL	N-CA-CB	5.57	119.01	111.21
1	A	61	PRO	CA-C-N	5.55	132.15	121.54
1	A	61	PRO	C-N-CA	5.55	132.15	121.54
1	A	63	ARG	N-CA-CB	5.54	118.63	110.49
1	B	140	ILE	O-C-N	5.53	128.99	123.18
1	A	54	ASN	CA-CB-CG	-5.53	107.07	112.60
1	A	173	ASN	CA-CB-CG	5.52	118.12	112.60
1	B	109	VAL	N-CA-CB	5.51	118.09	111.31
1	B	181	TYR	CA-CB-CG	5.50	123.81	113.90
1	B	33	ASN	CA-C-O	-5.48	113.81	119.51
1	A	165	THR	N-CA-C	5.42	117.46	108.20
1	A	81	GLN	CB-CG-CD	5.38	121.74	112.60
1	A	128	GLU	N-CA-C	-5.36	104.84	111.33
1	B	41	HIS	CA-CB-CG	5.34	119.14	113.80
1	A	53	VAL	CB-CA-C	5.33	120.03	111.29
1	B	22	CYS	CB-CA-C	5.31	119.65	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	GLY	N-CA-C	-5.28	104.98	112.37
1	A	207	GLU	CB-CG-CD	5.26	121.53	112.60
1	A	123	PRO	N-CA-C	5.25	115.51	110.47
1	A	77	VAL	CB-CA-C	5.14	116.85	110.73
1	B	68	LYS	N-CA-C	5.13	116.20	108.46
1	B	34	TYR	N-CA-CB	5.12	118.15	110.11
1	B	29	VAL	CB-CA-C	-5.11	104.78	110.96
1	A	186	PRO	N-CA-C	-5.10	106.77	113.65
1	B	157	SER	O-C-N	5.09	127.17	121.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PRO	Peptide
1	A	167	LYS	Peptide

## 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	1605	0	1540	103	0
1	B	1605	0	1540	105	0
2	P	37	0	29	9	0
All	All	3247	0	3109	206	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 32.

All (206) 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:B:28:ASP:O	1:B:32:TYR:HB2	1.69	0.93
1:B:4:LEU:HD23	1:B:22:CYS:SG	2.14	0.88
1:A:131:ALA:O	1:A:132:ASN:HB2	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PRO:HB3	1:A:143:PHE:HB3	1.57	0.87
1:B:10:ALA:O	1:B:107:VAL:HA	1.85	0.76
1:B:214:GLU:O	1:B:215:CYS:HB3	1.84	0.76
1:A:173:ASN:ND2	1:A:175:LYS:HB2	2.00	0.76
1:B:52:GLU:HG2	1:B:55:LYS:NZ	2.02	0.74
1:A:165:THR:HG22	1:A:167:LYS:HD3	1.69	0.73
1:A:171:GLN:HE21	1:A:177:ALA:HB2	1.52	0.73
1:A:63:ARG:O	1:A:77:VAL:HA	1.88	0.73
1:A:59:GLY:O	1:A:60:VAL:HG23	1.89	0.71
1:B:40:GLN:O	1:B:86:ALA:HB1	1.90	0.71
1:A:126:SER:O	1:A:129:LEU:HB2	1.91	0.71
1:A:126:SER:HA	1:A:129:LEU:HD12	1.72	0.71
1:B:37:TRP:HB2	1:B:50:ILE:HB	1.73	0.70
1:B:124:PRO:HD3	1:B:136:LEU:HG	1.71	0.69
1:A:48:VAL:O	1:A:57:PRO:HG2	1.93	0.68
1:B:45:ALA:HB1	1:B:46:PRO:CD	2.24	0.68
1:A:35:VAL:HA	1:A:91:SER:O	1.94	0.67
1:A:171:GLN:HB2	1:A:175:LYS:O	1.95	0.67
2:P:3:HIS:HB3	2:P:4:DPR:HD2	1.78	0.66
1:B:173:ASN:ND2	1:B:175:LYS:HG3	2.11	0.66
1:B:16:GLN:O	1:B:80:LEU:HB2	1.96	0.65
1:A:150:VAL:HG11	1:A:180:SER:OG	1.95	0.65
1:B:143:PHE:CE2	1:B:148:VAL:HB	2.31	0.65
1:A:65:SER:O	1:A:75:LEU:HD12	1.97	0.65
1:B:32:TYR:OH	1:B:93:TYR:N	2.30	0.65
1:B:149:THR:O	1:B:199:VAL:HA	1.97	0.65
1:A:198:GLN:NE2	1:A:205:THR:HG21	2.12	0.64
1:B:185:THR:OG1	1:B:188:GLN:HB2	1.97	0.64
1:B:153:LYS:HZ2	1:B:198:GLN:HB2	1.63	0.64
1:A:166:THR:HG21	1:B:166:THR:HG21	1.80	0.63
1:B:155:ASP:OD1	1:B:193:ARG:HD2	1.98	0.63
1:A:166:THR:HG21	1:B:166:THR:CG2	2.28	0.63
1:B:35:VAL:HA	1:B:91:SER:O	1.98	0.63
1:A:142:ASP:H	1:A:171:GLN:HE22	1.48	0.62
1:B:36:SER:OG	2:P:1:DPN:HD2	2.00	0.62
1:B:153:LYS:NZ	1:B:196:SER:HB2	2.15	0.61
1:B:52:GLU:HG2	1:B:55:LYS:HZ2	1.63	0.61
1:A:154:ALA:HB2	1:A:159:VAL:CG2	2.30	0.61
1:B:9:SER:HB2	1:B:147:ALA:HB3	1.82	0.60
1:B:32:TYR:OH	1:B:34:TYR:HB2	2.02	0.60
1:B:173:ASN:ND2	1:B:175:LYS:HZ3	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG23	1:A:180:SER:HB3	1.84	0.60
1:B:173:ASN:HD22	1:B:175:LYS:HZ3	1.50	0.59
1:A:155:ASP:OD2	1:A:193:ARG:HB2	2.02	0.59
1:B:149:THR:HB	1:B:200:THR:OG1	2.02	0.59
1:A:87:ASP:OD1	1:A:106:LYS:HG2	2.01	0.59
2:P:3:HIS:HB3	2:P:4:DPR:CD	2.32	0.59
1:B:41:HIS:HB2	1:B:44:LYS:CG	2.33	0.59
1:A:63:ARG:HB3	1:A:78:SER:H	1.66	0.58
1:B:41:HIS:HB2	1:B:44:LYS:HG2	1.85	0.58
1:A:159:VAL:C	1:A:160:LYS:HD2	2.28	0.58
1:A:14:LEU:HD22	1:A:110:LEU:O	2.03	0.58
1:A:121:LEU:HD23	1:A:210:VAL:HG13	1.85	0.58
1:A:54:ASN:OD1	1:A:65:SER:HA	2.04	0.58
1:B:56:ARG:HG3	1:B:60:VAL:HB	1.85	0.57
1:A:184:LEU:HA	1:A:188:GLN:OE1	2.05	0.56
1:B:214:GLU:O	1:B:215:CYS:CB	2.53	0.56
1:A:87:ASP:HA	1:A:105:THR:O	2.05	0.56
1:B:67:SER:HB3	1:B:74:SER:HB2	1.86	0.56
1:B:41:HIS:ND1	1:B:86:ALA:HB2	2.21	0.56
1:B:69:SER:O	1:B:71:ASN:N	2.39	0.55
1:B:17:SER:HB3	1:B:78:SER:HA	1.88	0.55
1:A:56:ARG:HD3	1:A:64:PHE:O	2.06	0.55
1:A:147:ALA:O	1:A:201:HIS:HD2	1.91	0.54
1:B:32:TYR:HH	1:B:93:TYR:HB3	1.72	0.54
1:A:80:LEU:HD22	1:A:109:VAL:HG21	1.89	0.54
1:B:171:GLN:HB2	1:B:173:ASN:OD1	2.08	0.54
1:B:38:TYR:HE1	1:B:91:SER:HB2	1.73	0.54
1:A:153:LYS:HD2	1:A:156:GLY:O	2.08	0.54
1:A:10:ALA:HB3	1:A:107:VAL:HG22	1.90	0.54
1:A:122:PHE:HB2	1:A:137:VAL:HG13	1.89	0.54
1:B:4:LEU:HA	1:B:24:GLY:HA2	1.90	0.54
1:B:45:ALA:HB1	1:B:46:PRO:HD3	1.90	0.54
1:B:122:PHE:O	1:B:136:LEU:HD23	2.08	0.54
1:B:64:PHE:CE1	1:B:77:VAL:HG22	2.44	0.53
1:B:186:PRO:O	1:B:190:LYS:HG2	2.09	0.53
1:B:41:HIS:O	1:B:43:GLY:N	2.42	0.53
1:A:117:PRO:HB2	1:A:140:ILE:HG23	1.90	0.53
1:B:108:THR:HG21	1:B:145:PRO:HB3	1.91	0.53
1:B:185:THR:OG1	1:B:187:GLU:HG3	2.08	0.53
1:B:52:GLU:HB3	1:B:55:LYS:HD3	1.90	0.53
1:B:171:GLN:OE1	1:B:177:ALA:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:CG	1:A:106:LYS:HG2	2.33	0.52
1:B:54:ASN:HD22	1:B:54:ASN:C	2.17	0.52
1:A:165:THR:CG2	1:A:167:LYS:HD3	2.40	0.52
1:A:136:LEU:HD11	1:A:184:LEU:HD11	1.92	0.52
2:P:4:DPR:HD3	2:P:5:NH2:N	2.25	0.51
1:B:1:PRO:O	1:B:3:ALA:N	2.43	0.51
1:B:198:GLN:HB2	1:B:207:GLU:HG3	1.91	0.51
1:A:38:TYR:HA	1:A:47:LYS:O	2.11	0.51
1:B:52:GLU:HG2	1:B:55:LYS:HZ3	1.72	0.51
1:A:19:THR:CG2	1:A:74:SER:HB3	2.41	0.51
1:A:140:ILE:HG13	1:A:199:VAL:HG21	1.92	0.51
1:A:150:VAL:HA	1:A:198:GLN:O	2.11	0.51
1:A:94:GLU:HG2	1:A:100:VAL:HG22	1.93	0.50
1:A:49:ILE:O	1:A:57:PRO:HD2	2.11	0.50
1:A:171:GLN:HG2	1:B:164:GLU:HG3	1.94	0.50
1:B:134:ALA:HB3	1:B:184:LEU:O	2.11	0.50
1:A:53:VAL:HG13	1:A:68:LYS:HB2	1.94	0.50
1:B:63:ARG:NH2	1:B:84:ASP:OD1	2.44	0.50
1:B:173:ASN:ND2	1:B:175:LYS:NZ	2.60	0.50
1:A:181:TYR:CD2	1:B:139:LEU:HD11	2.47	0.49
1:B:196:SER:OG	1:B:209:THR:HG22	2.11	0.49
2:P:1:DPN:CD1	2:P:1:DPN:C	2.91	0.49
1:A:81:GLN:OE1	1:A:84:ASP:OD2	2.31	0.49
1:A:4:LEU:HD23	1:A:22:CYS:SG	2.53	0.49
1:B:8:PRO:HG3	1:B:149:THR:HB	1.95	0.48
1:A:36:SER:O	1:A:90:CYS:HA	2.13	0.48
1:A:15:GLY:H	1:A:80:LEU:HB2	1.78	0.48
1:B:164:GLU:O	1:B:180:SER:HA	2.13	0.48
1:B:17:SER:HA	1:B:77:VAL:O	2.14	0.48
1:A:131:ALA:O	1:A:132:ASN:CB	2.53	0.48
1:A:114:LYS:HB2	1:A:114:LYS:NZ	2.29	0.48
1:A:149:THR:O	1:A:199:VAL:HA	2.13	0.48
1:A:114:LYS:HB2	1:A:114:LYS:HZ3	1.79	0.48
1:B:34:TYR:CD2	1:B:93:TYR:HD2	2.31	0.48
1:A:112:GLN:CD	1:A:174:ASN:HD21	2.21	0.48
1:A:151:ALA:HB3	1:A:198:GLN:HB3	1.96	0.48
1:A:124:PRO:HD3	1:A:136:LEU:HD22	1.97	0.47
1:A:169:SER:O	1:A:176:TYR:HA	2.14	0.47
1:A:171:GLN:C	1:A:173:ASN:H	2.23	0.47
1:A:186:PRO:O	1:A:189:TRP:HB3	2.15	0.47
1:A:54:ASN:C	1:A:54:ASN:ND2	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:HIS:CB	2:P:4:DPR:HD2	2.44	0.47
1:B:12:GLY:O	1:B:109:VAL:HA	2.15	0.46
1:B:39:GLN:O	1:B:39:GLN:HG3	2.15	0.46
1:A:167:LYS:HB3	1:A:168:PRO:CD	2.45	0.46
1:A:14:LEU:HD13	1:A:109:VAL:CG1	2.46	0.46
1:A:28:ASP:HB3	1:A:94:GLU:HB3	1.96	0.46
1:B:125:SER:OG	1:B:128:GLU:HG3	2.15	0.46
1:B:173:ASN:HD22	1:B:175:LYS:NZ	2.14	0.46
1:A:33:ASN:HA	1:A:68:LYS:NZ	2.30	0.46
1:A:60:VAL:HA	1:A:61:PRO:HD3	1.72	0.46
1:B:65:SER:O	1:B:75:LEU:HA	2.16	0.46
1:A:66:GLY:HA2	1:A:74:SER:O	2.16	0.46
1:B:32:TYR:OH	1:B:93:TYR:HB3	2.16	0.45
1:B:82:ALA:C	1:B:84:ASP:H	2.24	0.45
1:B:153:LYS:HZ2	1:B:198:GLN:CB	2.28	0.45
1:A:126:SER:CA	1:A:129:LEU:HD12	2.44	0.45
1:A:114:LYS:O	1:A:114:LYS:HG3	2.16	0.45
1:B:153:LYS:HZ1	1:B:207:GLU:HG3	1.82	0.45
1:A:49:ILE:HD11	1:A:75:LEU:HD21	1.98	0.45
1:B:85:GLU:O	1:B:86:ALA:HB2	2.16	0.45
1:A:91:SER:HA	1:A:100:VAL:O	2.17	0.45
2:P:2:BAL:O	2:P:3:HIS:CG	2.70	0.45
1:A:56:ARG:NH1	1:A:64:PHE:O	2.46	0.45
1:B:36:SER:CB	2:P:1:DPN:HD2	2.46	0.45
1:B:153:LYS:HZ1	1:B:207:GLU:CG	2.29	0.44
1:A:189:TRP:CZ2	1:A:212:PRO:HG3	2.53	0.44
1:B:124:PRO:HG2	1:B:189:TRP:NE1	2.32	0.44
1:A:14:LEU:HD13	1:A:109:VAL:HG11	1.99	0.44
1:B:170:LYS:HD2	1:B:176:TYR:CZ	2.53	0.44
1:B:211:ALA:HA	1:B:212:PRO:HD3	1.86	0.44
1:B:61:PRO:C	1:B:63:ARG:H	2.25	0.44
1:A:20:ILE:HD12	1:A:20:ILE:N	2.33	0.44
1:A:112:GLN:NE2	1:A:174:ASN:HD21	2.15	0.44
1:B:8:PRO:HG3	1:B:149:THR:CB	2.48	0.44
1:B:28:ASP:OD2	1:B:94:GLU:HB2	2.18	0.44
1:A:37:TRP:CE2	1:A:75:LEU:HB2	2.53	0.43
1:A:94:GLU:CD	1:A:100:VAL:HG22	2.43	0.43
1:A:115:ALA:CB	1:A:175:LYS:HZ3	2.31	0.43
1:A:116:ASN:HA	1:A:117:PRO:HD3	1.93	0.43
1:A:117:PRO:HB2	1:A:140:ILE:CG2	2.49	0.43
1:B:34:TYR:OH	2:P:3:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ALA:HA	1:A:100:VAL:CG1	2.48	0.43
1:A:57:PRO:HB3	1:B:97:ASP:OD1	2.19	0.43
1:B:3:ALA:HB3	1:B:100:VAL:HG11	2.00	0.43
1:B:128:GLU:O	1:B:131:ALA:HB3	2.19	0.43
1:B:28:ASP:HB3	1:B:94:GLU:HA	2.01	0.43
1:B:160:LYS:HD3	1:B:161:ALA:N	2.33	0.43
1:B:32:TYR:HE2	1:B:92:SER:HG	1.67	0.43
1:A:112:GLN:HA	1:A:113:PRO:HD3	1.76	0.42
1:A:115:ALA:HB2	1:A:175:LYS:NZ	2.34	0.42
1:A:19:THR:HG22	1:A:74:SER:HB3	2.00	0.42
1:A:41:HIS:O	1:A:42:ALA:C	2.63	0.42
1:A:215:CYS:SG	1:B:215:CYS:C	3.02	0.42
1:A:80:LEU:HD22	1:A:109:VAL:CG2	2.49	0.42
1:A:122:PHE:HB2	1:A:137:VAL:CG1	2.50	0.42
1:B:38:TYR:O	1:B:88:TYR:HA	2.19	0.42
1:A:146:GLY:O	1:A:168:PRO:HG2	2.20	0.42
1:A:115:ALA:CB	1:A:175:LYS:NZ	2.83	0.42
1:A:128:GLU:CD	1:A:135:THR:H	2.28	0.42
1:A:137:VAL:HG21	1:B:137:VAL:HG11	2.02	0.42
1:B:25:THR:HB	1:B:26:SER:H	1.61	0.41
1:A:49:ILE:HA	1:A:60:VAL:HG21	2.01	0.41
1:A:57:PRO:HB2	1:A:60:VAL:HG23	2.01	0.41
1:B:45:ALA:HB1	1:B:46:PRO:HD2	2.02	0.41
1:A:82:ALA:HB1	1:A:174:ASN:CG	2.45	0.41
1:B:33:ASN:O	1:B:53:VAL:HG23	2.20	0.41
1:B:61:PRO:C	1:B:63:ARG:N	2.78	0.41
1:A:34:TYR:O	1:A:92:SER:HA	2.21	0.41
1:A:215:CYS:SG	1:B:216:SER:N	2.94	0.41
1:B:91:SER:HA	1:B:100:VAL:O	2.20	0.41
1:B:22:CYS:HB3	1:B:73:ALA:HB3	2.02	0.41
1:B:94:GLU:HB3	1:B:98:ASN:OD1	2.21	0.41
1:B:7:PRO:HA	1:B:8:PRO:HD2	1.85	0.41
1:B:51:TYR:O	1:B:52:GLU:C	2.64	0.41
1:A:83:GLU:O	1:A:83:GLU:HG3	2.22	0.40
1:B:122:PHE:HA	1:B:123:PRO:HD3	1.87	0.40
1:A:4:LEU:HD13	1:A:100:VAL:HB	2.03	0.40
1:B:41:HIS:CD2	1:B:44:LYS:HE3	2.57	0.40
1:B:213:THR:O	1:B:214:GLU:HB2	2.21	0.40
1:B:57:PRO:O	1:B:60:VAL:HG23	2.21	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	A	214/216 (99%)	176 (82%)	27 (13%)	11 (5%)	1	1
1	B	214/216 (99%)	183 (86%)	23 (11%)	8 (4%)	2	2
2	P	1/6 (17%)	1 (100%)	0	0	100	100
All	All	429/438 (98%)	360 (84%)	50 (12%)	19 (4%)	2	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	155	ASP
1	B	25	THR
1	B	42	ALA
1	B	70	GLY
1	A	53	VAL
1	A	132	ASN
1	B	2	SER
1	B	214	GLU
1	B	215	CYS
1	A	14	LEU
1	A	172	SER
1	A	42	ALA
1	A	187	GLU
1	A	83	GLU
1	A	212	PRO
1	B	30	GLY
1	B	146	GLY
1	A	30	GLY

### 5.3.2 Protein sidechains [i](#)

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%)	137 (76%)	44 (24%)	1	1
1	B	181/181 (100%)	136 (75%)	45 (25%)	0	0
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	363/363 (100%)	274 (76%)	89 (24%)	1	1

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	11	SER
1	A	13	SER
1	A	14	LEU
1	A	17	SER
1	A	21	SER
1	A	22	CYS
1	A	23	THR
1	A	32	TYR
1	A	36	SER
1	A	44	LYS
1	A	50	ILE
1	A	51	TYR
1	A	52	GLU
1	A	58	SER
1	A	63	ARG
1	A	77	VAL
1	A	83	GLU
1	A	91	SER
1	A	92	SER
1	A	100	VAL
1	A	112	GLN
1	A	114	LYS
1	A	118	THR
1	A	120	THR
1	A	125	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	126	SER
1	A	127	GLU
1	A	132	ASN
1	A	133	LYS
1	A	135	THR
1	A	136	LEU
1	A	139	LEU
1	A	140	ILE
1	A	148	VAL
1	A	160	LYS
1	A	164	GLU
1	A	172	SER
1	A	173	ASN
1	A	183	SER
1	A	194	SER
1	A	198	GLN
1	A	204	SER
1	A	216	SER
1	B	13	SER
1	B	14	LEU
1	B	18	VAL
1	B	21	SER
1	B	23	THR
1	B	26	SER
1	B	27	SER
1	B	28	ASP
1	B	29	VAL
1	B	35	VAL
1	B	39	GLN
1	B	44	LYS
1	B	47	LYS
1	B	54	ASN
1	B	58	SER
1	B	65	SER
1	B	67	SER
1	B	72	THR
1	B	76	THR
1	B	78	SER
1	B	90	CYS
1	B	91	SER
1	B	92	SER
1	B	94	GLU

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Mol	Chain	Res	Type
1	B	97	ASP
1	B	103	THR
1	B	121	LEU
1	B	136	LEU
1	B	138	CYS
1	B	142	ASP
1	B	143	PHE
1	B	153	LYS
1	B	159	VAL
1	B	160	LYS
1	B	166	THR
1	B	167	LYS
1	B	184	LEU
1	B	187	GLU
1	B	188	GLN
1	B	193	ARG
1	B	196	SER
1	B	199	VAL
1	B	210	VAL
1	B	214	GLU
1	B	215	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	112	GLN
1	A	171	GLN
1	A	173	ASN
1	A	174	ASN
1	B	54	ASN
1	B	112	GLN
1	B	116	ASN
1	B	132	ASN
2	P	3	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	2	2	3,4,5	0.30	0	3,3,5	3.34	2 (66%)

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	2	2	-	0/1/2/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	P	2	BAL	CB-CA-C	-5.33	101.33	111.60
2	P	2	BAL	CA-CB-N	2.17	129.95	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	2	BAL	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

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.