



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 1MCE / pdb_00001mce
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

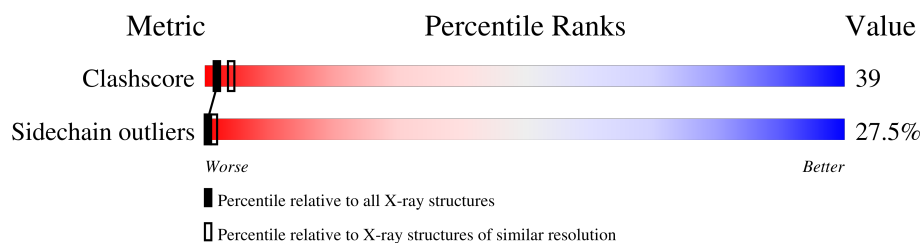
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

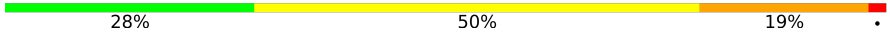
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
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	
1	B	216	
2	P	6	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3256 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-OH.

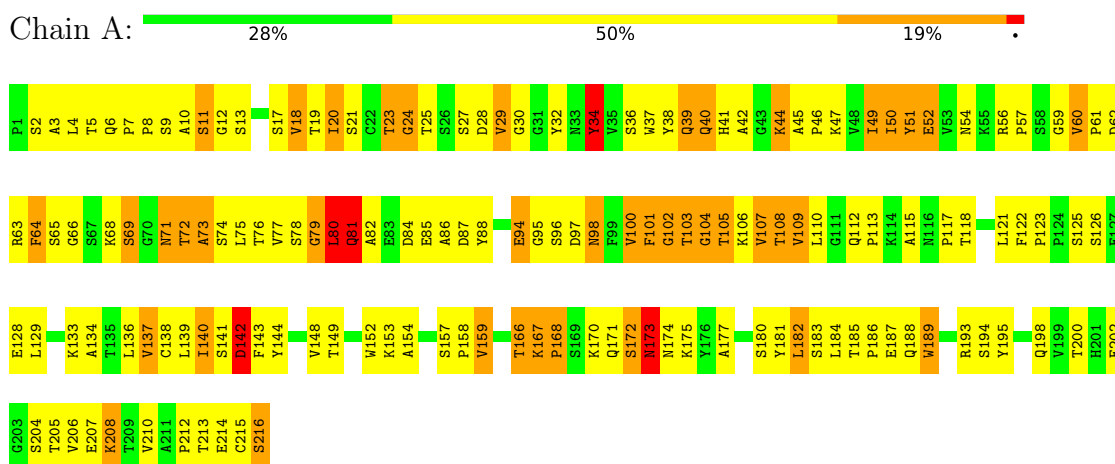
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			46	30	8	8			

3 Residue-property plots

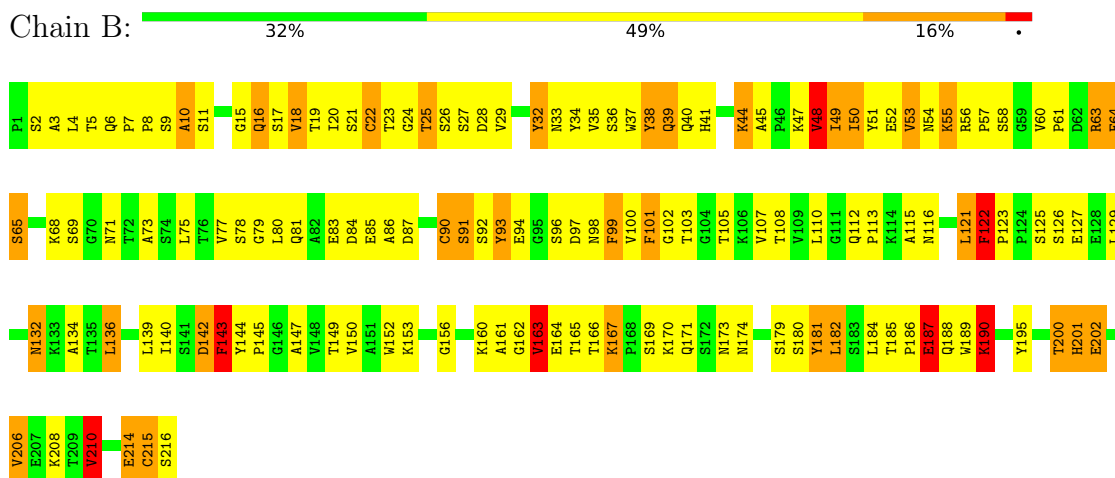
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

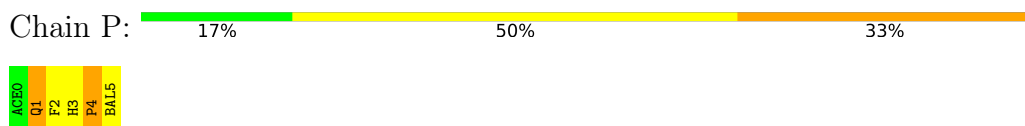
- Molecule 1: Immunoglobulin lambda-1 light chain



- Molecule 1: Immunoglobulin lambda-1 light chain



- Molecule 2: PEPTIDE N-ACETYL-L-GLN-D-PHE-L-HIS-D-PRO-B-ALA-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}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3256	wwPDB-VP
Average B, all atoms (Å ²)	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: BAL, DPN, DPR, 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	1.07	1/1644 (0.1%)	1.86	32/2241 (1.4%)
1	B	1.03	0/1644	1.82	32/2241 (1.4%)
2	P	1.24	0/19	2.02	0/23
All	All	1.05	1/3307 (0.0%)	1.84	64/4505 (1.4%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	GLY	N-CA	6.07	1.51	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ASN	CA-CB-CG	12.56	125.17	112.60
1	B	64	PHE	CA-CB-CG	11.85	125.65	113.80
1	A	98	ASN	CA-CB-CG	9.82	122.42	112.60
1	B	122	PHE	CA-CB-CG	9.41	123.21	113.80
1	B	87	ASP	CA-CB-CG	9.16	121.77	112.60
1	A	34	TYR	CA-CB-CG	8.78	129.70	113.90
1	B	25	THR	N-CA-C	8.70	121.31	108.60
1	A	173	ASN	CA-CB-CG	8.52	121.12	112.60
1	B	93	TYR	CA-CB-CG	8.14	128.55	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	THR	CA-C-N	-7.21	116.61	122.16
1	A	23	THR	C-N-CA	-7.21	116.61	122.16
1	B	202	GLU	CB-CG-CD	7.18	124.81	112.60
1	A	142	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	104	GLY	CA-C-N	7.06	135.02	121.54
1	A	104	GLY	C-N-CA	7.06	135.02	121.54
1	A	64	PHE	CA-CB-CG	7.02	120.82	113.80
1	A	214	GLU	N-CA-C	6.97	125.65	110.80
1	B	143	PHE	CA-CB-CG	6.93	120.73	113.80
1	B	142	ASP	N-CA-C	6.63	123.80	113.72
1	A	30	GLY	N-CA-C	-6.62	101.25	111.64
1	B	55	LYS	N-CA-C	6.47	119.50	109.07
1	A	102	GLY	N-CA-C	-6.37	102.77	112.51
1	B	202	GLU	CA-CB-CG	6.34	126.79	114.10
1	A	105	THR	N-CA-C	6.30	124.22	110.80
1	B	84	ASP	N-CA-C	-6.29	105.65	113.38
1	A	81	GLN	OE1-CD-NE2	-6.20	116.41	122.60
1	A	80	LEU	CB-CA-C	6.16	120.74	110.88
1	A	79	GLY	N-CA-C	-5.88	99.24	113.18
1	A	213	THR	CA-C-N	5.88	132.76	121.54
1	A	213	THR	C-N-CA	5.88	132.76	121.54
1	B	210	VAL	CB-CA-C	5.81	119.27	110.62
1	A	28	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	60	VAL	CA-C-O	5.72	122.92	119.94
1	A	181	TYR	CA-CB-CG	5.63	124.03	113.90
1	B	189	TRP	CA-CB-CG	5.60	124.23	113.60
1	A	140	ILE	CB-CA-C	5.57	117.94	110.42
1	A	94	GLU	CA-CB-CG	5.54	125.19	114.10
1	B	201	HIS	CA-CB-CG	5.53	119.33	113.80
1	B	190	LYS	CA-CB-CG	5.47	125.04	114.10
1	B	28	ASP	N-CA-CB	5.46	118.22	110.46
1	A	73	ALA	N-CA-C	-5.45	101.48	109.81
1	A	101	PHE	CA-CB-CG	-5.42	108.38	113.80
1	B	187	GLU	CA-CB-CG	5.34	124.78	114.10
1	B	16	GLN	CA-C-O	5.34	127.21	121.55
1	A	100	VAL	CB-CA-C	5.32	118.54	110.62
1	B	10	ALA	N-CA-C	-5.31	100.03	109.06
1	B	48	VAL	CB-CA-C	5.29	118.72	111.31
1	B	25	THR	CA-C-O	5.27	126.97	121.38
1	B	84	ASP	O-C-N	5.27	129.33	122.42
1	A	50	ILE	CA-C-O	-5.24	114.23	120.78
1	A	51	TYR	CA-CB-CG	5.24	123.33	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASN	CA-C-O	5.20	123.93	119.66
1	B	81	GLN	CA-C-N	5.19	127.49	120.38
1	B	81	GLN	C-N-CA	5.19	127.49	120.38
1	B	163	VAL	CA-C-O	-5.16	116.62	120.96
1	B	181	TYR	O-C-N	5.14	129.38	123.17
1	B	39	GLN	CA-CB-CG	5.09	124.28	114.10
1	B	122	PHE	O-C-N	5.08	125.91	121.39
1	A	81	GLN	N-CA-C	-5.08	103.00	110.52
1	B	84	ASP	CA-C-N	-5.08	113.84	120.95
1	B	84	ASP	C-N-CA	-5.08	113.84	120.95
1	A	52	GLU	CA-CB-CG	5.06	124.22	114.10
1	A	168	PRO	N-CA-C	5.06	118.82	111.03
1	A	71	ASN	O-C-N	5.04	128.64	122.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	4	DPR	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	136	0
1	B	1605	0	1540	123	0
2	P	46	0	37	10	0
All	All	3256	0	3117	251	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 39.

All (251) 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:2:SER:HA	1:B:100:VAL:HG13	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:HB	1:B:53:VAL:HG12	1.53	0.90
1:A:6:GLN:HB3	1:A:104:GLY:H	1.33	0.89
1:B:94:GLU:HB3	1:B:98:ASN:HB3	1.59	0.85
1:A:3:ALA:HB1	1:A:103:THR:OG1	1.81	0.80
1:B:10:ALA:O	1:B:107:VAL:HA	1.81	0.80
1:B:149:THR:HB	1:B:200:THR:HG23	1.62	0.80
1:A:69:SER:O	1:A:72:THR:HG22	1.82	0.79
1:A:57:PRO:HB3	1:B:99:PHE:HE1	1.47	0.79
1:A:57:PRO:HD2	1:A:60:VAL:HG21	1.64	0.79
1:A:166:THR:HG22	1:B:169:SER:HB2	1.64	0.79
1:A:20:ILE:O	1:A:74:SER:HA	1.83	0.79
1:A:122:PHE:HB2	1:A:137:VAL:HG12	1.65	0.78
1:B:38:TYR:HE1	1:B:91:SER:HB2	1.49	0.78
1:A:85:GLU:HA	1:A:107:VAL:O	1.84	0.77
1:A:115:ALA:HB3	1:A:144:TYR:H	1.49	0.75
1:A:94:GLU:HB3	1:A:98:ASN:HB2	1.67	0.75
1:A:12:GLY:HA3	1:A:80:LEU:HD23	1.69	0.74
1:A:11:SER:HA	1:A:108:THR:O	1.87	0.74
1:B:32:TYR:HE2	1:B:93:TYR:HD2	1.36	0.74
1:B:214:GLU:O	1:B:215:CYS:HB3	1.89	0.71
1:B:136:LEU:HD13	1:B:182:LEU:HB3	1.72	0.71
1:A:65:SER:O	1:A:75:LEU:HD12	1.93	0.69
1:A:152:TRP:HE1	1:A:180:SER:HB3	1.57	0.69
1:A:171:GLN:HB2	1:B:164:GLU:HG3	1.75	0.69
1:B:186:PRO:O	1:B:190:LYS:HB3	1.94	0.68
1:B:56:ARG:HD2	1:B:60:VAL:HG12	1.76	0.68
1:A:63:ARG:HB2	1:A:78:SER:O	1.95	0.67
1:A:122:PHE:O	1:A:136:LEU:HD12	1.93	0.67
1:B:153:LYS:HD2	1:B:156:GLY:O	1.95	0.67
1:B:166:THR:HG22	1:B:167:LYS:O	1.94	0.66
1:B:134:ALA:HB3	1:B:184:LEU:C	2.22	0.65
2:P:1:GLN:HE21	2:P:2:DPN:HB3	1.61	0.65
1:B:9:SER:HB2	1:B:147:ALA:HB3	1.77	0.65
1:B:47:LYS:HD2	1:B:49:ILE:HD12	1.79	0.65
1:A:54:ASN:HB2	1:A:66:GLY:O	1.97	0.64
1:A:86:ALA:O	1:A:106:LYS:HA	1.98	0.64
1:B:38:TYR:CE1	1:B:91:SER:HB2	2.31	0.64
1:B:134:ALA:HB3	1:B:184:LEU:O	1.98	0.64
1:B:49:ILE:HG13	1:B:60:VAL:HG13	1.80	0.63
1:B:143:PHE:HD1	1:B:143:PHE:H	1.46	0.63
1:A:19:THR:HA	1:A:75:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:C	1:A:173:ASN:H	2.06	0.63
1:A:12:GLY:HA3	1:A:80:LEU:CD2	2.28	0.62
1:A:17:SER:HA	1:A:77:VAL:O	1.98	0.62
1:A:5:THR:HB	1:A:23:THR:HB	1.80	0.62
1:B:121:LEU:HD13	1:B:210:VAL:HB	1.81	0.62
1:A:138:CYS:HB2	1:A:152:TRP:CZ2	2.36	0.61
1:B:4:LEU:HA	1:B:23:THR:O	2.01	0.61
1:A:115:ALA:HB3	1:A:144:TYR:N	2.15	0.61
1:B:18:VAL:HG12	1:B:80:LEU:HG	1.84	0.60
1:A:117:PRO:HB3	1:A:143:PHE:HB3	1.82	0.60
1:B:15:GLY:O	1:B:79:GLY:HA2	2.02	0.60
1:A:34:TYR:HD2	2:P:3:HIS:ND1	2.00	0.60
1:A:82:ALA:HA	1:A:109:VAL:HG21	1.84	0.60
1:B:49:ILE:HG13	1:B:60:VAL:CG1	2.32	0.59
1:A:25:THR:HA	1:A:71:ASN:ND2	2.17	0.59
1:B:23:THR:HA	1:B:71:ASN:O	2.02	0.59
1:B:32:TYR:HE2	1:B:93:TYR:CD2	2.21	0.59
1:A:46:PRO:HD2	1:B:101:PHE:HE2	1.68	0.58
1:B:163:VAL:HG23	1:B:181:TYR:O	2.02	0.58
1:A:84:ASP:O	1:A:85:GLU:C	2.45	0.58
1:A:101:PHE:HE2	1:B:48:VAL:HG12	1.68	0.58
1:B:3:ALA:O	1:B:24:GLY:HA2	2.02	0.58
1:B:68:LYS:HD2	1:B:69:SER:N	2.17	0.58
1:B:34:TYR:HE1	2:P:2:DPN:HA	1.68	0.58
1:A:125:SER:O	1:A:129:LEU:HB2	2.04	0.58
1:A:82:ALA:C	1:A:84:ASP:H	2.12	0.58
1:A:136:LEU:HD11	1:A:210:VAL:HG11	1.85	0.57
1:A:13:SER:H	1:A:80:LEU:HD23	1.69	0.57
1:B:17:SER:HA	1:B:77:VAL:O	2.05	0.57
1:A:57:PRO:O	1:A:59:GLY:N	2.34	0.56
1:A:173:ASN:C	1:A:175:LYS:H	2.12	0.56
1:B:39:GLN:HG2	1:B:49:ILE:HD13	1.87	0.56
1:A:10:ALA:HB1	1:A:18:VAL:HG21	1.88	0.56
1:A:12:GLY:O	1:A:13:SER:HB3	2.04	0.56
1:A:142:ASP:O	1:A:175:LYS:HD2	2.06	0.56
1:B:8:PRO:O	1:B:105:THR:HA	2.05	0.56
1:A:122:PHE:HB3	1:B:122:PHE:HD2	1.70	0.56
1:A:37:TRP:O	1:A:49:ILE:HG13	2.06	0.55
1:A:6:GLN:HB3	1:A:104:GLY:N	2.15	0.55
1:A:128:GLU:HG3	1:A:133:LYS:O	2.07	0.55
1:A:79:GLY:O	1:A:81:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LYS:NZ	1:B:174:ASN:ND2	2.55	0.55
1:A:68:LYS:HA	1:A:73:ALA:HA	1.89	0.55
1:B:61:PRO:HG2	1:B:64:PHE:CD1	2.42	0.55
1:B:184:LEU:HD11	1:B:195:TYR:CE1	2.41	0.55
1:A:215:CYS:SG	1:B:214:GLU:O	2.64	0.54
1:B:52:GLU:OE1	1:B:55:LYS:HE3	2.06	0.54
1:B:44:LYS:HG2	1:B:45:ALA:O	2.07	0.54
1:B:170:LYS:HZ1	1:B:174:ASN:ND2	2.06	0.54
1:A:46:PRO:HD2	1:B:101:PHE:CE2	2.42	0.54
1:A:57:PRO:HB3	1:B:99:PHE:CE1	2.37	0.54
1:A:121:LEU:HD21	1:A:210:VAL:HG12	1.90	0.54
1:A:87:ASP:OD2	1:A:106:LYS:HG3	2.08	0.53
1:B:57:PRO:HD2	1:B:60:VAL:HG21	1.90	0.53
1:A:60:VAL:HG12	1:A:64:PHE:HD2	1.73	0.53
1:A:95:GLY:O	1:A:97:ASP:N	2.42	0.53
1:A:139:LEU:C	1:A:140:ILE:HG13	2.34	0.53
1:B:170:LYS:HZ1	1:B:174:ASN:HD21	1.57	0.53
1:B:112:GLN:HB3	1:B:113:PRO:HD2	1.89	0.53
1:B:112:GLN:HB3	1:B:113:PRO:CD	2.39	0.52
1:B:162:GLY:O	1:B:182:LEU:HD23	2.08	0.52
1:A:62:ASP:OD1	1:A:79:GLY:HA3	2.10	0.51
1:A:140:ILE:HG22	1:A:143:PHE:CD1	2.46	0.51
1:A:198:GLN:HG3	1:A:206:VAL:O	2.10	0.51
1:A:153:LYS:O	1:A:195:TYR:HD1	1.93	0.51
1:B:164:GLU:O	1:B:180:SER:HA	2.11	0.51
2:P:1:GLN:NE2	2:P:2:DPN:HB3	2.25	0.51
1:B:187:GLU:O	1:B:190:LYS:HE2	2.11	0.51
1:B:48:VAL:HG21	2:P:2:DPN:HE2	1.93	0.51
1:A:66:GLY:HA2	1:A:74:SER:O	2.11	0.50
1:A:84:ASP:O	1:A:86:ALA:HB2	2.11	0.50
1:A:173:ASN:N	1:A:173:ASN:HD22	2.10	0.50
1:B:161:ALA:O	1:B:163:VAL:HG12	2.11	0.50
2:P:1:GLN:HB2	2:P:3:HIS:CD2	2.47	0.50
1:A:46:PRO:O	1:A:47:LYS:HE2	2.11	0.50
1:A:62:ASP:CG	1:A:63:ARG:H	2.20	0.50
1:A:154:ALA:HA	1:A:195:TYR:CD1	2.47	0.50
1:B:34:TYR:OH	2:P:3:HIS:HA	2.12	0.49
1:B:56:ARG:HB3	1:B:60:VAL:HB	1.94	0.49
1:B:171:GLN:C	1:B:173:ASN:H	2.21	0.49
1:B:56:ARG:HD2	1:B:60:VAL:CG1	2.42	0.49
1:B:165:THR:HA	1:B:179:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:O	1:B:188:GLN:N	2.45	0.49
1:A:140:ILE:HG22	1:A:143:PHE:CE1	2.48	0.49
1:A:21:SER:HA	1:A:73:ALA:O	2.12	0.49
1:B:49:ILE:O	1:B:60:VAL:HG11	2.13	0.49
1:B:184:LEU:HD11	1:B:195:TYR:CZ	2.47	0.49
1:B:144:TYR:CD1	1:B:145:PRO:HA	2.48	0.48
1:A:4:LEU:HD13	1:A:100:VAL:HG22	1.95	0.48
1:B:185:THR:O	1:B:187:GLU:N	2.46	0.48
1:A:115:ALA:HB2	1:A:175:LYS:NZ	2.29	0.48
1:B:20:ILE:HG23	1:B:105:THR:HG21	1.95	0.48
1:B:201:HIS:O	1:B:202:GLU:C	2.57	0.48
1:B:35:VAL:HG11	1:B:73:ALA:CB	2.43	0.48
1:B:115:ALA:O	1:B:143:PHE:HA	2.13	0.48
1:B:11:SER:HB3	1:B:110:LEU:HD21	1.96	0.48
1:A:134:ALA:O	1:A:184:LEU:O	2.32	0.48
1:A:167:LYS:HA	1:A:167:LYS:NZ	2.28	0.48
1:A:57:PRO:HD2	1:A:60:VAL:CG2	2.42	0.48
1:B:10:ALA:HB3	1:B:107:VAL:HG22	1.94	0.48
1:A:215:CYS:SG	1:A:216:SER:N	2.87	0.47
1:B:32:TYR:HD2	1:B:93:TYR:O	1.97	0.47
1:A:82:ALA:O	1:A:84:ASP:N	2.47	0.47
1:A:171:GLN:NE2	1:A:177:ALA:HB2	2.30	0.47
1:B:52:GLU:O	1:B:54:ASN:N	2.47	0.47
1:B:215:CYS:SG	1:B:216:SER:N	2.87	0.47
1:A:153:LYS:O	1:A:195:TYR:CD1	2.67	0.47
1:A:184:LEU:HD22	1:A:188:GLN:HB3	1.95	0.47
1:A:38:TYR:O	1:A:49:ILE:HD11	2.14	0.47
1:A:44:LYS:HE2	1:A:45:ALA:O	2.15	0.47
1:A:65:SER:O	1:A:75:LEU:HA	2.14	0.47
1:A:117:PRO:CB	1:A:143:PHE:HB3	2.44	0.47
1:A:121:LEU:CB	1:A:208:LYS:HG3	2.44	0.47
1:A:123:PRO:HA	1:A:136:LEU:CD1	2.45	0.47
1:B:52:GLU:HB2	1:B:55:LYS:HD3	1.96	0.47
1:A:117:PRO:HB2	1:A:140:ILE:HG23	1.97	0.47
1:B:140:ILE:HG22	1:B:143:PHE:CE1	2.50	0.47
2:P:3:HIS:HA	2:P:4:DPR:HD2	1.88	0.47
1:A:36:SER:HA	1:A:51:TYR:HA	1.98	0.46
1:B:4:LEU:O	1:B:102:GLY:HA2	2.14	0.46
1:A:57:PRO:CB	1:B:99:PHE:HE1	2.24	0.46
1:B:85:GLU:HG3	1:B:108:THR:HA	1.97	0.46
1:A:158:PRO:O	1:A:159:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLN:HB2	1:B:173:ASN:OD1	2.15	0.46
1:A:144:TYR:HD1	1:A:174:ASN:O	1.98	0.46
1:B:65:SER:O	1:B:75:LEU:HD12	2.15	0.46
1:B:171:GLN:NE2	1:B:173:ASN:OD1	2.49	0.46
1:B:152:TRP:CE3	1:B:182:LEU:HD12	2.51	0.45
1:B:57:PRO:HG2	1:B:60:VAL:HG21	1.98	0.45
1:A:38:TYR:HA	1:A:47:LYS:O	2.16	0.45
1:A:51:TYR:CD1	1:B:99:PHE:HZ	2.35	0.45
1:B:32:TYR:CD2	1:B:93:TYR:O	2.69	0.45
1:A:171:GLN:C	1:A:173:ASN:N	2.75	0.45
1:A:40:GLN:NE2	1:A:44:LYS:O	2.49	0.45
1:A:171:GLN:HG3	1:A:172:SER:N	2.32	0.45
1:B:214:GLU:O	1:B:215:CYS:CB	2.63	0.45
1:A:41:HIS:O	1:A:42:ALA:C	2.60	0.44
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.69	0.44
1:B:214:GLU:OE2	1:B:216:SER:HA	2.17	0.44
1:B:187:GLU:HA	1:B:190:LYS:HD3	2.00	0.44
1:A:79:GLY:O	1:A:81:GLN:HG3	2.18	0.44
1:A:144:TYR:HE1	1:A:174:ASN:ND2	2.15	0.44
1:B:26:SER:HB3	1:B:27:SER:H	1.56	0.44
1:B:37:TRP:HB2	1:B:50:ILE:HG22	2.00	0.44
1:B:123:PRO:HD3	1:B:210:VAL:HG21	2.00	0.44
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.84	0.44
1:B:96:SER:O	1:B:98:ASN:N	2.50	0.44
1:A:40:GLN:O	1:A:40:GLN:HG3	2.17	0.44
1:A:117:PRO:HB3	1:A:143:PHE:CD1	2.53	0.44
1:A:144:TYR:CD1	1:A:174:ASN:O	2.70	0.44
1:A:118:THR:HG23	1:A:142:ASP:OD2	2.17	0.44
1:A:153:LYS:HA	1:A:158:PRO:O	2.18	0.43
1:B:40:GLN:HA	1:B:44:LYS:HD3	1.99	0.43
1:B:123:PRO:HB3	1:B:210:VAL:HG11	2.00	0.43
1:B:19:THR:C	1:B:20:ILE:HG13	2.43	0.43
1:A:13:SER:HA	1:A:110:LEU:O	2.19	0.43
1:B:61:PRO:C	1:B:63:ARG:H	2.25	0.43
1:A:19:THR:HG22	1:A:74:SER:OG	2.18	0.43
1:A:82:ALA:C	1:A:84:ASP:N	2.76	0.43
1:A:121:LEU:HD12	1:A:137:VAL:O	2.18	0.43
1:B:35:VAL:HA	1:B:91:SER:O	2.18	0.43
1:B:206:VAL:HG11	1:B:208:LYS:HZ2	1.83	0.43
1:A:173:ASN:C	1:A:175:LYS:N	2.77	0.43
1:B:6:GLN:HG3	1:B:90:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TRP:HB2	1:B:50:ILE:CG2	2.48	0.43
1:B:51:TYR:O	1:B:55:LYS:HB2	2.19	0.43
1:A:137:VAL:HA	1:A:180:SER:O	2.19	0.43
1:A:189:TRP:CH2	1:A:212:PRO:HA	2.53	0.43
1:A:7:PRO:HA	1:A:8:PRO:HD3	1.75	0.42
1:A:171:GLN:HB2	1:B:164:GLU:CG	2.47	0.42
1:A:184:LEU:HD22	1:A:188:GLN:CB	2.48	0.42
1:B:68:LYS:HD2	1:B:69:SER:H	1.84	0.42
1:A:112:GLN:HA	1:A:113:PRO:HD3	1.68	0.42
1:B:99:PHE:N	1:B:99:PHE:CD1	2.87	0.42
1:B:18:VAL:CG1	1:B:80:LEU:HG	2.49	0.42
1:B:50:ILE:HG23	1:B:51:TYR:N	2.34	0.42
1:B:125:SER:O	1:B:129:LEU:HG	2.19	0.42
1:A:171:GLN:HG3	1:A:172:SER:H	1.84	0.42
1:A:61:PRO:HB2	1:A:64:PHE:CE2	2.54	0.42
1:A:87:ASP:CG	1:A:106:LYS:HG3	2.44	0.42
1:A:3:ALA:HB1	1:A:103:THR:CB	2.49	0.42
1:B:126:SER:O	1:B:129:LEU:HB2	2.20	0.42
1:A:38:TYR:C	1:A:49:ILE:HD11	2.45	0.42
1:A:39:GLN:HG2	1:A:88:TYR:CE2	2.54	0.42
1:B:167:LYS:NZ	1:B:167:LYS:HB3	2.35	0.41
1:A:44:LYS:O	1:A:46:PRO:HD3	2.19	0.41
1:B:150:VAL:HG11	1:B:180:SER:CB	2.50	0.41
1:B:152:TRP:CD1	1:B:163:VAL:HG21	2.56	0.41
1:A:24:GLY:N	1:A:29:VAL:HG21	2.36	0.41
1:B:9:SER:CB	1:B:147:ALA:HB3	2.48	0.41
1:B:34:TYR:OH	2:P:4:DPR:HD2	2.20	0.41
1:A:171:GLN:O	1:A:173:ASN:N	2.54	0.41
1:B:41:HIS:CD2	1:B:86:ALA:HB2	2.55	0.41
1:A:85:GLU:HA	1:A:107:VAL:HG12	2.03	0.41
1:A:171:GLN:HG3	1:A:172:SER:OG	2.21	0.41
1:A:208:LYS:HD3	1:A:208:LYS:HA	1.90	0.41
1:A:65:SER:HB2	1:A:76:THR:HB	2.02	0.41
1:A:121:LEU:HB3	1:A:208:LYS:HG3	2.03	0.41
1:A:167:LYS:HA	1:A:168:PRO:HD3	1.81	0.41
1:B:136:LEU:N	1:B:136:LEU:HD12	2.35	0.41
1:A:17:SER:OG	1:A:18:VAL:N	2.54	0.41
1:B:6:GLN:HG3	1:B:22:CYS:HB2	2.02	0.41
1:B:143:PHE:HB2	1:B:201:HIS:NE2	2.36	0.41
1:A:185:THR:HB	1:A:186:PRO:CD	2.52	0.40
1:B:7:PRO:HA	1:B:8:PRO:HD2	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.89	0.40
1:A:6:GLN:OE1	1:A:102:GLY:HA3	2.22	0.40
1:A:38:TYR:OH	2:P:1:GLN:CG	2.70	0.40
1:B:96:SER:C	1:B:98:ASN:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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%)	129 (71%)	52 (29%)	0	1
1	B	181/181 (100%)	134 (74%)	47 (26%)	0	2
2	P	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	364/364 (100%)	264 (72%)	100 (28%)	0	1

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	9	SER
1	A	11	SER
1	A	18	VAL
1	A	20	ILE
1	A	27	SER
1	A	29	VAL
1	A	32	TYR

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Mol	Chain	Res	Type
1	A	34	TYR
1	A	39	GLN
1	A	40	GLN
1	A	44	LYS
1	A	49	ILE
1	A	50	ILE
1	A	52	GLU
1	A	56	ARG
1	A	69	SER
1	A	72	THR
1	A	80	LEU
1	A	81	GLN
1	A	96	SER
1	A	103	THR
1	A	105	THR
1	A	107	VAL
1	A	108	THR
1	A	109	VAL
1	A	126	SER
1	A	137	VAL
1	A	141	SER
1	A	142	ASP
1	A	148	VAL
1	A	149	THR
1	A	157	SER
1	A	159	VAL
1	A	166	THR
1	A	167	LYS
1	A	170	LYS
1	A	172	SER
1	A	173	ASN
1	A	182	LEU
1	A	183	SER
1	A	187	GLU
1	A	189	TRP
1	A	193	ARG
1	A	194	SER
1	A	200	THR
1	A	202	GLU
1	A	204	SER
1	A	205	THR
1	A	207	GLU

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Mol	Chain	Res	Type
1	A	208	LYS
1	A	216	SER
1	B	5	THR
1	B	16	GLN
1	B	18	VAL
1	B	21	SER
1	B	22	CYS
1	B	25	THR
1	B	29	VAL
1	B	32	TYR
1	B	33	ASN
1	B	36	SER
1	B	38	TYR
1	B	44	LYS
1	B	48	VAL
1	B	49	ILE
1	B	50	ILE
1	B	53	VAL
1	B	58	SER
1	B	63	ARG
1	B	65	SER
1	B	78	SER
1	B	83	GLU
1	B	90	CYS
1	B	91	SER
1	B	92	SER
1	B	97	ASP
1	B	99	PHE
1	B	101	PHE
1	B	103	THR
1	B	121	LEU
1	B	122	PHE
1	B	127	GLU
1	B	132	ASN
1	B	136	LEU
1	B	139	LEU
1	B	142	ASP
1	B	143	PHE
1	B	160	LYS
1	B	163	VAL
1	B	167	LYS
1	B	182	LEU

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Mol	Chain	Res	Type
1	B	187	GLU
1	B	190	LYS
1	B	200	THR
1	B	206	VAL
1	B	210	VAL
1	B	214	GLU
1	B	215	CYS
2	P	1	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	16	GLN
1	A	40	GLN
1	A	132	ASN
1	A	171	GLN
1	A	173	ASN
1	B	39	GLN
1	B	40	GLN
1	B	41	HIS
1	B	171	GLN
1	B	174	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	5	2	5,5,5	1.06	0	5,5,5	2.40	1 (20%)

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	5	2	-	0/3/3/3	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	BAL	OXT-C-CA	-4.78	98.90	114.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.