



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:47 PM UTC

PDB ID : 1MCH / pdb_00001mch
Title : PRINCIPLES AND PITFALLS IN DESIGNING SITE DIRECTED PEPTIDE 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

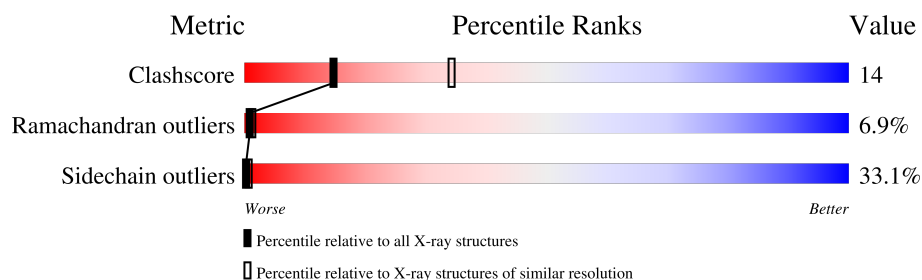
1 Overall quality at a glance

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	
1	B	216	
2	P	7	

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	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 DIMER MCG (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 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	PHE	conflict	PIR S14675
A	23	THR	SER	conflict	PIR S14675
A	29	VAL	ILE	conflict	PIR S14675
A	31	GLY	ASN	conflict	PIR S14675
A	39	GLN	ARG	conflict	PIR S14675
A	42	ALA	PRO	conflict	PIR S14675
A	48	VAL	LEU	conflict	PIR S14675
A	49	ILE	MET	conflict	PIR S14675
A	54	ASN	THR	conflict	PIR S14675
A	62	ASP	ASN	conflict	PIR S14675
A	94	GLU	ALA	conflict	PIR S14675
A	97	ASP	ASN	conflict	PIR S14675
A	98	ASN	SER	conflict	PIR S14675
A	99	PHE	LEU	conflict	PIR S14675
A	100	VAL	ILE	conflict	PIR S14675
A	103	THR	GLY	conflict	PIR S14675
A	106	LYS	ARG	conflict	PIR S14675
A	107	VAL	LEU	conflict	PIR S14675
A	116	ASN	ALA	conflict	PIR S14675
A	118	THR	SER	conflict	PIR S14675
A	156	GLY	SER	conflict	PIR S14675
A	167	LYS	THR	conflict	PIR S14675
B	20	ILE	PHE	conflict	PIR S14675
B	23	THR	SER	conflict	PIR S14675

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	VAL	ILE	conflict	PIR S14675
B	31	GLY	ASN	conflict	PIR S14675
B	39	GLN	ARG	conflict	PIR S14675
B	42	ALA	PRO	conflict	PIR S14675
B	48	VAL	LEU	conflict	PIR S14675
B	49	ILE	MET	conflict	PIR S14675
B	54	ASN	THR	conflict	PIR S14675
B	62	ASP	ASN	conflict	PIR S14675
B	94	GLU	ALA	conflict	PIR S14675
B	97	ASP	ASN	conflict	PIR S14675
B	98	ASN	SER	conflict	PIR S14675
B	99	PHE	LEU	conflict	PIR S14675
B	100	VAL	ILE	conflict	PIR S14675
B	103	THR	GLY	conflict	PIR S14675
B	106	LYS	ARG	conflict	PIR S14675
B	107	VAL	LEU	conflict	PIR S14675
B	116	ASN	ALA	conflict	PIR S14675
B	118	THR	SER	conflict	PIR S14675
B	156	GLY	SER	conflict	PIR S14675
B	167	LYS	THR	conflict	PIR S14675

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

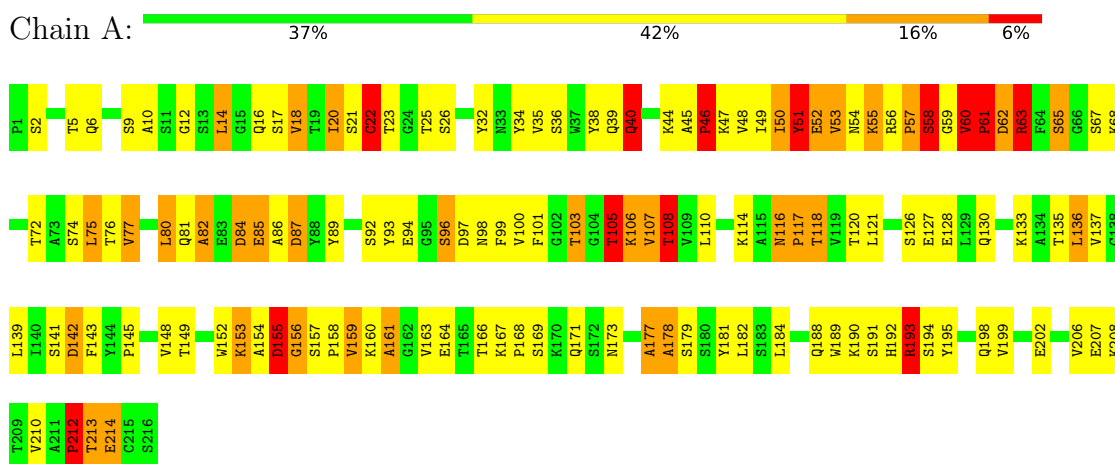
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			51	33	9	9			

3 Residue-property plots

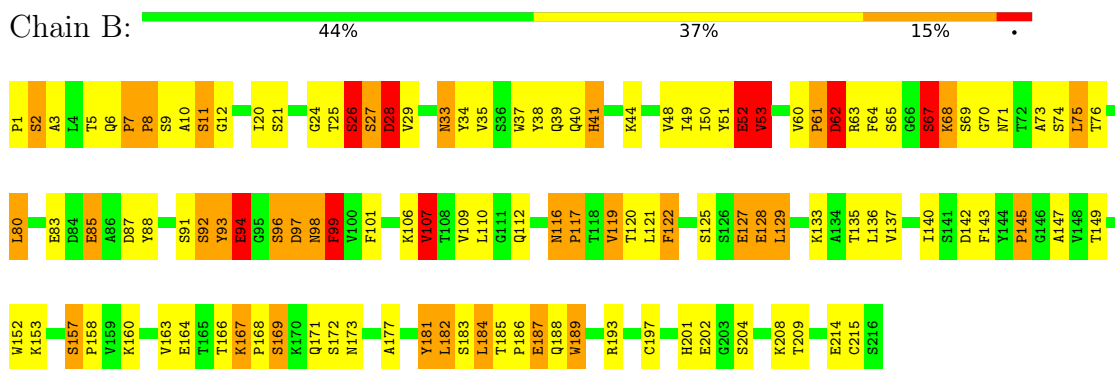
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

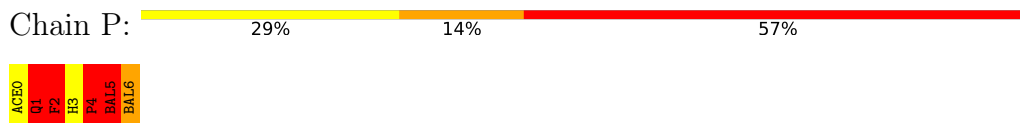
• Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN)



• Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (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}	0.252 , (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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BAL, 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	1.20	6/1644 (0.4%)	2.09	61/2241 (2.7%)
1	B	1.20	6/1644 (0.4%)	2.12	66/2241 (2.9%)
2	P	1.58	0/40	3.80	9/54 (16.7%)
All	All	1.21	12/3328 (0.4%)	2.13	136/4536 (3.0%)

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	1
1	B	0	2
2	P	2	2
All	All	2	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	THR	N-CA	8.84	1.57	1.46
1	A	5	THR	CA-CB	6.68	1.61	1.53
1	B	41	HIS	CA-CB	6.65	1.61	1.53
1	B	164	GLU	N-CA	5.96	1.53	1.46
1	B	96	SER	CA-C	5.65	1.57	1.52
1	B	201	HIS	N-CA	5.55	1.53	1.46
1	A	105	THR	CA-CB	5.29	1.61	1.53
1	A	12	GLY	N-CA	5.29	1.50	1.44
1	B	64	PHE	CA-CB	5.19	1.60	1.53
1	A	85	GLU	N-CA	5.15	1.52	1.46
1	A	118	THR	N-CA	5.07	1.52	1.46
1	B	24	GLY	N-CA	5.01	1.49	1.44

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASP	CA-CB-CG	16.16	128.76	112.60
1	B	99	PHE	CA-CB-CG	14.54	128.34	113.80
2	P	2	PHE	N-CA-C	13.71	139.99	110.80
1	B	187	GLU	CA-CB-CG	11.77	137.65	114.10
1	B	96	SER	N-CA-C	-10.55	95.61	111.34
1	B	3	ALA	N-CA-C	10.31	126.14	107.99
1	A	177	ALA	CA-C-N	10.21	141.04	121.54
1	A	177	ALA	C-N-CA	10.21	141.04	121.54
1	A	51	TYR	N-CA-C	9.92	125.70	113.50
2	P	1	GLN	CA-C-N	9.91	140.46	121.54
2	P	1	GLN	C-N-CA	9.91	140.46	121.54
1	B	63	ARG	N-CA-C	9.19	121.37	111.36
1	A	87	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	193	ARG	CA-CB-CG	8.64	131.38	114.10
1	B	28	ASP	CA-CB-CG	8.47	121.07	112.60
1	A	173	ASN	CA-CB-CG	8.25	120.85	112.60
1	A	108	THR	CB-CA-C	8.21	123.50	110.19
1	B	93	TYR	CA-CB-CG	8.20	128.66	113.90
1	A	107	VAL	CA-C-N	-8.06	112.05	122.77
1	A	107	VAL	C-N-CA	-8.06	112.05	122.77
1	A	107	VAL	O-C-N	8.02	131.93	123.03
1	B	164	GLU	CB-CG-CD	8.02	126.23	112.60
1	B	181	TYR	CA-CB-CG	7.91	128.13	113.90
1	B	41	HIS	N-CA-C	7.89	125.86	110.56
2	P	3	HIS	CA-CB-CG	-7.80	106.00	113.80
1	A	173	ASN	N-CA-C	-7.78	103.37	113.17
1	B	65	SER	N-CA-C	7.78	121.14	107.61
1	B	97	ASP	CA-CB-CG	7.59	120.19	112.60
1	B	87	ASP	CA-CB-CG	7.59	120.19	112.60
1	A	84	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	46	PRO	CA-C-N	7.49	132.06	120.75
1	A	46	PRO	C-N-CA	7.49	132.06	120.75
1	B	117	PRO	N-CA-C	7.49	122.56	111.03
1	A	177	ALA	N-CA-C	7.41	123.87	114.31
1	B	69	SER	N-CA-C	-7.40	100.32	111.34
1	B	83	GLU	CA-CB-CG	7.38	128.87	114.10
1	A	177	ALA	O-C-N	-7.33	114.28	122.34
1	B	94	GLU	CA-CB-CG	7.30	128.70	114.10
1	B	189	TRP	CA-CB-CG	7.17	127.22	113.60
1	B	145	PRO	N-CA-C	7.12	130.60	112.10
1	A	214	GLU	CA-CB-CG	7.02	128.13	114.10
1	A	52	GLU	CA-CB-CG	6.91	127.92	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	SER	N-CA-C	6.80	118.84	109.18
1	B	88	TYR	CA-CB-CG	6.79	126.12	113.90
1	B	2	SER	N-CA-C	6.75	125.18	110.80
1	A	47	LYS	N-CA-C	6.69	119.45	110.35
1	A	178	ALA	N-CA-C	6.69	125.06	110.80
1	A	34	TYR	CA-CB-CG	6.67	125.91	113.90
1	A	141	SER	CA-C-N	6.60	134.15	121.54
1	A	141	SER	C-N-CA	6.60	134.15	121.54
1	B	169	SER	CA-C-N	6.59	130.78	121.02
1	B	169	SER	C-N-CA	6.59	130.78	121.02
1	A	192	HIS	N-CA-C	6.56	120.53	110.36
1	A	55	LYS	N-CA-C	6.50	120.09	109.76
1	A	143	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	105	THR	N-CA-C	6.42	118.94	109.69
1	A	101	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	191	SER	N-CA-C	6.29	118.14	111.28
1	A	117	PRO	CA-C-N	-6.29	114.41	122.77
1	A	117	PRO	C-N-CA	-6.29	114.41	122.77
1	B	52	GLU	CA-CB-CG	6.28	126.65	114.10
1	B	187	GLU	CB-CA-C	6.28	119.92	109.56
1	B	85	GLU	CA-CB-CG	6.26	126.61	114.10
1	B	143	PHE	CA-CB-CG	6.25	120.05	113.80
1	A	207	GLU	CB-CG-CD	6.23	123.19	112.60
2	P	4	PRO	CA-N-CD	-6.20	103.32	112.00
1	B	163	VAL	O-C-N	6.07	129.56	123.18
1	B	62	ASP	CA-C-N	6.06	128.90	120.29
1	B	62	ASP	C-N-CA	6.06	128.90	120.29
1	B	142	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	158	PRO	N-CA-C	6.03	120.70	111.11
1	A	108	THR	CA-CB-CG2	6.00	120.71	110.50
1	B	33	ASN	N-CA-C	-5.98	103.11	110.65
1	B	51	TYR	CA-C-N	5.95	132.91	121.54
1	B	51	TYR	C-N-CA	5.95	132.91	121.54
1	B	97	ASP	CA-C-N	5.91	132.83	121.54
1	B	97	ASP	C-N-CA	5.91	132.83	121.54
1	B	107	VAL	CB-CA-C	5.91	119.16	110.77
1	A	181	TYR	CA-CB-CG	5.87	124.47	113.90
1	B	215	CYS	N-CA-CB	5.84	121.18	112.30
1	B	67	SER	N-CA-C	5.81	116.76	108.74
1	A	61	PRO	N-CA-C	5.80	124.41	112.47
1	A	44	LYS	N-CA-C	5.75	117.48	110.41
1	A	206	VAL	O-C-N	5.72	128.26	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	THR	N-CA-C	5.69	118.04	110.53
1	B	61	PRO	CA-C-N	5.68	132.38	121.54
1	B	61	PRO	C-N-CA	5.68	132.38	121.54
1	A	46	PRO	N-CA-C	5.67	124.16	112.47
1	A	107	VAL	N-CA-CB	5.67	117.79	110.99
1	A	58	SER	N-CA-C	5.66	122.86	110.80
1	B	52	GLU	CB-CG-CD	5.64	122.19	112.60
1	B	96	SER	O-C-N	5.62	127.30	121.79
2	P	2	PHE	CA-C-O	5.61	128.54	120.51
1	B	53	VAL	N-CA-CB	5.58	120.45	111.23
1	B	37	TRP	CA-CB-CG	5.51	124.06	113.60
2	P	2	PHE	N-CA-CB	-5.50	101.19	110.49
2	P	1	GLN	CA-C-O	5.49	130.13	120.80
1	B	25	THR	CA-C-N	5.49	132.01	121.54
1	B	25	THR	C-N-CA	5.49	132.01	121.54
1	A	68	LYS	CA-CB-CG	5.48	125.06	114.10
1	A	63	ARG	CB-CG-CD	5.46	123.86	111.30
1	A	57	PRO	CA-C-N	5.45	131.95	121.54
1	A	57	PRO	C-N-CA	5.45	131.95	121.54
1	B	33	ASN	CA-CB-CG	5.43	118.03	112.60
1	B	127	GLU	CA-C-O	-5.42	115.13	120.82
1	A	22	CYS	CB-CA-C	5.41	118.47	110.14
1	B	40	GLN	CA-C-N	5.40	129.22	121.71
1	B	40	GLN	C-N-CA	5.40	129.22	121.71
1	B	197	CYS	CA-C-N	5.40	130.60	123.05
1	B	197	CYS	C-N-CA	5.40	130.60	123.05
1	A	99	PHE	N-CA-C	5.39	117.75	109.07
1	B	116	ASN	CA-C-N	5.38	125.64	119.83
1	B	116	ASN	C-N-CA	5.38	125.64	119.83
1	B	166	THR	CA-C-N	5.38	127.86	120.39
1	B	166	THR	C-N-CA	5.38	127.86	120.39
1	B	41	HIS	CA-CB-CG	-5.37	108.43	113.80
1	B	214	GLU	CA-C-N	5.34	130.14	122.40
1	B	214	GLU	C-N-CA	5.34	130.14	122.40
1	A	93	TYR	CA-CB-CG	5.34	123.51	113.90
1	A	155	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	40	GLN	CA-CB-CG	5.29	124.67	114.10
1	B	69	SER	O-C-N	5.28	126.97	121.79
1	A	86	ALA	N-CA-C	5.21	116.75	108.79
1	A	169	SER	CA-C-N	5.19	128.24	120.87
1	A	169	SER	C-N-CA	5.19	128.24	120.87
1	A	206	VAL	N-CA-CB	5.16	118.49	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	GLU	CA-CB-CG	5.14	124.38	114.10
1	B	26	SER	N-CA-C	5.13	121.73	110.80
1	A	152	TRP	CA-CB-CG	5.12	123.34	113.60
1	A	141	SER	N-CA-C	5.07	118.34	110.17
2	P	1	GLN	CB-CG-CD	5.06	121.20	112.60
1	B	204	SER	N-CA-C	5.04	117.74	110.28
1	A	118	THR	N-CA-CB	5.04	118.63	110.42
1	B	6	GLN	CA-C-N	5.02	125.55	120.38
1	B	6	GLN	C-N-CA	5.02	125.55	120.38
1	B	127	GLU	CB-CG-CD	5.01	121.12	112.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	2	PHE	CA
2	P	4	PRO	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	VAL	Peptide
1	B	157	SER	Peptide
1	B	33	ASN	Peptide
2	P	1	GLN	Peptide
2	P	5	BAL	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	47	0
1	B	1605	0	1540	43	0
2	P	51	0	43	5	0
All	All	3261	0	3123	89	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 14.

All (89) 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:101:PHE:HZ	2:P:0:ACE:H2	1.39	0.87
1:A:108:THR:HG22	1:A:110:LEU:HD11	1.58	0.85
1:A:18:VAL:HG22	1:A:80:LEU:HD21	1.61	0.82
1:A:114:LYS:HG2	1:A:145:PRO:HD3	1.72	0.72
1:A:18:VAL:HG23	1:A:77:VAL:HG13	1.76	0.66
1:A:108:THR:HG22	1:A:110:LEU:CD1	2.29	0.61
1:A:193:ARG:HB2	1:A:193:ARG:HH11	1.66	0.61
1:A:51:TYR:HB2	1:B:99:PHE:HZ	1.67	0.60
1:B:7:PRO:HD2	1:B:21:SER:O	2.01	0.59
1:A:62:ASP:H	1:A:63:ARG:HE	1.50	0.59
1:B:128:GLU:OE2	1:B:133:LYS:HB3	2.02	0.59
1:B:49:ILE:O	1:B:50:ILE:HD12	2.03	0.58
1:A:155:ASP:OD1	1:A:193:ARG:HB3	2.05	0.56
1:A:81:GLN:O	1:A:82:ALA:CB	2.54	0.56
1:B:27:SER:O	1:B:28:ASP:HB3	2.05	0.55
1:B:34:TYR:OH	2:P:2:PHE:HE1	1.89	0.54
1:B:38:TYR:CE1	1:B:48:VAL:HG22	2.44	0.53
1:B:20:ILE:HD13	1:B:75:LEU:HD13	1.90	0.52
1:B:26:SER:O	1:B:27:SER:HB2	2.09	0.52
1:B:183:SER:O	1:B:184:LEU:HD13	2.10	0.51
1:B:12:GLY:O	1:B:109:VAL:HA	2.10	0.51
1:A:9:SER:HA	1:A:106:LYS:O	2.11	0.51
1:A:50:ILE:CG2	1:A:56:ARG:HG3	2.41	0.51
1:A:105:THR:O	1:A:106:LYS:HB2	2.11	0.51
1:A:53:VAL:HG13	1:A:54:ASN:H	1.75	0.51
1:B:171:GLN:HE21	1:B:173:ASN:HD21	1.59	0.50
1:A:53:VAL:HG13	1:A:54:ASN:N	2.25	0.50
1:B:67:SER:O	1:B:73:ALA:HA	2.12	0.50
1:B:11:SER:OG	1:B:145:PRO:HG2	2.12	0.50
1:A:137:VAL:HG11	1:B:137:VAL:HG11	1.93	0.49
2:P:5:BAL:N	2:P:6:BAL:N	2.56	0.49
1:A:136:LEU:HD23	1:A:136:LEU:N	2.27	0.49
1:B:10:ALA:O	1:B:107:VAL:HA	2.13	0.49
1:B:26:SER:O	1:B:27:SER:CB	2.61	0.49
1:A:6:GLN:HG2	1:A:22:CYS:HB2	1.95	0.49
1:B:9:SER:HB2	1:B:147:ALA:HB3	1.95	0.49
1:A:25:THR:HG22	1:A:26:SER:N	2.29	0.48
1:A:52:GLU:O	1:A:54:ASN:N	2.47	0.48
1:A:171:GLN:HG2	1:A:177:ALA:HB2	1.95	0.48
1:A:38:TYR:CD1	1:A:48:VAL:HG22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG22	1:A:26:SER:H	1.77	0.48
1:A:184:LEU:HD22	1:A:188:GLN:HB3	1.96	0.48
1:A:35:VAL:HG22	1:A:92:SER:HB3	1.96	0.48
1:B:171:GLN:NE2	1:B:173:ASN:HD21	2.12	0.47
1:B:101:PHE:CZ	2:P:0:ACE:H2	2.31	0.47
1:A:62:ASP:H	1:A:63:ARG:NE	2.13	0.47
1:A:136:LEU:HD21	1:A:184:LEU:HD12	1.95	0.47
1:A:40:GLN:HG2	1:A:89:TYR:HE2	1.80	0.47
1:B:171:GLN:OE1	1:B:177:ALA:HB2	2.15	0.47
1:B:34:TYR:O	1:B:53:VAL:HG13	2.16	0.46
1:A:20:ILE:HD12	1:A:75:LEU:O	2.15	0.46
1:A:38:TYR:HD1	1:A:48:VAL:HG22	1.80	0.46
1:B:28:ASP:OD1	1:B:28:ASP:C	2.58	0.46
1:B:136:LEU:HD21	1:B:189:TRP:CZ3	2.52	0.45
1:B:167:LYS:HA	1:B:168:PRO:HD3	1.77	0.45
1:A:81:GLN:O	1:A:82:ALA:HB3	2.17	0.44
1:A:10:ALA:HB3	1:A:107:VAL:HG12	1.98	0.44
1:A:160:LYS:O	1:A:161:ALA:CB	2.66	0.44
1:B:152:TRP:CE3	1:B:182:LEU:HD12	2.53	0.44
1:B:185:THR:OG1	1:B:188:GLN:HB2	2.18	0.43
1:B:68:LYS:HE2	1:B:68:LYS:HB3	1.84	0.43
1:A:61:PRO:HB2	1:A:63:ARG:HE	1.83	0.43
1:A:96:SER:O	1:A:97:ASP:HB2	2.17	0.43
1:B:49:ILE:C	1:B:50:ILE:HD12	2.43	0.43
1:B:94:GLU:HG3	1:B:98:ASN:HB3	2.00	0.43
1:A:16:GLN:HB3	1:A:17:SER:H	1.61	0.43
1:A:137:VAL:HG23	1:B:122:PHE:CZ	2.53	0.43
1:B:20:ILE:N	1:B:20:ILE:HD12	2.34	0.43
1:B:183:SER:C	1:B:184:LEU:HD13	2.42	0.42
1:B:116:ASN:HA	1:B:117:PRO:HD3	1.74	0.42
1:B:38:TYR:HE1	1:B:48:VAL:HG22	1.84	0.42
1:A:65:SER:O	1:A:75:LEU:HD23	2.19	0.42
1:A:59:GLY:O	1:A:60:VAL:HG22	2.20	0.42
1:A:116:ASN:HA	1:A:117:PRO:HD3	1.83	0.42
1:B:129:LEU:HD12	1:B:186:PRO:HB3	2.02	0.42
1:A:23:THR:OG1	1:A:72:THR:HG23	2.19	0.41
1:B:60:VAL:HA	1:B:61:PRO:HD2	1.83	0.41
1:A:53:VAL:CG1	1:A:54:ASN:H	2.33	0.41
1:B:7:PRO:HA	1:B:8:PRO:HD2	1.91	0.41
1:A:154:ALA:C	1:A:156:GLY:H	2.27	0.41
2:P:4:PRO:HA	2:P:6:BAL:C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HA	1:A:57:PRO:HD2	1.90	0.41
1:B:119:VAL:HG22	1:B:140:ILE:HG23	2.02	0.41
1:B:157:SER:HA	1:B:158:PRO:HD3	1.95	0.41
1:A:45:ALA:HA	1:A:46:PRO:HD3	1.66	0.41
1:A:153:LYS:HA	1:A:159:VAL:HG23	2.02	0.40
1:B:122:PHE:CD1	1:B:122:PHE:N	2.89	0.40
1:B:121:LEU:HD23	1:B:208:LYS:O	2.21	0.40
1:A:212:PRO:O	1:A:214:GLU:N	2.55	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%)	175 (82%)	23 (11%)	16 (8%)	1	1
1	B	214/216 (99%)	173 (81%)	29 (14%)	12 (6%)	1	2
2	P	4/7 (57%)	1 (25%)	1 (25%)	2 (50%)	0	0
All	All	432/439 (98%)	349 (81%)	53 (12%)	30 (7%)	1	1

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO
1	A	82	ALA
1	A	161	ALA
1	A	178	ALA
1	A	213	THR
1	B	26	SER
1	B	27	SER
1	B	28	ASP
1	B	98	ASN

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Mol	Chain	Res	Type
2	P	2	PHE
2	P	4	PRO
1	A	53	VAL
1	A	58	SER
1	A	155	ASP
1	A	212	PRO
1	B	52	GLU
1	B	202	GLU
1	A	46	PRO
1	A	85	GLU
1	A	106	LYS
1	A	142	ASP
1	B	62	ASP
1	A	14	LEU
1	B	35	VAL
1	B	70	GLY
1	B	92	SER
1	A	60	VAL
1	B	8	PRO
1	B	80	LEU
1	A	156	GLY

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%)	113 (62%)	68 (38%)	0	0
1	B	181/181 (100%)	129 (71%)	52 (29%)	0	1
2	P	4/4 (100%)	3 (75%)	1 (25%)	0	2
All	All	366/366 (100%)	245 (67%)	121 (33%)	0	1

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER

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Mol	Chain	Res	Type
1	A	14	LEU
1	A	18	VAL
1	A	20	ILE
1	A	21	SER
1	A	22	CYS
1	A	32	TYR
1	A	36	SER
1	A	39	GLN
1	A	40	GLN
1	A	49	ILE
1	A	50	ILE
1	A	51	TYR
1	A	55	LYS
1	A	58	SER
1	A	60	VAL
1	A	63	ARG
1	A	65	SER
1	A	67	SER
1	A	74	SER
1	A	75	LEU
1	A	76	THR
1	A	77	VAL
1	A	80	LEU
1	A	84	ASP
1	A	87	ASP
1	A	94	GLU
1	A	96	SER
1	A	98	ASN
1	A	100	VAL
1	A	103	THR
1	A	105	THR
1	A	108	THR
1	A	116	ASN
1	A	118	THR
1	A	120	THR
1	A	121	LEU
1	A	126	SER
1	A	128	GLU
1	A	130	GLN
1	A	133	LYS
1	A	135	THR
1	A	136	LEU

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Mol	Chain	Res	Type
1	A	139	LEU
1	A	142	ASP
1	A	148	VAL
1	A	149	THR
1	A	153	LYS
1	A	157	SER
1	A	159	VAL
1	A	163	VAL
1	A	164	GLU
1	A	166	THR
1	A	167	LYS
1	A	168	PRO
1	A	182	LEU
1	A	189	TRP
1	A	190	LYS
1	A	193	ARG
1	A	194	SER
1	A	195	TYR
1	A	198	GLN
1	A	199	VAL
1	A	202	GLU
1	A	208	LYS
1	A	210	VAL
1	A	212	PRO
1	A	213	THR
1	B	1	PRO
1	B	2	SER
1	B	5	THR
1	B	7	PRO
1	B	11	SER
1	B	28	ASP
1	B	29	VAL
1	B	39	GLN
1	B	41	HIS
1	B	44	LYS
1	B	52	GLU
1	B	53	VAL
1	B	62	ASP
1	B	67	SER
1	B	68	LYS
1	B	71	ASN
1	B	74	SER

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Mol	Chain	Res	Type
1	B	75	LEU
1	B	76	THR
1	B	80	LEU
1	B	85	GLU
1	B	91	SER
1	B	92	SER
1	B	93	TYR
1	B	94	GLU
1	B	96	SER
1	B	97	ASP
1	B	99	PHE
1	B	106	LYS
1	B	107	VAL
1	B	110	LEU
1	B	112	GLN
1	B	119	VAL
1	B	120	THR
1	B	122	PHE
1	B	125	SER
1	B	127	GLU
1	B	128	GLU
1	B	129	LEU
1	B	135	THR
1	B	149	THR
1	B	153	LYS
1	B	160	LYS
1	B	167	LYS
1	B	169	SER
1	B	172	SER
1	B	181	TYR
1	B	182	LEU
1	B	184	LEU
1	B	187	GLU
1	B	193	ARG
1	B	209	THR
2	P	1	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	B	39	GLN

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Mol	Chain	Res	Type
1	B	40	GLN
1	B	54	ASN
1	B	71	ASN
1	B	98	ASN
1	B	173	ASN
1	B	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	1.34	1 (20%)	5,5,5	3.06	3 (60%)
2	BAL	P	5	2	3,4,5	1.33	1 (33%)	3,3,5	0.87	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	-	0/1/2/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	5	BAL	CB-CA	2.20	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	6	BAL	O-C	2.16	1.29	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	6	BAL	OXT-C-O	-4.19	112.57	123.33
2	P	6	BAL	OXT-C-CA	4.13	127.06	114.00
2	P	6	BAL	CB-CA-C	2.87	119.19	112.98

There are no chirality outliers.

All (3) 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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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.