



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:51 PM GMT

PDB ID : 1MCD  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

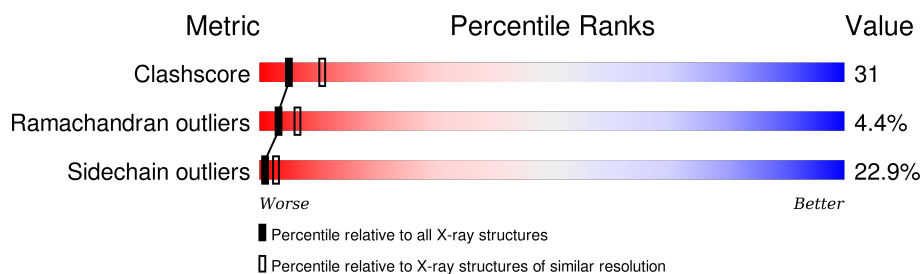
# 1 Overall quality at a glance

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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
6	DPR	P	8	-	-	X	-

## 2 Entry composition

There are 7 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 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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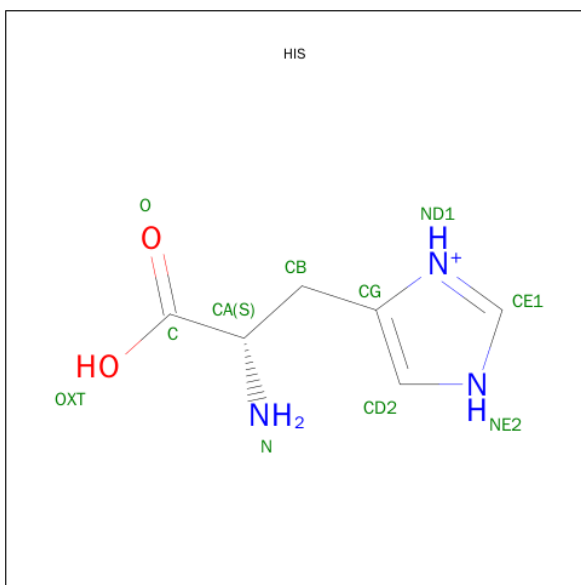
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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	VAL	ILE	CONFLICT	PIR S14675
B	31	GLY	ASN	CONFLICT	PIR S14675
B	39	GLN	ARG	CONFLICT	PIR S14675
B	42	ALA	PRO	CONFLICT	PIR S14675
B	48	VAL	LEU	CONFLICT	PIR S14675
B	49	ILE	MET	CONFLICT	PIR S14675
B	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-D-PHE-B-ALA-L-HIS-D-PRO-NH<sub>2</sub>.

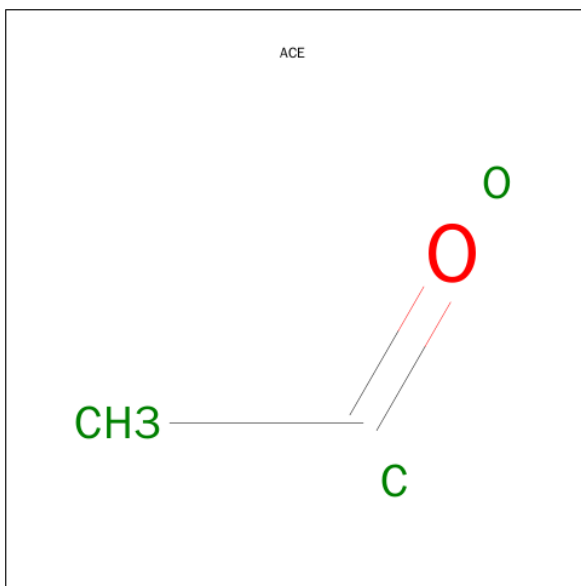
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	1	Total	C	N	O	0	0	0
			5	3	1	1			

- Molecule 3 is HISTIDINE (three-letter code: HIS) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>3</sub>O<sub>2</sub>).



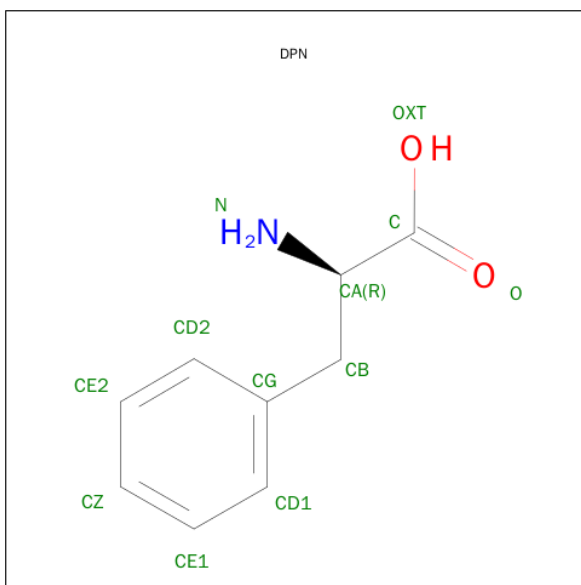
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 4 is ACETYL GROUP (three-letter code: ACE) (formula:  $C_2H_4O$ ).



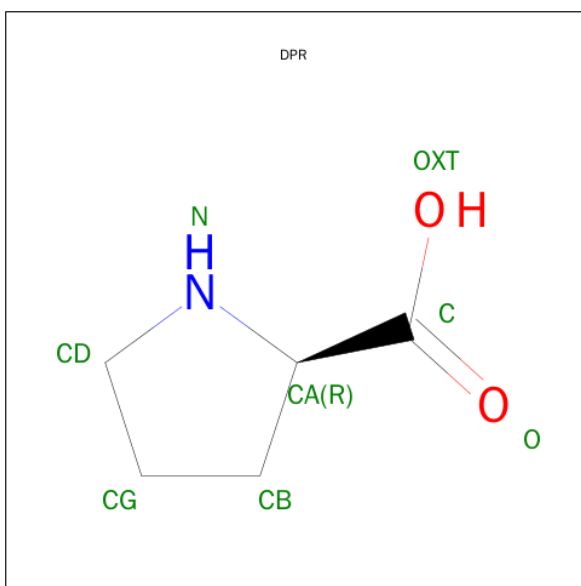
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	2	1		

- Molecule 5 is D-PHENYLALANINE (three-letter code: DPN) (formula:  $C_9H_{11}NO_2$ ).



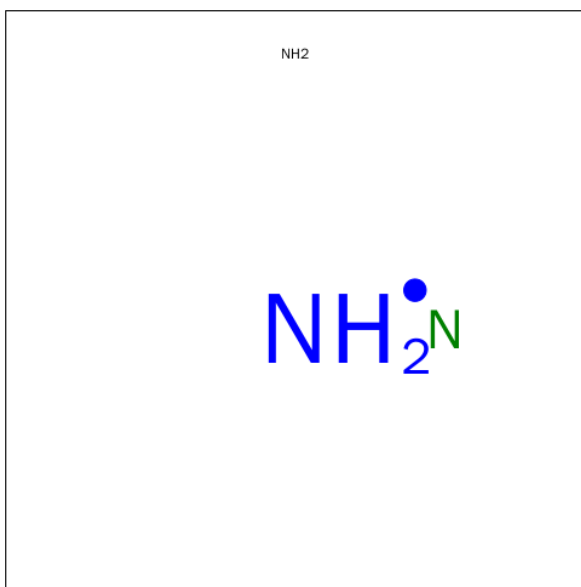
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	P	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 6 is D-PROLINE (three-letter code: DPR) (formula:  $C_5H_9NO_2$ ).



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

- Molecule 7 is AMINO GROUP (three-letter code: NH2) (formula:  $H_2N$ ).



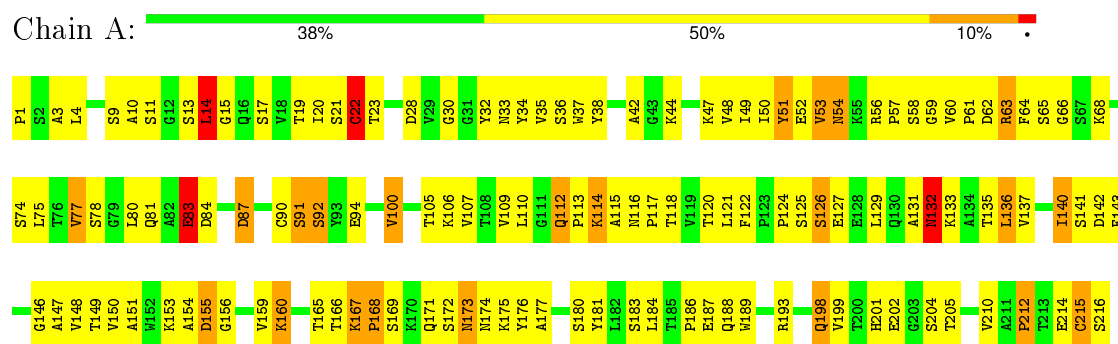
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N 1 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3247	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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, BAL, DPR, ACE, NH2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.83	0/1644	1.38	9/2241 (0.4%)
1	B	0.89	1/1644 (0.1%)	1.42	11/2241 (0.5%)
All	All	0.86	1/3288 (0.0%)	1.40	20/4482 (0.4%)

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
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	CYS	CB-SG	-5.56	1.72	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	CYS	CA-CB-SG	12.37	136.27	114.00
1	B	34	TYR	CA-CB-CG	8.08	128.75	113.40
1	A	22	CYS	CA-CB-SG	7.96	128.33	114.00
1	A	215	CYS	CA-CB-SG	7.81	128.06	114.00
1	A	214	GLU	CA-CB-CG	6.99	128.78	113.40
1	A	51	TYR	CA-CB-CG	6.85	126.42	113.40
1	B	193	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	B	99	PHE	CA-CB-CG	6.83	130.28	113.90
1	A	202	GLU	CA-CB-CG	6.19	127.02	113.40
1	B	31	GLY	N-CA-C	-5.92	98.31	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	TRP	CA-CB-CG	5.86	124.84	113.70
1	B	32	TYR	CA-CB-CG	-5.84	102.30	113.40
1	A	83	GLU	CA-CB-CG	5.62	125.77	113.40
1	B	97	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	30	GLY	N-CA-C	-5.48	99.40	113.10
1	B	181	TYR	CA-CB-CG	5.48	123.81	113.40
1	A	215	CYS	N-CA-CB	5.25	120.05	110.60
1	B	22	CYS	CA-CB-SG	5.10	123.19	114.00
1	A	54	ASN	N-CA-CB	5.07	119.72	110.60
1	A	168	PRO	N-CA-C	5.02	125.16	112.10

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	98	0
1	B	1605	0	1540	100	0
2	P	5	0	4	1	0
3	P	10	0	6	5	0
4	A	3	0	3	0	0
5	P	11	0	8	3	0
6	P	7	0	7	4	0
7	A	1	0	0	1	0
All	All	3247	0	3108	197	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 31.

All (197) 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
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:171:GLN:HB2	1:A:175:LYS:O	1.95	0.67
1:A:35:VAL:HA	1:A:91:SER:O	1.94	0.67
1:B:153:LYS:HZ2	1:B:198:GLN:HB2	1.57	0.67
3:P:6:HIS:HB3	6:P:8: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: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	5:P:7: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:32:TYR:OH	1:B:34:TYR:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:SER:HB2	1:B:147:ALA:HB3	1.82	0.60
1:B:173:ASN:ND2	1:B:175:LYS:HZ3	1.99	0.60
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
3:P:6:HIS:HB3	6:P:8: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: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:B:214:GLU:O	1:B:215:CYS:CB	2.53	0.56
1:A:184:LEU:HA	1:A:188:GLN:OE1	2.05	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:171:GLN:HB2	1:B:173:ASN:OD1	2.08	0.54
1:A:80:LEU:HD22	1:A:109:VAL:HG21	1.89	0.54
1:B:32:TYR:HH	1:B:93:TYR:HB3	1.73	0.54
1:B:38:TYR:HE1	1:B:91:SER:HB2	1.73	0.54
1:A:159:VAL:C	1:A:160:LYS:HD2	2.28	0.54
1:A:153:LYS:HD2	1:A:156:GLY:O	2.08	0.54
1:B:4:LEU:HA	1:B:24:GLY:HA2	1.90	0.54
1:B:122:PHE:O	1:B:136:LEU:HD23	2.08	0.54
1:B:45:ALA:HB1	1:B:46:PRO:HD3	1.90	0.54
1:A:122:PHE:HB2	1:A:137:VAL:HG13	1.89	0.54
1:A:10:ALA:HB3	1:A:107:VAL:HG22	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:A:217:NH2:N	6:P:8:DPR:HD3	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:B:52:GLU:HG2	1:B:55:LYS:HZ3	1.72	0.51
1:A:38:TYR:HA	1:A:47:LYS:O	2.11	0.51
1:A:140:ILE:HG13	1:A:199:VAL:HG21	1.92	0.51
1:A:19:THR:CG2	1:A:74:SER:HB3	2.41	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:B:173:ASN:ND2	1:B:175:LYS:NZ	2.60	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: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
5:P:7:DPN:C	5:P:7:DPN:CD1	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:B:164:GLU:O	1:B:180:SER:HA	2.13	0.48
1:A:15:GLY:H	1:A:80:LEU:HB2	1.78	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:149:THR:O	1:A:199:VAL:HA	2.13	0.48
1:A:114:LYS:NZ	1:A:114:LYS:HB2	2.29	0.48
1:B:34:TYR:CD2	1:B:93:TYR:HD2	2.31	0.48
1:A:114:LYS:HB2	1:A:114:LYS:HZ3	1.79	0.48
1:A:151:ALA:HB3	1:A:198:GLN:HB3	1.96	0.48
1:B:153:LYS:HZ2	1:B:198:GLN:CB	2.27	0.47
1:A:87:ASP:CG	1:A:106:LYS:HG2	2.33	0.47
1:A:124:PRO:HD3	1:A:136:LEU:HD22	1.97	0.47
1:B:54:ASN:C	1:B:54:ASN:HD22	2.17	0.47
1:A:169:SER:O	1:A:176:TYR:HA	2.14	0.47
1:B:153:LYS:HZ1	1:B:196:SER:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PRO:O	1:A:189:TRP:HB3	2.15	0.47
3:P:6:HIS:CB	6:P:8:DPR:HD2	2.44	0.47
1:B:12:GLY:O	1:B:109:VAL:HA	2.15	0.46
1:B:39:GLN:HG3	1:B:39:GLN:O	2.15	0.46
1:A:167:LYS:HB3	1:A:168:PRO:CD	2.45	0.46
1:A:28:ASP:HB3	1:A:94:GLU:HB3	1.96	0.46
1:A:14:LEU:HD13	1:A:109:VAL:CG1	2.46	0.46
1:B:125:SER:OG	1:B:128:GLU:HG3	2.15	0.46
1:B:85:GLU:O	1:B:86:ALA:HB2	2.16	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: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:A:49:ILE:HD11	1:A:75:LEU:HD21	1.98	0.45
2:P:2:BAL:O	3:P:6:HIS:CG	2.70	0.45
1:A:91:SER:HA	1:A:100:VAL:O	2.17	0.45
1:B:36:SER:CB	5:P:7:DPN:HD2	2.46	0.45
1:A:56:ARG:NH1	1:A:64:PHE:O	2.46	0.45
1:B:124:PRO:HG2	1:B:189:TRP:NE1	2.32	0.44
1:A:189:TRP:CZ2	1:A:212:PRO:HG3	2.53	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:32:TYR:HE2	1:B:92:SER:HG	1.66	0.44
1:B:8:PRO:HG3	1:B:149:THR:CB	2.48	0.44
1:A:112:GLN:NE2	1:A:174:ASN:HD21	2.15	0.44
1:A:20:ILE:HD12	1:A:20:ILE:N	2.33	0.44
1:B:28:ASP:OD2	1:B:94:GLU:HB2	2.18	0.44
1:A:116:ASN:HA	1:A:117:PRO:HD3	1.93	0.43
1:A:37:TRP:CE2	1:A:75:LEU:HB2	2.53	0.43
1:A:117:PRO:HB2	1:A:140:ILE:CG2	2.49	0.43
1:B:34:TYR:OH	3:P:6:HIS:CE1	2.71	0.43
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:A:112:GLN:CD	1:A:174:ASN:HD21	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:115:ALA:CB	1:A:175:LYS:HZ3	2.32	0.42
1:A:115:ALA:HB2	1:A:175:LYS:NZ	2.34	0.42
1:A:112:GLN:HA	1:A:113:PRO:HD3	1.76	0.42
1:A:19:THR:HG22	1:A:74:SER:HB3	2.00	0.42
1:B:38:TYR:O	1:B:88:TYR:HA	2.19	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:A:171:GLN:C	1:A:173:ASN:H	2.23	0.42
1:A:146:GLY:O	1:A:168:PRO:HG2	2.20	0.42
1:A:54:ASN:C	1:A:54:ASN:ND2	2.73	0.42
1:A:115:ALA:CB	1:A:175:LYS:NZ	2.83	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:B:33:ASN:O	1:B:53:VAL:HG23	2.20	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:82:ALA:C	1:B:84:ASP:H	2.24	0.41
1:B:122:PHE:HA	1:B:123:PRO:HD3	1.87	0.40
1:A:83:GLU:O	1:A:83:GLU:HG3	2.22	0.40
1:B:213:THR:O	1:B:214:GLU:HB2	2.21	0.40
1:B:41:HIS:CD2	1:B:44:LYS:HE3	2.57	0.40
1:A:4:LEU:HD13	1:A:100:VAL:HB	2.03	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

### 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%)	176 (82%)	27 (13%)	11 (5%)	2	4
1	B	214/216 (99%)	183 (86%)	23 (11%)	8 (4%)	4	9
All	All	428/432 (99%)	359 (84%)	50 (12%)	19 (4%)	3	6

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 ⓘ

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%)	140 (77%)	41 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	181/181 (100%)	139 (77%)	42 (23%)	1	2
All	All	362/362 (100%)	279 (77%)	83 (23%)	1	3

All (83) 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	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	87	ASP
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
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	140	ILE
1	A	141	SER
1	A	148	VAL
1	A	160	LYS

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	183	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	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	90	CYS
1	B	91	SER
1	B	92	SER
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

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Mol	Chain	Res	Type
1	B	196	SER
1	B	199	VAL
1	B	210	VAL
1	B	214	GLU
1	B	215	CYS

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

Mol	Chain	Res	Type
1	A	112	GLN
1	A	171	GLN
1	A	173	ASN
1	A	174	ASN
1	B	39	GLN
1	B	54	ASN
1	B	116	ASN
1	B	132	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	3	3,4,5	2.25	1 (33%)	0,3,5	0.00	-

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	3	-	0/1/2/3	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	BAL	CA-C	3.89	1.60	1.49

There are no bond angle outliers.

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is modelled with single atom - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
4	ACE	A	0	-	2,2,2	1.17	0	0,1,1	0.00	-
3	HIS	P	6	2	5,10,11	0.75	0	3,12,14	1.15	0
5	DPN	P	7	-	10,11,12	1.76	1 (10%)	10,13,15	1.11	1 (10%)
6	DPR	P	8	-	6,7,8	0.81	0	7,8,10	1.75	2 (28%)

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
4	ACE	A	0	-	-	0/0/0/0	0/0/0/0
3	HIS	P	6	2	-	0/4/6/8	0/1/1/1
5	DPN	P	7	-	-	0/4/6/8	0/1/1/1
6	DPR	P	8	-	-	0/0/9/11	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	7	DPN	CA-N	-5.33	1.30	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	8	DPR	CD-N-CA	-3.25	99.31	107.20
5	P	7	DPN	O-C-CA	-2.97	117.74	125.49
6	P	8	DPR	CG-CD-N	-2.41	99.34	105.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	6	HIS	5	0
5	P	7	DPN	3	0
6	P	8	DPR	4	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.