



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:12 PM GMT

PDB ID : 1YDP  
Title : 1.9A crystal structure of HLA-G  
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Deposited on : 2004-12-25  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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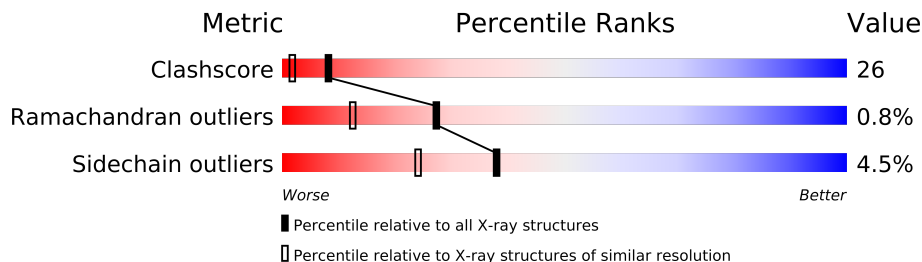
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	100	
3	P	9	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3590 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2242	1397	404	429	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	SER	CYS	ENGINEERED	UNP P17693

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1A	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called histone 2a peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	0	0	0
			81	52	18	11			

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Co	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		

- Molecule 6 is water.

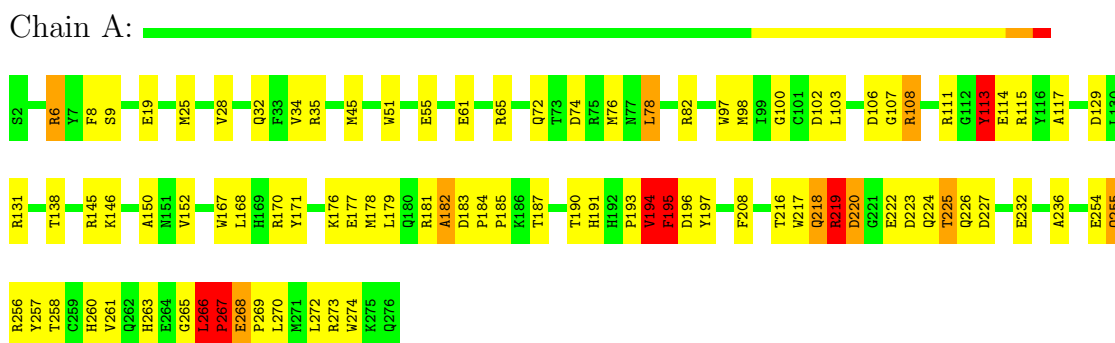
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	311	Total	O	0	0
			311	311		
6	B	105	Total	O	0	0
			105	105		
6	P	11	Total	O	0	0
			11	11		

### 3 Residue-property plots

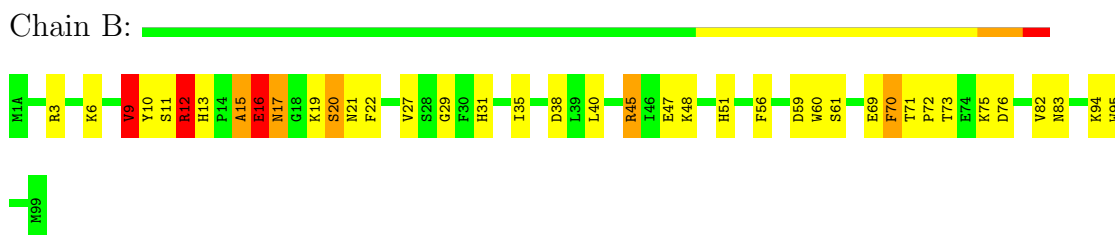
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: MHC class I antigen



- Molecule 2: Beta-2-microglobulin



- Molecule 3: histone 2a peptide



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.15Å 77.15Å 151.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.235 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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: CO, CL

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	0.85	12/2303 (0.5%)	1.30	27/3124 (0.9%)
2	B	1.21	7/860 (0.8%)	1.08	8/1162 (0.7%)
3	P	0.38	0/82	0.82	0/108
All	All	0.95	19/3245 (0.6%)	1.23	35/4394 (0.8%)

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	4
2	B	0	4
All	All	0	8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	12	ARG	CD-NE	-16.82	1.17	1.46
1	A	268	GLU	CB-CG	-16.16	1.21	1.52
2	B	9	VAL	C-N	-16.00	0.97	1.34
2	B	15	ALA	C-N	13.59	1.65	1.34
1	A	182	ALA	C-N	12.37	1.62	1.34
2	B	16	GLU	C-N	-11.29	1.08	1.34
2	B	82	VAL	C-N	11.15	1.59	1.34
1	A	267	PRO	N-CD	11.14	1.63	1.47
1	A	266	LEU	CB-CG	10.53	1.83	1.52
1	A	217	TRP	C-N	9.71	1.56	1.34
2	B	83	ASN	C-N	-9.59	1.11	1.34
1	A	190	THR	C-N	-8.85	1.13	1.34
1	A	176	LYS	C-N	-8.68	1.14	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	PRO	CB-CG	8.19	1.90	1.50
2	B	17	ASN	CB-CG	-8.02	1.32	1.51
1	A	268	GLU	C-N	-7.02	1.21	1.34
1	A	219	ARG	CA-CB	-6.87	1.38	1.53
1	A	219	ARG	CD-NE	-5.78	1.36	1.46
1	A	220	ASP	C-N	-5.30	1.23	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	CD-NE-CZ	28.68	163.75	123.60
1	A	220	ASP	CB-CG-OD2	21.32	137.49	118.30
1	A	220	ASP	CB-CG-OD1	-20.91	99.48	118.30
2	B	9	VAL	O-C-N	-19.23	91.93	122.70
1	A	195	PHE	CB-CG-CD1	-15.11	110.22	120.80
1	A	195	PHE	CB-CG-CD2	14.37	130.86	120.80
2	B	9	VAL	CA-C-N	13.58	147.07	117.20
1	A	266	LEU	CB-CG-CD1	10.88	129.50	111.00
1	A	268	GLU	CA-CB-CG	10.51	136.52	113.40
1	A	176	LYS	O-C-N	-10.28	106.26	122.70
1	A	220	ASP	CA-CB-CG	9.12	133.47	113.40
1	A	194	VAL	C-N-CA	-8.86	99.55	121.70
1	A	190	THR	O-C-N	-8.49	109.12	122.70
1	A	219	ARG	CB-CA-C	-7.83	94.75	110.40
2	B	83	ASN	O-C-N	-7.55	110.62	122.70
2	B	15	ALA	C-N-CA	-7.49	102.99	121.70
1	A	176	LYS	CA-C-N	7.45	133.60	117.20
1	A	113	TYR	CB-CA-C	-7.41	95.57	110.40
1	A	195	PHE	CA-CB-CG	6.87	130.38	113.90
1	A	113	TYR	CB-CG-CD2	-6.86	116.89	121.00
2	B	82	VAL	C-N-CA	-6.85	104.58	121.70
1	A	182	ALA	C-N-CA	-6.83	104.62	121.70
1	A	78	LEU	C-N-CA	-6.83	104.63	121.70
1	A	6	ARG	CB-CA-C	-6.54	97.31	110.40
1	A	267	PRO	N-CA-CB	6.35	110.92	103.30
1	A	190	THR	CA-C-N	6.29	131.04	117.20
2	B	83	ASN	CA-C-N	6.23	130.90	117.20
2	B	16	GLU	O-C-N	-5.86	113.32	122.70
2	B	9	VAL	C-N-CA	5.81	136.22	121.70
1	A	138	THR	O-C-N	-5.74	113.52	122.70
1	A	267	PRO	CA-CB-CG	-5.59	93.39	104.00
1	A	218	GLN	CB-CG-CD	-5.52	97.24	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	267	PRO	CA-N-CD	-5.37	103.98	111.50
1	A	220	ASP	O-C-N	5.09	131.85	123.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ASP	Mainchain
1	A	194	VAL	Peptide
1	A	219	ARG	Sidechain
1	A	268	GLU	Mainchain
2	B	12	ARG	Sidechain
2	B	15	ALA	Mainchain
2	B	16	GLU	Mainchain
2	B	9	VAL	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2242	0	2094	121	1
2	B	837	0	800	45	0
3	P	81	0	94	2	0
4	B	1	0	0	0	0
5	B	2	0	0	0	0
6	A	311	0	0	28	1
6	B	105	0	0	5	0
6	P	11	0	0	1	0
All	All	3590	0	2988	163	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (163) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:LEU:CG	1:A:266:LEU:CB	1.83	1.53
1:A:266:LEU:CD1	1:A:270:LEU:HD22	1.43	1.47
1:A:267:PRO:CG	1:A:267:PRO:CB	1.90	1.39
1:A:266:LEU:CB	1:A:266:LEU:HG	1.50	1.30
1:A:108:ARG:CD	6:A:385:HOH:O	1.93	1.17
1:A:108:ARG:HD2	6:A:385:HOH:O	1.43	1.16
1:A:6:ARG:NH1	1:A:113:TYR:HE1	1.42	1.15
1:A:6:ARG:NH1	1:A:113:TYR:CE1	2.17	1.12
1:A:266:LEU:HD12	1:A:270:LEU:HD22	1.18	1.11
1:A:266:LEU:HD12	1:A:270:LEU:CD2	1.86	1.05
1:A:266:LEU:CD1	1:A:270:LEU:CD2	2.35	1.04
1:A:102:ASP:OD2	1:A:111:ARG:NE	1.98	0.96
2:B:16:GLU:OE2	2:B:19:LYS:HB2	1.68	0.94
1:A:266:LEU:HD11	1:A:270:LEU:HD22	1.46	0.92
1:A:222:GLU:HB2	6:A:522:HOH:O	1.71	0.89
1:A:194:VAL:HG12	1:A:197:TYR:CE2	2.10	0.87
1:A:218:GLN:HB2	1:A:258:THR:OG1	1.77	0.85
1:A:34:VAL:CG2	1:A:45:MET:HG3	2.07	0.84
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.60	0.84
1:A:111:ARG:NE	6:A:462:HOH:O	2.11	0.84
1:A:103:LEU:HD13	1:A:168:LEU:HD23	1.59	0.83
2:B:16:GLU:OE2	2:B:19:LYS:CB	2.29	0.80
2:B:16:GLU:O	2:B:17:ASN:C	2.17	0.78
2:B:19:LYS:HG3	6:B:1093:HOH:O	1.84	0.78
1:A:263:HIS:O	1:A:266:LEU:HB2	1.85	0.77
1:A:111:ARG:CZ	6:A:462:HOH:O	2.32	0.76
1:A:270:LEU:H	1:A:270:LEU:HD23	1.53	0.73
1:A:187:THR:HB	1:A:272:LEU:HD21	1.71	0.73
1:A:218:GLN:O	1:A:257:TYR:HA	1.91	0.71
1:A:34:VAL:HG22	1:A:45:MET:HG3	1.73	0.71
2:B:16:GLU:CG	2:B:19:LYS:HB2	2.20	0.71
1:A:194:VAL:O	1:A:195:PHE:C	2.26	0.71
1:A:107:GLY:HA3	6:A:579:HOH:O	1.91	0.71
2:B:16:GLU:OE2	2:B:19:LYS:CG	2.39	0.70
1:A:76:MET:HE3	1:A:76:MET:O	1.91	0.70
1:A:266:LEU:CG	1:A:266:LEU:CA	2.68	0.69
2:B:11:SER:HB2	2:B:21:ASN:ND2	2.08	0.69
2:B:3:ARG:HH21	2:B:61:SER:HB3	1.58	0.68
1:A:194:VAL:O	1:A:195:PHE:O	2.12	0.67
1:A:266:LEU:HD13	1:A:270:LEU:HD22	1.66	0.67
2:B:19:LYS:O	2:B:72:PRO:HD2	1.94	0.67
1:A:98:MET:HG3	6:B:1096:HOH:O	1.94	0.66
2:B:22:PHE:CE1	2:B:69:GLU:HG2	2.30	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:VAL:HB	1:A:270:LEU:HD21	1.77	0.66
1:A:218:GLN:HE21	1:A:260:HIS:HB2	1.61	0.66
1:A:194:VAL:CG1	1:A:197:TYR:CE2	2.80	0.65
2:B:21:ASN:ND2	2:B:22:PHE:H	1.95	0.65
2:B:73:THR:HG22	2:B:75:LYS:H	1.61	0.65
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.78	0.64
1:A:194:VAL:HG11	1:A:197:TYR:CZ	2.34	0.62
1:A:178:MET:HG2	6:A:458:HOH:O	2.00	0.62
1:A:266:LEU:HB2	1:A:266:LEU:HG	1.73	0.61
1:A:102:ASP:HB2	1:A:111:ARG:HG2	1.82	0.61
1:A:236:ALA:O	2:B:12:ARG:HD3	2.00	0.61
2:B:20:SER:HA	2:B:70:PHE:O	2.01	0.61
2:B:13:HIS:HB2	2:B:21:ASN:OD1	2.01	0.61
1:A:72:GLN:HB3	6:A:545:HOH:O	2.01	0.61
2:B:16:GLU:CD	2:B:19:LYS:HB2	2.22	0.60
1:A:6:ARG:HH11	1:A:113:TYR:HE1	1.42	0.60
1:A:187:THR:CB	1:A:272:LEU:HD21	2.32	0.59
1:A:185:PRO:HD2	1:A:266:LEU:HD23	1.83	0.59
1:A:194:VAL:HG11	1:A:197:TYR:OH	2.03	0.59
2:B:13:HIS:H	2:B:21:ASN:HD21	1.49	0.59
1:A:6:ARG:NH1	1:A:113:TYR:CZ	2.70	0.58
1:A:19:GLU:HB2	6:A:557:HOH:O	2.03	0.58
1:A:108:ARG:CG	6:A:385:HOH:O	2.43	0.57
1:A:181:ARG:HB3	6:A:563:HOH:O	2.04	0.57
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.36	0.56
1:A:191:HIS:HB2	1:A:274:TRP:NE1	2.19	0.56
1:A:261:VAL:HB	1:A:270:LEU:CD2	2.36	0.56
2:B:16:GLU:HG3	2:B:16:GLU:O	2.06	0.56
1:A:34:VAL:HG21	1:A:45:MET:HG3	1.86	0.56
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.40	0.55
1:A:108:ARG:CZ	1:A:108:ARG:HB2	2.27	0.55
2:B:6:LYS:HE2	2:B:29:GLY:HA3	1.87	0.55
1:A:65:ARG:NH1	6:A:460:HOH:O	2.40	0.55
1:A:273:ARG:HH11	1:A:273:ARG:HB2	1.71	0.54
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.43	0.54
1:A:6:ARG:CZ	1:A:113:TYR:CE1	2.89	0.54
1:A:260:HIS:CE1	1:A:269:PRO:HB2	2.43	0.54
1:A:218:GLN:O	1:A:258:THR:N	2.36	0.53
1:A:167:TRP:CE2	3:P:1:ARG:HG3	2.43	0.53
1:A:61:GLU:HG2	6:A:449:HOH:O	2.08	0.53
1:A:273:ARG:NH1	1:A:273:ARG:HB2	2.24	0.53
1:A:194:VAL:CG1	1:A:197:TYR:CZ	2.92	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:224:GLN:HA	6:A:468:HOH:O	2.09	0.53
1:A:115:ARG:HD3	6:A:560:HOH:O	2.09	0.53
1:A:216:THR:OG1	1:A:260:HIS:HB3	2.09	0.53
1:A:265:GLY:HA2	6:A:569:HOH:O	2.09	0.52
1:A:191:HIS:CD2	1:A:193:PRO:HG3	2.45	0.51
2:B:3:ARG:NH2	2:B:61:SER:HB3	2.25	0.51
2:B:73:THR:HB	2:B:76:ASP:HB2	1.92	0.51
1:A:184:PRO:HB2	1:A:266:LEU:CD2	2.41	0.50
2:B:20:SER:OG	2:B:71:THR:HG22	2.12	0.50
2:B:11:SER:HB2	2:B:21:ASN:HD22	1.74	0.50
1:A:196:ASP:OD1	6:A:454:HOH:O	2.20	0.50
2:B:31:HIS:CD2	6:B:1072:HOH:O	2.65	0.49
2:B:16:GLU:OE2	2:B:19:LYS:HG2	2.11	0.49
2:B:10:TYR:N	2:B:10:TYR:CD1	2.80	0.49
1:A:227:ASP:HB2	6:A:541:HOH:O	2.12	0.49
1:A:150:ALA:HB3	1:A:152:VAL:HG13	1.92	0.49
1:A:270:LEU:HA	6:A:529:HOH:O	2.12	0.49
1:A:266:LEU:HD11	1:A:270:LEU:CD2	2.25	0.49
1:A:6:ARG:HD3	1:A:100:GLY:HA3	1.94	0.49
1:A:102:ASP:CG	1:A:113:TYR:OH	2.52	0.48
1:A:219:ARG:HA	1:A:256:ARG:O	2.12	0.48
1:A:218:GLN:HA	1:A:222:GLU:O	2.14	0.48
1:A:194:VAL:HG12	1:A:195:PHE:N	2.28	0.47
1:A:9:SER:OG	1:A:97:TRP:HB3	2.15	0.47
1:A:145:ARG:HD3	6:A:523:HOH:O	2.15	0.47
1:A:28:VAL:HG11	1:A:179:LEU:CD1	2.39	0.46
1:A:184:PRO:CB	1:A:266:LEU:CD2	2.93	0.46
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.34	0.46
1:A:182:ALA:HB1	1:A:265:GLY:HA2	1.96	0.46
1:A:218:GLN:NE2	1:A:260:HIS:HB2	2.30	0.46
2:B:47:GLU:O	2:B:48:LYS:HG2	2.15	0.46
2:B:16:GLU:O	2:B:16:GLU:CG	2.63	0.46
1:A:218:GLN:N	1:A:258:THR:O	2.42	0.46
1:A:272:LEU:N	1:A:272:LEU:HD12	2.31	0.46
1:A:270:LEU:H	1:A:270:LEU:CD2	2.24	0.46
1:A:51:TRP:CZ3	1:A:171:TYR:HB3	2.51	0.45
1:A:34:VAL:CG2	1:A:45:MET:CG	2.88	0.45
2:B:11:SER:HA	2:B:22:PHE:O	2.16	0.45
1:A:146:LYS:HD3	6:A:410:HOH:O	2.15	0.45
3:P:5:ARG:HG2	6:P:19:HOH:O	2.16	0.45
2:B:94:LYS:HE3	6:B:1081:HOH:O	2.16	0.45
2:B:20:SER:CB	2:B:71:THR:HG22	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:GLN:OE1	1:A:35:ARG:HD3	2.17	0.45
1:A:82:ARG:NH1	6:A:377:HOH:O	2.50	0.45
2:B:21:ASN:CG	2:B:22:PHE:H	2.21	0.45
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.44
1:A:224:GLN:O	1:A:226:GLN:N	2.51	0.44
1:A:34:VAL:HG22	1:A:45:MET:CG	2.46	0.43
1:A:185:PRO:HB3	1:A:208:PHE:HB3	1.99	0.43
2:B:38:ASP:OD1	2:B:45:ARG:NH1	2.51	0.43
1:A:191:HIS:CE1	1:A:254:GLU:HG2	2.54	0.43
1:A:182:ALA:HB3	6:A:569:HOH:O	2.17	0.43
1:A:8:PHE:HB3	2:B:56:PHE:CZ	2.53	0.43
1:A:255:GLN:HG3	1:A:273:ARG:HD3	1.99	0.43
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.52	0.43
1:A:170:ARG:NH2	6:A:546:HOH:O	2.52	0.42
1:A:232:GLU:HB2	6:A:530:HOH:O	2.19	0.42
1:A:218:GLN:NE2	6:A:339:HOH:O	2.52	0.42
1:A:273:ARG:HH11	1:A:273:ARG:CB	2.31	0.42
1:A:194:VAL:HG12	1:A:197:TYR:HE2	1.74	0.42
2:B:27:VAL:HG11	2:B:35:ILE:HD11	2.02	0.42
2:B:27:VAL:HG11	2:B:35:ILE:HD13	2.02	0.42
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.89	0.42
1:A:196:ASP:CG	6:A:454:HOH:O	2.58	0.41
1:A:191:HIS:HB2	1:A:274:TRP:CE2	2.55	0.41
1:A:182:ALA:HB1	1:A:265:GLY:CA	2.51	0.41
1:A:184:PRO:CB	1:A:266:LEU:HD22	2.51	0.41
1:A:270:LEU:N	1:A:270:LEU:HD23	2.30	0.41
1:A:115:ARG:HG3	2:B:60:TRP:CH2	2.56	0.41
1:A:185:PRO:HB3	1:A:208:PHE:CD1	2.56	0.41
1:A:34:VAL:HG21	1:A:45:MET:CG	2.50	0.41
1:A:129:ASP:O	1:A:131:ARG:HG3	2.21	0.41
1:A:106:ASP:N	1:A:106:ASP:OD1	2.51	0.41
2:B:45:ARG:HG3	2:B:45:ARG:O	2.21	0.41
1:A:225:THR:HA	6:A:551:HOH:O	2.21	0.41
2:B:51:HIS:NE2	6:B:1004:HOH:O	2.37	0.40
1:A:254:GLU:H	1:A:254:GLU:CD	2.24	0.40
2:B:9:VAL:CG1	2:B:95:TRP:HB2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:PHE:CZ	6:A:568:HOH:O[5_565]	2.10	0.10

## 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	273/275 (99%)	261 (96%)	9 (3%)	3 (1%)	21	7
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100
All	All	378/384 (98%)	362 (96%)	13 (3%)	3 (1%)	27	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	195	PHE
1	A	225	THR

### 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	232/232 (100%)	221 (95%)	11 (5%)	36	22
2	B	95/95 (100%)	92 (97%)	3 (3%)	51	39
3	P	9/9 (100%)	8 (89%)	1 (11%)	9	3
All	All	336/336 (100%)	321 (96%)	15 (4%)	38	24

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	74	ASP
1	A	108	ARG

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Mol	Chain	Res	Type
1	A	113	TYR
1	A	177	GLU
1	A	195	PHE
1	A	220	ASP
1	A	223	ASP
1	A	255	GLN
1	A	266	LEU
1	A	267	PRO
2	B	20	SER
2	B	45	ARG
2	B	70	PHE
3	P	1	ARG

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

Mol	Chain	Res	Type
1	A	87	GLN
1	A	127	ASN
1	A	180	GLN
1	A	191	HIS
1	A	218	GLN
1	A	255	GLN
1	A	260	HIS
2	B	21	ASN
2	B	83	ASN
2	B	89	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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