



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:13 PM UTC

PDB ID : 1YDP / pdb_00001ydp
Title : 1.9A crystal structure of HLA-G
Authors : Clements, C.S.; Kjer-nielsen, L.; Kostenko, L.; Hoare, H.L.; Dunstone, M.A.;
Moses, E.; Freed, K.; Brooks, A.G.; Rossjohn, J.; McCluskey, J.
Deposited on : 2004-12-25
Resolution : 1.90 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
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

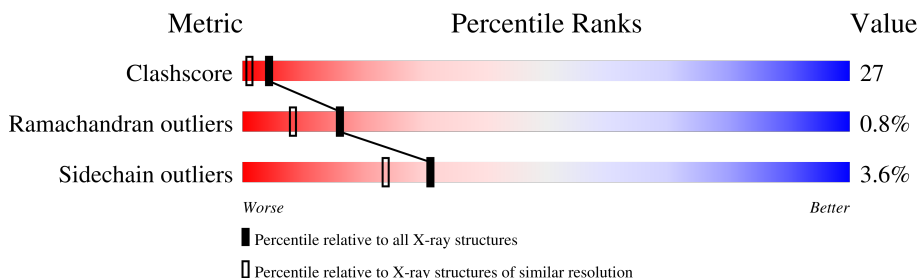
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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	275	 64% 29% 5% •
2	B	100	 59% 34% • •
3	P	9	 56% 33% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3590 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 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 mutation	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 (CCD ID: CO) (formula: Co).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is water.

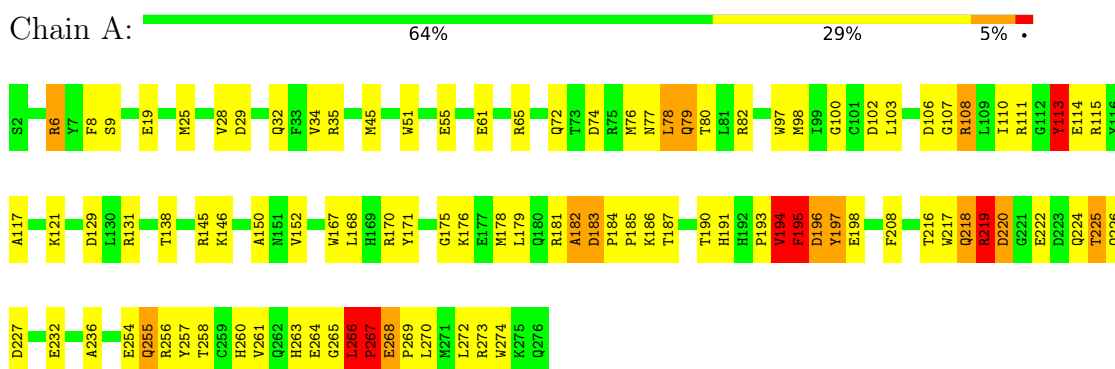
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	311	Total	O	0	0
			311	311		
6	B	105	Total	O	0	0
			105	105		
6	P	11	Total	O	0	0
			11	11		

3 Residue-property plots

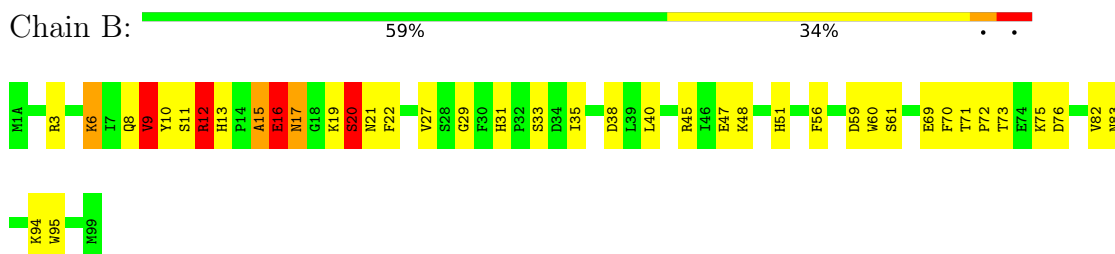
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	48.0	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: 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	1.11	17/2303 (0.7%)	1.53	48/3124 (1.5%)
2	B	1.82	9/860 (1.0%)	1.49	17/1162 (1.5%)
3	P	0.48	0/82	1.20	2/108 (1.9%)
All	All	1.32	26/3245 (0.8%)	1.51	67/4394 (1.5%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	VAL	C-N	-27.31	0.97	1.33
2	B	15	ALA	C-N	20.49	1.65	1.33
2	B	12	ARG	CD-NE	-20.28	1.17	1.46
2	B	16	GLU	C-N	-18.72	1.08	1.33
1	A	182	ALA	C-N	18.24	1.62	1.33
2	B	82	VAL	C-N	18.20	1.59	1.33
2	B	83	ASN	C-N	-17.69	1.11	1.33
1	A	217	TRP	C-N	15.92	1.56	1.33
1	A	190	THR	C-N	-14.94	1.13	1.33
1	A	176	LYS	C-N	-14.83	1.14	1.34
1	A	266	LEU	CB-CG	14.82	1.83	1.53
1	A	267	PRO	N-CD	11.22	1.63	1.47
1	A	268	GLU	C-N	-10.55	1.21	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	GLU	CB-CG	-10.34	1.21	1.52
1	A	219	ARG	CA-CB	-9.58	1.38	1.53
1	A	267	PRO	CB-CG	8.25	1.90	1.49
1	A	138	THR	C-N	-8.17	1.23	1.33
2	B	17	ASN	CB-CG	-7.78	1.32	1.52
1	A	80	THR	N-CA	7.15	1.55	1.46
1	A	78	LEU	CA-C	-7.03	1.43	1.52
1	A	219	ARG	CD-NE	-6.87	1.36	1.46
1	A	220	ASP	C-N	-6.84	1.23	1.33
2	B	8	GLN	C-N	6.79	1.43	1.33
2	B	20	SER	C-N	-6.20	1.28	1.33
1	A	113	TYR	CA-C	-5.94	1.46	1.53
1	A	175	GLY	C-N	5.90	1.41	1.33

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	CD-NE-CZ	28.11	163.75	124.40
2	B	9	VAL	O-C-N	-20.88	91.93	122.20
1	A	220	ASP	CA-CB-CG	20.86	133.47	112.60
1	A	195	PHE	CA-CB-CG	16.58	130.38	113.80
1	A	176	LYS	O-C-N	-13.79	106.26	122.11
2	B	82	VAL	CA-C-N	-12.24	104.58	122.94
2	B	82	VAL	C-N-CA	-12.24	104.58	122.94
2	B	15	ALA	CA-C-N	-12.19	102.99	122.73
2	B	15	ALA	C-N-CA	-12.19	102.99	122.73
1	A	194	VAL	CA-C-N	-11.51	99.55	121.54
1	A	194	VAL	C-N-CA	-11.51	99.55	121.54
1	A	268	GLU	CA-CB-CG	11.21	136.52	114.10
1	A	182	ALA	CA-C-N	-11.18	104.62	120.49
1	A	182	ALA	C-N-CA	-11.18	104.62	120.49
1	A	190	THR	O-C-N	-11.14	109.12	123.16
2	B	17	ASN	CA-CB-CG	10.70	123.30	112.60
1	A	218	GLN	OE1-CD-NE2	-10.46	112.14	122.60
1	A	78	LEU	CA-C-N	-10.00	104.63	121.92
1	A	78	LEU	C-N-CA	-10.00	104.63	121.92
1	A	219	ARG	CB-CA-C	-9.93	94.75	110.74
2	B	83	ASN	O-C-N	-9.70	110.62	123.23
1	A	218	GLN	CB-CG-CD	-9.03	97.24	112.60
1	A	79	GLN	OE1-CD-NE2	-9.03	113.57	122.60
2	B	9	VAL	CA-C-N	8.66	136.22	122.36
2	B	9	VAL	C-N-CA	8.66	136.22	122.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	CB-CG-OD2	8.30	137.49	118.40
1	A	220	ASP	CB-CG-OD1	-8.23	99.48	118.40
1	A	113	TYR	CB-CA-C	-8.19	95.57	114.41
2	B	16	GLU	O-C-N	-8.15	113.32	123.27
1	A	79	GLN	CG-CD-NE2	7.56	127.74	116.40
1	A	267	PRO	N-CA-CB	7.31	110.92	103.25
1	A	268	GLU	CB-CG-CD	6.98	124.47	112.60
2	B	17	ASN	CB-CG-ND2	-6.76	106.26	116.40
1	A	138	THR	O-C-N	-6.65	113.52	122.43
2	B	8	GLN	CA-C-N	-6.57	114.98	122.93
2	B	8	GLN	C-N-CA	-6.57	114.98	122.93
2	B	16	GLU	CA-C-N	-6.39	111.80	120.82
2	B	16	GLU	C-N-CA	-6.39	111.80	120.82
1	A	218	GLN	CG-CD-NE2	6.37	125.95	116.40
1	A	197	TYR	N-CA-C	6.36	119.16	111.40
1	A	78	LEU	N-CA-C	-6.35	103.64	111.33
1	A	183	ASP	O-C-N	-6.35	114.32	121.43
1	A	266	LEU	CB-CG-CD1	6.27	129.50	110.70
1	A	195	PHE	CB-CG-CD1	-6.16	110.22	120.70
1	A	80	THR	N-CA-C	6.04	117.86	111.28
1	A	220	ASP	O-C-N	5.98	131.85	122.23
1	A	195	PHE	CB-CG-CD2	5.97	130.86	120.70
1	A	195	PHE	N-CA-C	5.92	123.42	110.80
1	A	267	PRO	CA-CB-CG	-5.85	93.39	104.50
2	B	33	SER	N-CA-C	5.85	119.68	112.54
1	A	264	GLU	O-C-N	-5.78	116.08	122.09
1	A	267	PRO	CA-N-CD	-5.73	103.98	112.00
1	A	79	GLN	CB-CG-CD	5.60	122.12	112.60
1	A	196	ASP	CA-C-N	5.60	130.06	120.71
1	A	196	ASP	C-N-CA	5.60	130.06	120.71
1	A	176	LYS	CA-C-N	5.56	128.28	120.28
1	A	176	LYS	C-N-CA	5.56	128.28	120.28
1	A	198	GLU	N-CA-C	5.55	117.71	108.99
1	A	6	ARG	CB-CA-C	-5.52	97.31	109.56
2	B	6	LYS	N-CA-C	-5.39	100.91	109.96
1	A	113	TYR	CA-CB-CG	-5.30	104.35	113.90
3	P	6	HIS	N-CA-C	-5.26	102.73	110.52
1	A	110	ILE	N-CA-C	-5.26	107.70	112.96
1	A	186	LYS	N-CA-C	-5.25	101.21	109.25
3	P	3	ILE	N-CA-C	-5.14	103.30	108.96
1	A	29	ASP	CB-CA-C	-5.06	110.76	116.63
1	A	218	GLN	CA-CB-CG	-5.05	103.99	114.10

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 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	2242	0	2094	123	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	165	1

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 27.

All (165) 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:A:266:LEU:CB	1:A:266:LEU:CG	1.83	1.53
1:A:266:LEU:CD1	1:A:270:LEU:HD22	1.43	1.47
1:A:267:PRO:CB	1:A:267:PRO:CG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.80
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:194:VAL:O	1:A:195:PHE:C	2.26	0.76
1:A:187:THR:HB	1:A:272:LEU:HD21	1.71	0.73
1:A:270:LEU:H	1:A:270:LEU:HD23	1.53	0.73
1:A:34:VAL:HG22	1:A:45:MET:HG3	1.73	0.71
1:A:218:GLN:O	1:A:257:TYR:HA	1.91	0.71
2:B:16:GLU:CG	2:B:19:LYS:HB2	2.20	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: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
1:A:76:MET:O	1:A:76:MET:HE3	1.94	0.66
2:B:22:PHE:CE1	2:B:69:GLU:HG2	2.30	0.66
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
2:B:16:GLU:CD	2:B:19:LYS:HB2	2.22	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:ASP:HB2	1:A:111:ARG:HG2	1.82	0.61
1:A:266:LEU:HG	1:A:266:LEU:HB2	1.73	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
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:O	2:B:16:GLU:HG3	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:HB2	1:A:108:ARG:CZ	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:HB2	1:A:273:ARG:HH11	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:61:GLU:HG2	6:A:449:HOH:O	2.08	0.53
1:A:167:TRP:CE2	3:P:1:ARG:HG3	2.43	0.53
1:A:273:ARG:HB2	1:A:273:ARG:NH1	2.24	0.53
1:A:194:VAL:CG1	1:A:197:TYR:CZ	2.92	0.53
1:A:102:ASP:CG	1:A:113:TYR:OH	2.52	0.53
1:A:224:GLN:HA	6:A:468:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:227:ASP:HB2	6:A:541:HOH:O	2.12	0.49
2:B:10:TYR:CD1	2:B:10:TYR:N	2.80	0.49
2:B:16:GLU:OE2	2:B:19:LYS:HG2	2.11	0.49
1:A:150:ALA:HB3	1:A:152:VAL:HG13	1.92	0.49
2:B:21:ASN:CG	2:B:22:PHE:H	2.21	0.49
1:A:270:LEU:HA	6:A:529:HOH:O	2.12	0.49
1:A:6:ARG:HD3	1:A:100:GLY:HA3	1.94	0.49
1:A:266:LEU:HD11	1:A:270:LEU:CD2	2.25	0.49
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
1:A:218:GLN:N	1:A:258:THR:O	2.42	0.46
1:A:272:LEU:HD12	1:A:272:LEU:N	2.31	0.46
2:B:16:GLU:O	2:B:16:GLU:CG	2.63	0.46
1:A:270:LEU:CD2	1:A:270:LEU:H	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
1:A:146:LYS:HD3	6:A:410:HOH:O	2.15	0.45
2:B:11:SER:HA	2:B:22:PHE:O	2.16	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
1:A:32:GLN:OE1	1:A:35:ARG:HD3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:SER:CB	2:B:71:THR:HG22	2.47	0.45
1:A:82:ARG:NH1	6:A:377:HOH:O	2.50	0.45
1:A:196:ASP:CG	6:A:454:HOH:O	2.58	0.44
1:A:254:GLU:H	1:A:254:GLU:CD	2.24	0.44
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:77:ASN:C	1:A:79:GLN:N	2.75	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
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.89	0.42
2:B:27:VAL:HG11	2:B:35:ILE:HD13	2.02	0.42
1:A:182:ALA:HB1	1:A:265:GLY:CA	2.51	0.41
1:A:191:HIS:HB2	1:A:274:TRP:CE2	2.55	0.41
1:A:76:MET:HE3	1:A:79:GLN:HG3	2.02	0.41
1:A:184:PRO:CB	1:A:266:LEU:HD22	2.51	0.41
1:A:270:LEU:HD23	1:A:270:LEU:N	2.30	0.41
1:A:115:ARG:HG3	2:B:60:TRP:CH2	2.56	0.41
1:A:34:VAL:HG21	1:A:45:MET:CG	2.50	0.41
1:A:106:ASP:OD1	1:A:106:ASP:N	2.51	0.41
1:A:129:ASP:O	1:A:131:ARG:HG3	2.21	0.41
1:A:185:PRO:HB3	1:A:208:PHE:CD1	2.56	0.41
1:A:225:THR:HA	6:A:551:HOH:O	2.21	0.41
2:B:45:ARG:O	2:B:45:ARG:HG3	2.21	0.41
2:B:51:HIS:NE2	6:B:1004:HOH:O	2.37	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PHE:CZ	6:A:568:HOH:O[5_565]	2.10	0.10

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	273/275 (99%)	261 (96%)	9 (3%)	3 (1%)	11	4
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%)	16	8

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 [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	232/232 (100%)	222 (96%)	10 (4%)	26	18
2	B	95/95 (100%)	94 (99%)	1 (1%)	65	67
3	P	9/9 (100%)	8 (89%)	1 (11%)	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	336/336 (100%)	324 (96%)	12 (4%)	31	23

All (12) 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
1	A	113	TYR
1	A	121	LYS
1	A	195	PHE
1	A	220	ASP
1	A	255	GLN
1	A	266	LEU
1	A	267	PRO
2	B	20	SER
3	P	1	ARG

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

Mol	Chain	Res	Type
1	A	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
1	A	262	GLN
2	B	21	ASN
2	B	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	4
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	15:ALA	C	16:GLU	N	1.65
1	A	182:ALA	C	183:ASP	N	1.62
1	A	176:LYS	C	177:GLU	N	1.14
1	A	190:THR	C	191:HIS	N	1.13
1	B	83:ASN	C	84:HIS	N	1.12
1	B	16:GLU	C	17:ASN	N	1.08
1	B	9:VAL	C	10:TYR	N	0.97

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.