



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:22 AM UTC

PDB ID : 6QZA / pdb_00006qza
Title : HLA-DR1 with GMF Influenza PB1 Peptide
Authors : Greenshields-Watson, A.; Rizkallah, P.J.
Deposited on : 2019-03-11
Resolution : 3.09 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

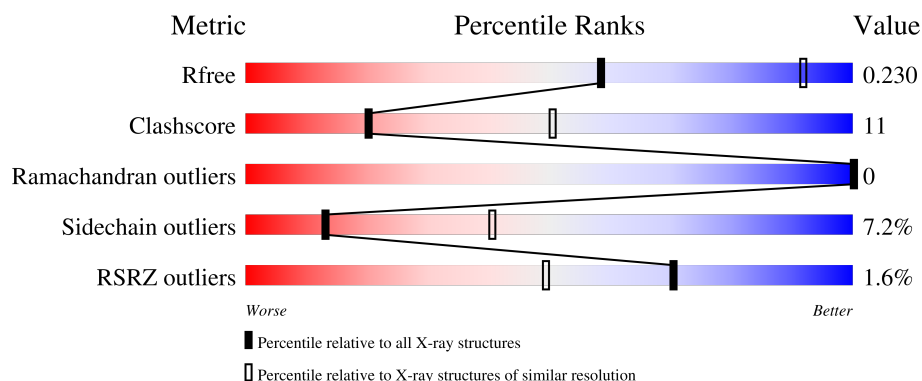
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	AAA	183	0% 65% 30% ..
1	DDD	183	0% 66% 30% ..
2	BBB	191	3% 69% 26% ..
2	EEE	191	2% 66% 27% 5%
3	CCC	20	65% 10% 25%

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Mol	Chain	Length	Quality of chain
3	FFF	20	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6148 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	179	Total	C	N	O	S	0	0	0
			1469	951	238	275	5			
1	DDD	179	Total	C	N	O	S	0	0	0
			1465	948	237	275	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP P01903
DDD	0	MET	-	initiating methionine	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	187	Total	C	N	O	S	0	0	0
			1525	957	273	289	6			
2	EEE	181	Total	C	N	O	S	0	0	0
			1481	933	263	279	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	MET	-	initiating methionine	UNP P04229
EEE	0	MET	-	initiating methionine	UNP P04229

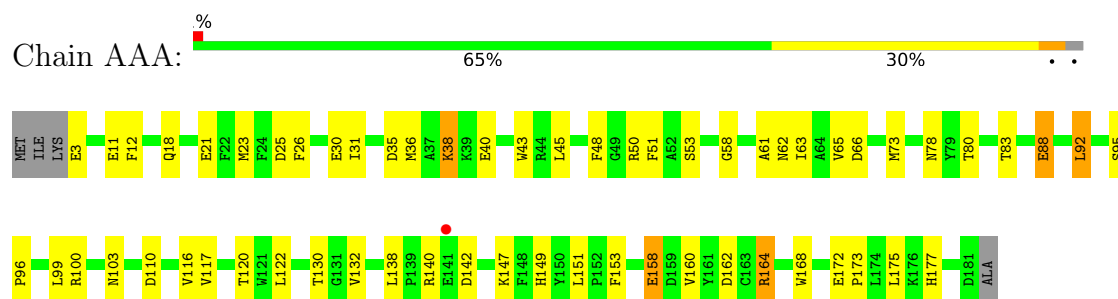
- Molecule 3 is a protein called PB1-410-422-GMF-Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	15	Total	C	N	O	S	0	0	0
			108	70	16	19	3			
3	FFF	14	Total	C	N	O	S	0	0	0
			100	65	15	18	2			

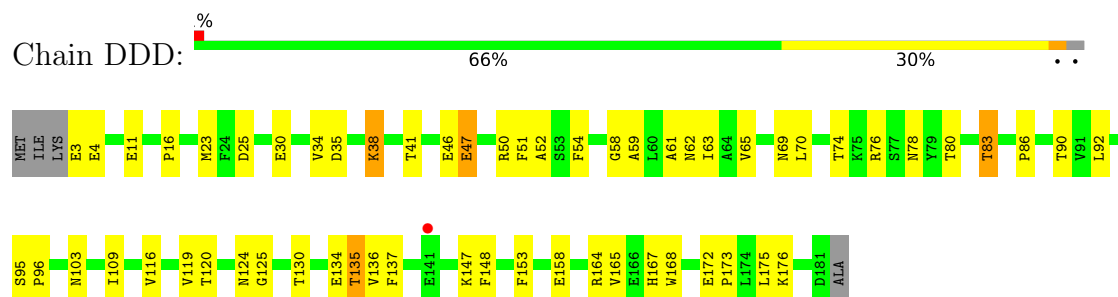
3 Residue-property plots [i](#)

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 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.

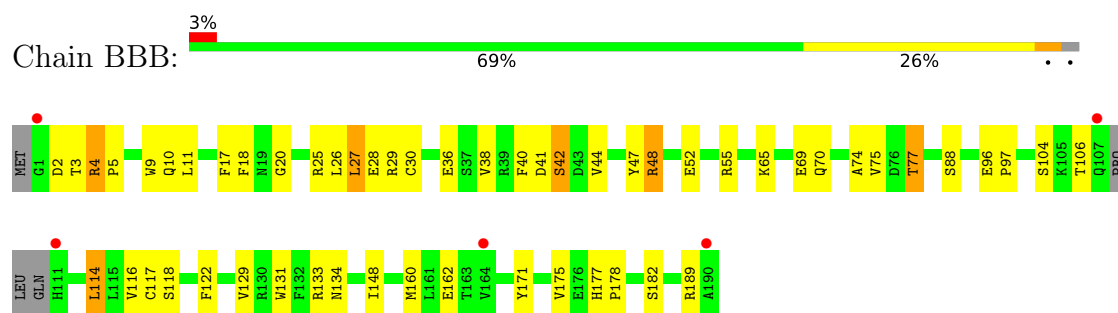
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



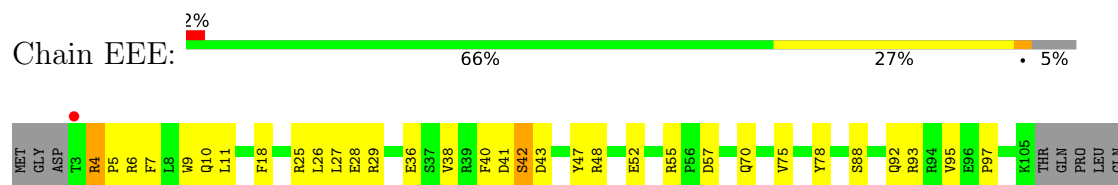
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

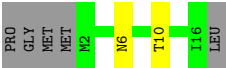


- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

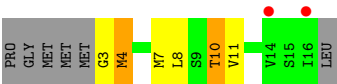




● Molecule 3: PB1-410-422-GMF-Peptide



● Molecule 3: PB1-410-422-GMF-Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.02Å 184.02Å 87.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.01 – 3.09 92.01 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (92.01-3.09) 99.5 (92.01-3.09)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.226 0.185 , 0.230	Depositor DCC
R_{free} test set	1533 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6148	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	AAA	0.62	0/1514	1.22	10/2066 (0.5%)
1	DDD	0.55	0/1510	1.14	6/2062 (0.3%)
2	BBB	0.67	0/1563	1.23	7/2122 (0.3%)
2	EEE	0.58	0/1517	1.12	3/2058 (0.1%)
3	CCC	0.69	0/108	1.32	1/143 (0.7%)
3	FFF	0.63	0/100	1.13	0/133
All	All	0.61	0/6312	1.18	27/8584 (0.3%)

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	DDD	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	3	THR	CB-CA-C	8.83	125.28	110.44
1	AAA	80	THR	CA-CB-OG1	-7.67	98.10	109.60
3	CCC	6	ASN	CB-CA-C	-7.40	97.60	109.80
2	BBB	3	THR	CA-CB-OG1	-7.11	98.93	109.60
1	AAA	78	ASN	CA-CB-CG	-6.68	105.92	112.60
1	DDD	78	ASN	CB-CA-C	-6.11	103.06	111.73
1	DDD	80	THR	CA-CB-OG1	-6.09	100.46	109.60
2	BBB	3	THR	N-CA-C	-6.08	103.97	113.02
1	AAA	88	GLU	CB-CA-C	5.94	120.23	109.37
1	AAA	73	MET	CG-SD-CE	-5.90	87.92	100.90
2	BBB	162	GLU	CB-CG-CD	5.90	122.63	112.60
1	DDD	83	THR	CB-CA-C	5.76	119.68	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EEE	41	ASP	CA-CB-CG	5.68	118.28	112.60
1	AAA	110	ASP	CA-CB-CG	5.52	118.12	112.60
1	AAA	50	ARG	CB-CA-C	5.50	120.09	110.64
1	AAA	18	GLN	CB-CG-CD	-5.47	103.31	112.60
1	AAA	83	THR	CB-CA-C	5.40	119.06	109.72
2	BBB	5	PRO	CB-CA-C	-5.21	104.12	110.95
2	EEE	48	ARG	CB-CG-CD	5.20	123.26	111.30
1	AAA	164	ARG	CG-CD-NE	-5.19	100.58	112.00
1	AAA	92	LEU	N-CA-CB	-5.17	101.91	111.52
2	EEE	162	GLU	CB-CG-CD	5.13	121.32	112.60
2	BBB	4	ARG	CG-CD-NE	-5.12	100.73	112.00
1	DDD	4	GLU	CB-CA-C	5.12	119.31	110.86
2	BBB	41	ASP	CA-CB-CG	5.02	117.62	112.60
1	DDD	124	ASN	CB-CA-C	5.02	122.31	116.54
1	DDD	158	GLU	CB-CA-C	5.00	118.81	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	125	GLY	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	AAA	1469	0	1396	34	0
1	DDD	1465	0	1385	45	0
2	BBB	1525	0	1439	34	0
2	EEE	1481	0	1411	37	0
3	CCC	108	0	115	1	0
3	FFF	100	0	106	8	0
All	All	6148	0	5852	136	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 11.

All (136) 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)
2:BBB:48:ARG:HH11	2:BBB:48:ARG:HG2	1.03	1.09
1:DDD:135:THR:HG22	1:DDD:148:PHE:H	1.37	0.89
2:EEE:114:LEU:HD12	2:EEE:160:MET:HB3	1.57	0.86
2:EEE:133:ARG:HD2	2:EEE:171:TYR:CE1	2.11	0.85
2:BBB:74:ALA:HA	2:BBB:77:THR:HG23	1.64	0.80
1:DDD:135:THR:CG2	1:DDD:148:PHE:H	1.94	0.79
2:BBB:48:ARG:HG2	2:BBB:48:ARG:NH1	1.81	0.79
1:AAA:158:GLU:HA	1:AAA:158:GLU:OE1	1.87	0.75
2:EEE:133:ARG:HD2	2:EEE:171:TYR:HE1	1.53	0.73
1:DDD:46:GLU:HG3	1:DDD:47:GLU:N	2.08	0.69
2:BBB:48:ARG:HH11	2:BBB:48:ARG:CG	1.95	0.67
1:DDD:41:THR:HG21	1:DDD:54:PHE:HD2	1.59	0.67
2:EEE:29:ARG:HG2	2:EEE:36:GLU:OE2	1.96	0.66
2:BBB:29:ARG:HG2	2:BBB:36:GLU:OE2	1.96	0.66
2:EEE:97:PRO:HB3	2:EEE:122:PHE:HB3	1.77	0.66
2:EEE:4:ARG:HB2	2:EEE:5:PRO:HD2	1.79	0.65
2:EEE:78:TYR:CG	3:FFF:8:LEU:HD13	2.31	0.65
1:AAA:160:VAL:HB	1:AAA:177:HIS:HE1	1.63	0.64
1:AAA:66:ASP:OD1	3:CCC:10:THR:HG21	1.97	0.64
2:BBB:97:PRO:HB3	2:BBB:122:PHE:HB3	1.80	0.63
2:EEE:116:VAL:HG22	2:EEE:160:MET:HG2	1.81	0.63
1:DDD:134:GLU:OE1	1:DDD:147:LYS:NZ	2.32	0.63
2:BBB:114:LEU:CD1	2:BBB:160:MET:HB3	2.28	0.62
1:DDD:58:GLY:O	1:DDD:62:ASN:ND2	2.30	0.62
1:DDD:11:GLU:HG3	2:EEE:11:LEU:HB2	1.81	0.62
1:AAA:3:GLU:HB3	2:BBB:18:PHE:CE2	2.35	0.62
2:EEE:93:ARG:NH1	2:EEE:95:VAL:HG21	2.17	0.60
1:DDD:109:ILE:CD1	1:DDD:119:VAL:HG21	2.31	0.60
1:DDD:109:ILE:HD11	1:DDD:119:VAL:HG21	1.83	0.60
2:EEE:93:ARG:HH11	2:EEE:95:VAL:HG21	1.66	0.60
1:DDD:136:VAL:HG22	1:DDD:137:PHE:N	2.19	0.58
2:BBB:69:GLU:OE1	2:EEE:140:ALA:HB1	2.03	0.58
1:DDD:135:THR:HG23	1:DDD:136:VAL:O	2.04	0.58
1:AAA:3:GLU:HB3	2:BBB:18:PHE:CD2	2.38	0.58
2:BBB:177:HIS:CD2	2:BBB:178:PRO:HD2	2.39	0.58
1:DDD:50:ARG:O	1:DDD:50:ARG:HG3	2.04	0.58
1:DDD:16:PRO:HD2	2:EEE:6:ARG:HD3	1.84	0.58
1:DDD:76:ARG:NH2	2:EEE:57:ASP:OD2	2.35	0.58
1:DDD:62:ASN:ND2	3:FFF:7:MET:HE1	2.19	0.57
1:AAA:36:MET:CE	1:AAA:63:ILE:HG13	2.34	0.57
2:EEE:52:GLU:HG2	2:EEE:55:ARG:HH22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:133:ARG:HG3	2:BBB:171:TYR:CE2	2.40	0.57
2:BBB:116:VAL:HG22	2:BBB:160:MET:HG2	1.87	0.56
2:BBB:104:SER:HB3	2:BBB:114:LEU:HB3	1.87	0.56
1:DDD:172:GLU:HG2	1:DDD:173:PRO:HD2	1.88	0.56
1:DDD:46:GLU:HG3	1:DDD:47:GLU:HG3	1.89	0.54
1:DDD:3:GLU:HB3	2:EEE:18:PHE:CE2	2.43	0.53
2:EEE:177:HIS:CD2	2:EEE:178:PRO:HD2	2.43	0.53
1:DDD:38:LYS:O	1:DDD:38:LYS:HG2	2.09	0.53
2:EEE:129:VAL:HG22	2:EEE:175:VAL:HG22	1.91	0.53
1:AAA:43:TRP:CZ2	1:AAA:53:SER:HA	2.44	0.52
1:DDD:136:VAL:HG22	1:DDD:137:PHE:H	1.72	0.52
1:DDD:46:GLU:HG3	1:DDD:47:GLU:H	1.74	0.52
1:DDD:23:MET:HE2	1:DDD:30:GLU:HG3	1.92	0.52
2:EEE:133:ARG:CD	2:EEE:171:TYR:HE1	2.21	0.52
2:BBB:129:VAL:HG22	2:BBB:175:VAL:HG22	1.92	0.51
1:DDD:74:THR:HG23	2:EEE:7:PHE:CD1	2.46	0.51
1:AAA:23:MET:HE3	1:AAA:138:LEU:HD23	1.92	0.51
1:DDD:116:VAL:HG11	1:DDD:168:TRP:CH2	2.45	0.51
2:BBB:177:HIS:CG	2:BBB:178:PRO:HD2	2.46	0.51
2:BBB:114:LEU:HD12	2:BBB:160:MET:HB3	1.92	0.51
2:BBB:117:CYS:HB2	2:BBB:131:TRP:CZ2	2.46	0.50
2:BBB:25:ARG:HE	2:BBB:27:LEU:HD11	1.76	0.50
1:DDD:47:GLU:O	1:DDD:51:PHE:CD2	2.65	0.50
1:DDD:54:PHE:HA	3:FFF:4:MET:HE3	1.93	0.50
2:EEE:11:LEU:HD11	3:FFF:10:THR:HG21	1.93	0.50
1:AAA:158:GLU:OE1	1:AAA:158:GLU:CA	2.59	0.50
1:AAA:11:GLU:OE1	1:AAA:62:ASN:HB3	2.12	0.50
1:AAA:11:GLU:HG3	2:BBB:11:LEU:HB2	1.93	0.49
1:AAA:132:VAL:HG12	1:AAA:151:LEU:HD13	1.94	0.49
2:EEE:117:CYS:HB2	2:EEE:131:TRP:CZ2	2.47	0.49
1:AAA:36:MET:HE3	1:AAA:63:ILE:HG13	1.94	0.49
1:AAA:35:ASP:OD2	1:AAA:38:LYS:HB2	2.13	0.49
1:DDD:164:ARG:HB2	1:DDD:175:LEU:CD2	2.43	0.49
1:AAA:147:LYS:HE3	1:AAA:149:HIS:NE2	2.28	0.48
1:DDD:95:SER:HB2	1:DDD:96:PRO:HD2	1.95	0.48
2:BBB:2:ASP:CG	2:BBB:4:ARG:HH11	2.20	0.48
1:DDD:176:LYS:HB2	1:DDD:176:LYS:HE2	1.67	0.47
1:DDD:59:ALA:O	1:DDD:63:ILE:HG12	2.15	0.47
1:AAA:164:ARG:HB2	1:AAA:175:LEU:CD2	2.44	0.47
2:BBB:48:ARG:NH1	2:BBB:48:ARG:CG	2.62	0.47
2:BBB:133:ARG:O	2:BBB:134:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EEE:28:GLU:HB3	2:EEE:40:PHE:HB3	1.96	0.47
1:AAA:95:SER:HB2	1:AAA:96:PRO:HD2	1.96	0.47
1:DDD:35:ASP:OD2	1:DDD:38:LYS:HB3	2.14	0.46
1:DDD:168:TRP:CH2	2:EEE:6:ARG:NH2	2.83	0.46
1:AAA:122:LEU:HB2	1:AAA:162:ASP:HB2	1.98	0.46
1:DDD:119:VAL:HG22	1:DDD:165:VAL:HG22	1.98	0.46
1:DDD:86:PRO:HA	1:DDD:167:HIS:HD2	1.80	0.46
2:EEE:26:LEU:H	2:EEE:42:SER:HB3	1.80	0.46
1:AAA:43:TRP:HZ2	1:AAA:53:SER:HA	1.78	0.46
1:AAA:140:ARG:NH1	1:AAA:142:ASP:OD2	2.49	0.46
2:BBB:96:GLU:HG3	2:BBB:97:PRO:HD2	1.98	0.46
2:EEE:187:GLU:H	2:EEE:187:GLU:HG2	1.53	0.46
2:EEE:78:TYR:CG	3:FFF:8:LEU:CD1	2.97	0.46
1:AAA:45:LEU:HD12	1:AAA:48:PHE:CZ	2.51	0.45
1:AAA:103:ASN:HB3	1:AAA:153:PHE:CE1	2.51	0.45
2:BBB:52:GLU:OE2	2:BBB:55:ARG:HD2	2.15	0.45
1:DDD:52:ALA:HA	3:FFF:3:GLY:O	2.16	0.45
2:BBB:114:LEU:HD11	2:BBB:160:MET:HB3	1.97	0.45
2:EEE:133:ARG:O	2:EEE:134:ASN:HB2	2.15	0.45
2:EEE:25:ARG:HE	2:EEE:27:LEU:HD11	1.82	0.45
2:EEE:177:HIS:CG	2:EEE:178:PRO:HD2	2.51	0.45
1:AAA:58:GLY:O	1:AAA:61:ALA:HB3	2.16	0.45
1:AAA:61:ALA:O	1:AAA:65:VAL:HG23	2.16	0.45
1:DDD:70:LEU:HD13	2:EEE:9:TRP:HB2	2.00	0.44
2:BBB:28:GLU:HB3	2:BBB:40:PHE:HB3	1.99	0.44
1:DDD:61:ALA:O	1:DDD:65:VAL:HG23	2.17	0.44
1:AAA:117:VAL:O	1:AAA:117:VAL:CG1	2.65	0.44
2:BBB:26:LEU:H	2:BBB:42:SER:HB3	1.82	0.44
1:DDD:103:ASN:HB3	1:DDD:153:PHE:CE1	2.53	0.43
1:AAA:99:LEU:O	1:AAA:100:ARG:HB2	2.17	0.43
1:AAA:92:LEU:HD21	2:BBB:148:ILE:HG21	1.99	0.43
1:AAA:175:LEU:HD23	1:AAA:175:LEU:HA	1.86	0.43
1:AAA:12:PHE:CZ	1:AAA:21:GLU:HG3	2.53	0.43
2:BBB:65:LYS:O	2:BBB:69:GLU:HG2	2.19	0.43
1:AAA:116:VAL:HG11	1:AAA:168:TRP:CH2	2.54	0.43
2:BBB:40:PHE:HB2	2:BBB:47:TYR:CE2	2.54	0.43
1:DDD:46:GLU:OE2	1:DDD:50:ARG:NH2	2.52	0.43
2:EEE:88:SER:HA	2:EEE:92:GLN:NE2	2.34	0.43
2:BBB:9:TRP:CH2	2:BBB:30:CYS:HB3	2.54	0.42
2:BBB:44:VAL:HG13	2:EEE:144:SER:O	2.18	0.42
1:DDD:135:THR:CG2	1:DDD:148:PHE:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EEE:40:PHE:HB2	2:EEE:47:TYR:CE2	2.55	0.42
1:DDD:86:PRO:HA	1:DDD:167:HIS:CD2	2.54	0.42
1:AAA:160:VAL:HB	1:AAA:177:HIS:CE1	2.50	0.42
1:DDD:54:PHE:CA	3:FFF:4:MET:HE3	2.49	0.42
2:EEE:78:TYR:CD2	3:FFF:8:LEU:HD13	2.54	0.42
1:DDD:11:GLU:OE1	1:DDD:62:ASN:HB3	2.21	0.41
1:DDD:69:ASN:ND2	2:EEE:9:TRP:CH2	2.88	0.41
1:DDD:109:ILE:HD13	1:DDD:119:VAL:HG21	2.03	0.41
2:EEE:25:ARG:NH1	2:EEE:43:ASP:OD2	2.54	0.41
1:AAA:26:PHE:HB2	1:AAA:31:ILE:HD11	2.02	0.41
2:BBB:17:PHE:HB3	2:BBB:20:GLY:O	2.20	0.41
1:AAA:172:GLU:HB3	1:AAA:173:PRO:HD2	2.04	0.40
1:AAA:23:MET:HE2	1:AAA:30:GLU:HG3	2.03	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	AAA	177/183 (97%)	169 (96%)	8 (4%)	0	100	100
1	DDD	177/183 (97%)	171 (97%)	6 (3%)	0	100	100
2	BBB	183/191 (96%)	171 (93%)	12 (7%)	0	100	100
2	EEE	177/191 (93%)	170 (96%)	7 (4%)	0	100	100
3	CCC	13/20 (65%)	13 (100%)	0	0	100	100
3	FFF	12/20 (60%)	12 (100%)	0	0	100	100
All	All	739/788 (94%)	706 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	163/167 (98%)	155 (95%)	8 (5%)	22	53
1	DDD	162/167 (97%)	152 (94%)	10 (6%)	16	46
2	BBB	166/172 (96%)	152 (92%)	14 (8%)	10	35
2	EEE	162/172 (94%)	148 (91%)	14 (9%)	10	34
3	CCC	13/17 (76%)	13 (100%)	0	100	100
3	FFF	12/17 (71%)	9 (75%)	3 (25%)	0	2
All	All	678/712 (95%)	629 (93%)	49 (7%)	13	40

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	25	ASP
1	AAA	38	LYS
1	AAA	40	GLU
1	AAA	51	PHE
1	AAA	88	GLU
1	AAA	120	THR
1	AAA	130	THR
1	AAA	158	GLU
2	BBB	10	GLN
2	BBB	27	LEU
2	BBB	38	VAL
2	BBB	42	SER
2	BBB	48	ARG
2	BBB	70	GLN
2	BBB	75	VAL
2	BBB	77	THR
2	BBB	88	SER
2	BBB	106	THR
2	BBB	114	LEU
2	BBB	118	SER
2	BBB	182	SER
2	BBB	189	ARG

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Mol	Chain	Res	Type
1	DDD	25	ASP
1	DDD	34	VAL
1	DDD	38	LYS
1	DDD	47	GLU
1	DDD	83	THR
1	DDD	90	THR
1	DDD	92	LEU
1	DDD	120	THR
1	DDD	130	THR
1	DDD	135	THR
2	EEE	4	ARG
2	EEE	10	GLN
2	EEE	38	VAL
2	EEE	42	SER
2	EEE	70	GLN
2	EEE	75	VAL
2	EEE	114	LEU
2	EEE	120	SER
2	EEE	138	GLU
2	EEE	172	THR
2	EEE	182	SER
2	EEE	185	THR
2	EEE	187	GLU
2	EEE	189	ARG
3	FFF	4	MET
3	FFF	10	THR
3	FFF	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	179/183 (97%)	-0.50	1 (0%) 85 70	32, 61, 106, 118	0
1	DDD	179/183 (97%)	-0.03	1 (0%) 85 70	59, 96, 141, 164	0
2	BBB	187/191 (97%)	-0.41	5 (2%) 56 35	39, 62, 106, 155	0
2	EEE	181/191 (94%)	-0.08	3 (1%) 69 48	54, 88, 136, 165	0
3	CCC	15/20 (75%)	-0.04	0 100 100	64, 70, 119, 141	0
3	FFF	14/20 (70%)	1.06	2 (14%) 6 3	94, 117, 161, 169	0
All	All	755/788 (95%)	-0.23	12 (1%) 70 49	32, 77, 133, 169	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	FFF	16	ILE	4.7
2	EEE	3	THR	3.0
2	BBB	111	HIS	2.9
2	BBB	1	GLY	2.9
1	DDD	141	GLU	2.7
2	EEE	113	ASN	2.6
2	BBB	190	ALA	2.3
3	FFF	14	VAL	2.2
2	EEE	164	VAL	2.1
1	AAA	141	GLU	2.1
2	BBB	164	VAL	2.0
2	BBB	107	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.