Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 03:39 AM EDT

PDB ID	:	7LKI
Title	:	The crystal structure of Epitope III of HCV envelop protein E2 in complex with antibody 1H8
Authors	:	Deng, L.; Zhang, P.
Deposited on	:	2021-02-02
Resolution	:	2.00 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:

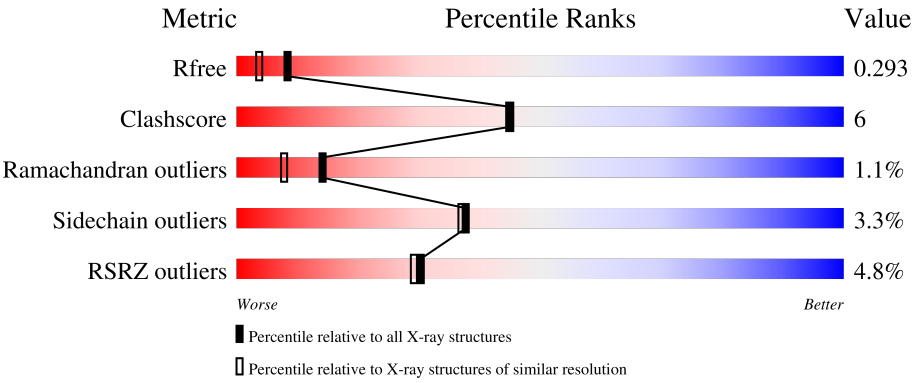
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	217	2% 85% 10%
1	DDD	217	4% 81% 12% 5%
2	BBB	218	% 83% 16%
2	EEE	218	12% 77% 17%
3	CCC	15	53% 47%

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Mol	Chain	Length	Quality of chain
3	FFF	15	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6986 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 antibody 1H8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	210	Total	C	N	O	S	0	0	0
			1585	999	260	318	8			
1	DDD	206	Total	C	N	O	S	0	0	0
			1554	981	255	310	8			

- Molecule 2 is a protein called antibody 1H8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	218	Total	C	N	O	S	0	0	0
			1686	1060	284	336	6			
2	EEE	209	Total	C	N	O	S	0	0	0
			1614	1021	268	319	6			

- Molecule 3 is a protein called Epitope III peptide GLY-ALA-PRO-THR-TYR-SER-TRP-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	8	Total	C	N	O	0	0	0
			59	39	9	11			
3	FFF	8	Total	C	N	O	0	0	0
			59	39	9	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	115	Total	O	0	0
			115	115		
4	BBB	116	Total	O	0	0
			116	116		
4	CCC	1	Total	O	0	0
			1	1		
4	DDD	114	Total	O	0	0
			114	114		

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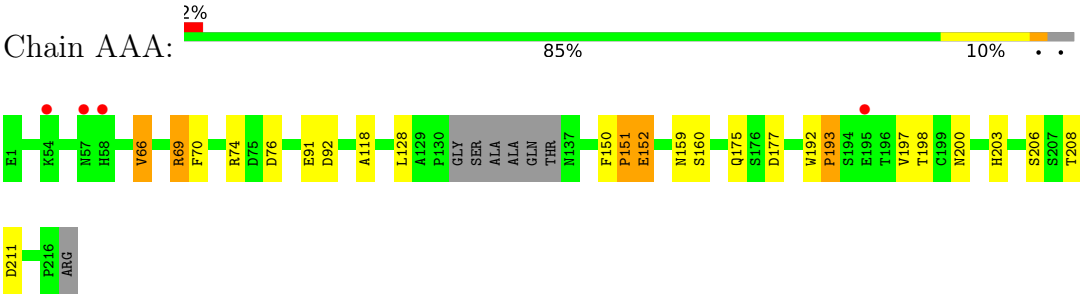
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	EEE	83	Total O 83 83	0	0

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.

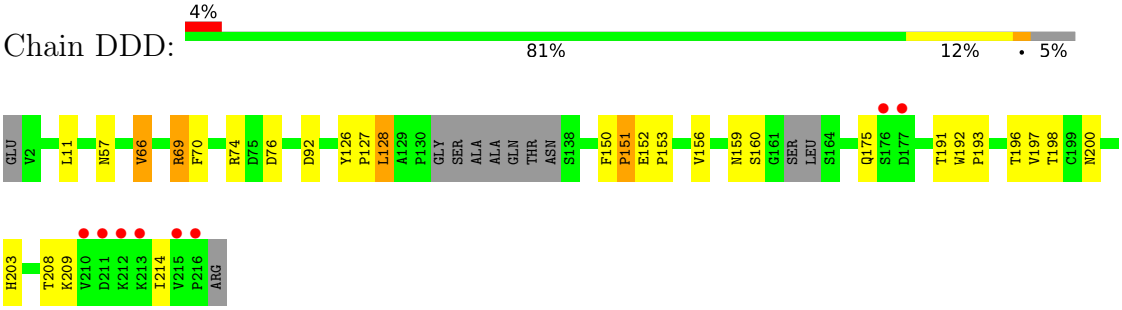
• Molecule 1: antibody 1H8 heavy chain

Chain AAA:



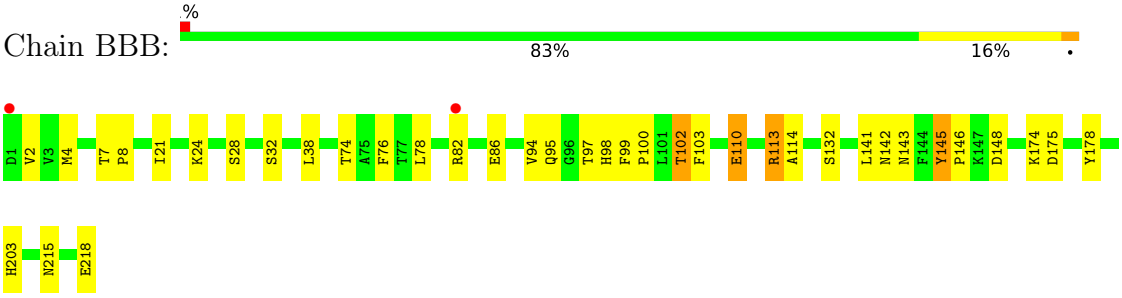
• Molecule 1: antibody 1H8 heavy chain

Chain DDD:



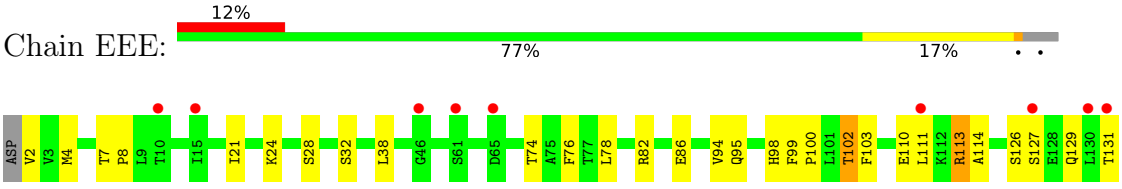
• Molecule 2: antibody 1H8 light chain

Chain BBB:



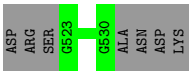
• Molecule 2: antibody 1H8 light chain

Chain EEE:



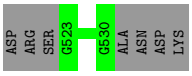
• Molecule 3: Epitope III peptide GLY-ALA-PRO-THR-TYR-SER-TRP-GLY

Chain CCC:



• Molecule 3: Epitope III peptide GLY-ALA-PRO-THR-TYR-SER-TRP-GLY

Chain FFF:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	201.68Å 42.79Å 110.82Å 90.00° 109.53° 90.00°	Depositor
Resolution (Å)	35.70 – 2.00 35.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.70-2.00) 98.4 (35.67-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.245 , 0.294 0.247 , 0.293	Depositor DCC
R_{free} test set	3030 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.72	1/1624 (0.1%)	0.89	2/2215 (0.1%)
1	DDD	0.69	0/1592	0.90	2/2170 (0.1%)
2	BBB	0.67	0/1723	0.82	0/2339
2	EEE	0.67	0/1650	0.81	0/2239
3	CCC	0.64	0/62	0.76	0/85
3	FFF	0.66	0/62	0.77	0/85
All	All	0.69	1/6713 (0.0%)	0.85	4/9133 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	5
1	DDD	0	6
2	BBB	0	4
2	EEE	0	4
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	152	GLU	CD-OE2	5.25	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DDD	69	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	AAA	69	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	DDD	69	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	AAA	69	ARG	NE-CZ-NH1	5.97	123.28	120.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	150	PHE	Peptide,Mainchain
1	AAA	152	GLU	Peptide,Mainchain
1	AAA	192	TRP	Peptide
2	BBB	145	TYR	Peptide
2	BBB	7	THR	Peptide
2	BBB	99	PHE	Peptide,Mainchain
1	DDD	150	PHE	Peptide,Mainchain
1	DDD	152	GLU	Peptide,Mainchain
1	DDD	192	TRP	Peptide,Mainchain
2	EEE	145	TYR	Peptide
2	EEE	7	THR	Peptide
2	EEE	99	PHE	Peptide,Mainchain

5.2 Too-close contacts (i)

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	1585	0	1540	20	0
1	DDD	1554	0	1508	23	0
2	BBB	1686	0	1654	22	0
2	EEE	1614	0	1589	27	1
3	CCC	59	0	48	0	0
3	FFF	59	0	48	0	0
4	AAA	115	0	0	4	0
4	BBB	116	0	0	1	0
4	CCC	1	0	0	0	0
4	DDD	114	0	0	4	0
4	EEE	83	0	0	3	0
All	All	6986	0	6387	84	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 6.

All (84) 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:EEE:111:LEU:HD23	2:EEE:176:SER:OG	1.40	1.17
2:BBB:95:GLN:HE22	2:BBB:98:HIS:H	1.11	0.98
2:EEE:95:GLN:HE22	2:EEE:98:HIS:H	1.05	0.95
2:EEE:95:GLN:NE2	2:EEE:98:HIS:H	1.63	0.94
2:BBB:95:GLN:NE2	2:BBB:98:HIS:H	1.69	0.89
2:EEE:95:GLN:HE22	2:EEE:98:HIS:N	1.78	0.81
1:AAA:160:SER:H	1:AAA:200:ASN:HD21	1.30	0.79
1:AAA:69:ARG:HD3	4:AAA:360:HOH:O	1.84	0.78
1:DDD:160:SER:H	1:DDD:200:ASN:HD21	1.32	0.76
2:EEE:111:LEU:HD23	2:EEE:176:SER:HG	1.48	0.74
1:DDD:74:ARG:HD3	1:DDD:76:ASP:OD1	1.89	0.73
2:BBB:95:GLN:HE22	2:BBB:98:HIS:N	1.86	0.73
2:EEE:127:SER:O	4:EEE:301:HOH:O	2.11	0.68
2:BBB:82:ARG:HG3	4:BBB:303:HOH:O	1.94	0.67
2:EEE:2:VAL:O	2:EEE:102:THR:HG21	1.95	0.66
1:AAA:177:ASP:CG	1:DDD:196:THR:HG23	2.16	0.65
2:BBB:215:ASN:HB3	2:BBB:218:GLU:HG2	1.79	0.65
2:BBB:2:VAL:O	2:BBB:102:THR:HG21	1.97	0.64
1:AAA:151:PRO:O	1:AAA:203:HIS:HE1	1.81	0.62
1:DDD:159:ASN:ND2	1:DDD:198:THR:H	1.98	0.61
1:AAA:74:ARG:HD3	1:AAA:76:ASP:OD1	2.01	0.60
1:DDD:160:SER:H	1:DDD:200:ASN:ND2	2.00	0.59
2:BBB:38:LEU:HD22	2:BBB:76:PHE:CG	2.37	0.59
1:DDD:57:ASN:ND2	4:DDD:301:HOH:O	2.12	0.59
2:EEE:113:ARG:HD3	2:EEE:114:ALA:O	2.02	0.59
1:AAA:66:VAL:HG13	1:AAA:70:PHE:HB2	1.85	0.58
2:EEE:146:PRO:HD2	2:EEE:203:HIS:CE1	2.39	0.58
1:AAA:160:SER:H	1:AAA:200:ASN:ND2	2.00	0.58
1:DDD:66:VAL:HG13	1:DDD:70:PHE:HB2	1.85	0.58
1:AAA:69:ARG:CD	4:AAA:360:HOH:O	2.45	0.58
1:DDD:151:PRO:O	1:DDD:203:HIS:HE1	1.85	0.57
1:AAA:177:ASP:OD2	1:DDD:196:THR:CG2	2.52	0.57
1:AAA:159:ASN:ND2	1:AAA:198:THR:H	2.03	0.57
1:DDD:127:PRO:O	2:EEE:126:SER:HB3	2.06	0.56
2:EEE:38:LEU:HD22	2:EEE:76:PHE:CG	2.40	0.56
2:EEE:82:ARG:NH1	4:EEE:302:HOH:O	2.37	0.55
2:BBB:28:SER:O	2:BBB:98:HIS:HE1	1.89	0.55
2:EEE:28:SER:O	2:EEE:98:HIS:HE1	1.89	0.55
1:AAA:177:ASP:OD2	1:DDD:196:THR:HG23	2.08	0.54
1:AAA:69:ARG:NH2	1:AAA:92:ASP:OD2	2.35	0.52
2:BBB:113:ARG:HD3	2:BBB:114:ALA:O	2.10	0.52
1:DDD:69:ARG:HD3	4:DDD:328:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:91:GLU:HG3	1:DDD:191:THR:CG2	2.40	0.52
1:AAA:159:ASN:HD21	1:AAA:197:VAL:HA	1.76	0.51
2:EEE:141:LEU:N	2:EEE:141:LEU:HD12	2.26	0.51
2:EEE:24:LYS:HA	2:EEE:74:THR:O	2.11	0.50
1:DDD:159:ASN:HD21	1:DDD:198:THR:H	1.58	0.50
1:DDD:214:ILE:O	4:DDD:302:HOH:O	2.19	0.50
2:BBB:21:ILE:HD11	2:BBB:78:LEU:HD23	1.94	0.50
1:AAA:208:THR:HG21	4:AAA:329:HOH:O	2.12	0.49
1:AAA:211:ASP:OD2	4:AAA:301:HOH:O	2.20	0.49
2:BBB:145:TYR:C	2:BBB:145:TYR:CD1	2.86	0.49
2:BBB:141:LEU:HD12	2:BBB:141:LEU:N	2.29	0.48
1:DDD:159:ASN:HD21	1:DDD:197:VAL:HA	1.80	0.47
2:EEE:131:THR:OG1	4:EEE:301:HOH:O	2.07	0.47
2:BBB:95:GLN:NE2	2:BBB:97:THR:N	2.63	0.47
2:BBB:110:GLU:CD	2:BBB:178:TYR:OH	2.54	0.46
2:BBB:4:MET:HG2	2:BBB:102:THR:HG23	1.98	0.46
2:BBB:24:LYS:HA	2:BBB:74:THR:O	2.16	0.46
2:EEE:145:TYR:CD1	2:EEE:145:TYR:C	2.88	0.46
2:EEE:142:ASN:HB3	2:EEE:143:ASN:ND2	2.32	0.45
2:EEE:21:ILE:HD11	2:EEE:78:LEU:HD23	1.98	0.45
1:DDD:203:HIS:HB3	1:DDD:208:THR:HB	1.99	0.45
2:BBB:95:GLN:HE21	2:BBB:97:THR:H	1.63	0.45
1:AAA:118:ALA:HB2	1:AAA:177:ASP:HB3	1.98	0.45
2:BBB:95:GLN:NE2	2:BBB:97:THR:H	2.14	0.45
1:DDD:11:LEU:HD22	1:DDD:151:PRO:HD3	1.99	0.44
2:BBB:146:PRO:O	2:BBB:203:HIS:HE1	2.00	0.44
2:EEE:4:MET:HG2	2:EEE:102:THR:HG23	2.00	0.44
1:DDD:69:ARG:NH2	1:DDD:92:ASP:OD2	2.33	0.44
2:EEE:111:LEU:CD2	2:EEE:176:SER:OG	2.35	0.44
2:EEE:95:GLN:NE2	2:EEE:98:HIS:N	2.46	0.44
2:BBB:142:ASN:HB3	2:BBB:143:ASN:ND2	2.33	0.43
2:BBB:94:VAL:HG22	2:BBB:103:PHE:CD2	2.53	0.43
1:DDD:156:VAL:O	4:DDD:303:HOH:O	2.21	0.42
2:EEE:94:VAL:HG22	2:EEE:103:PHE:CD2	2.53	0.42
1:AAA:66:VAL:HG13	1:AAA:70:PHE:CG	2.54	0.42
1:AAA:203:HIS:HD2	1:AAA:206:SER:OG	2.01	0.42
2:BBB:146:PRO:HD2	2:BBB:203:HIS:CE1	2.54	0.42
1:DDD:128:LEU:HD21	2:EEE:138:VAL:HG21	2.03	0.41
1:DDD:126:TYR:CE1	2:EEE:129:GLN:HA	2.56	0.41
1:DDD:127:PRO:HG2	2:EEE:126:SER:HB2	2.04	0.40
1:AAA:203:HIS:HB3	1:AAA:208:THR:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EEE:172:ASP:OD2	2:EEE:175:ASP:HB2	2.22	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)
2:EEE:131:THR:O	2:EEE:131:THR:O[2_556]	1.80	0.40

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	206/217 (95%)	200 (97%)	4 (2%)	2 (1%)	15 9
1	DDD	200/217 (92%)	197 (98%)	0	3 (2%)	10 4
2	BBB	216/218 (99%)	210 (97%)	4 (2%)	2 (1%)	17 11
2	EEE	205/218 (94%)	198 (97%)	5 (2%)	2 (1%)	15 9
3	CCC	6/15 (40%)	6 (100%)	0	0	100 100
3	FFF	6/15 (40%)	6 (100%)	0	0	100 100
All	All	839/900 (93%)	817 (97%)	13 (2%)	9 (1%)	14 8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	EEE	8	PRO
2	BBB	8	PRO
1	DDD	151	PRO
1	DDD	153	PRO
1	AAA	151	PRO
2	BBB	100	PRO
2	EEE	100	PRO

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Mol	Chain	Res	Type
1	DDD	193	PRO
1	AAA	193	PRO

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	AAA	181/185 (98%)	176 (97%)	5 (3%)	43	44
1	DDD	177/185 (96%)	173 (98%)	4 (2%)	50	53
2	BBB	194/194 (100%)	185 (95%)	9 (5%)	27	23
2	EEE	186/194 (96%)	179 (96%)	7 (4%)	33	31
3	CCC	5/11 (46%)	5 (100%)	0	100	100
3	FFF	5/11 (46%)	5 (100%)	0	100	100
All	All	748/780 (96%)	723 (97%)	25 (3%)	38	37

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	66	VAL
1	AAA	128	LEU
1	AAA	175	GLN
1	AAA	193	PRO
1	AAA	209	LYS
2	BBB	32	SER
2	BBB	86	GLU
2	BBB	102	THR
2	BBB	110	GLU
2	BBB	113	ARG
2	BBB	132	SER
2	BBB	148	ASP
2	BBB	174	LYS
2	BBB	175	ASP
1	DDD	66	VAL
1	DDD	128	LEU

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Mol	Chain	Res	Type
1	DDD	175	GLN
1	DDD	209	LYS
2	EEE	32	SER
2	EEE	86	GLU
2	EEE	102	THR
2	EEE	110	GLU
2	EEE	113	ARG
2	EEE	132	SER
2	EEE	174	LYS

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	210/217 (96%)	0.03	4 (1%) 66 65	13, 22, 42, 52	0
1	DDD	206/217 (94%)	0.32	8 (3%) 39 38	17, 28, 47, 63	0
2	BBB	218/218 (100%)	0.03	2 (0%) 84 83	15, 28, 42, 54	0
2	EEE	209/218 (95%)	0.66	27 (12%) 3 3	22, 35, 62, 84	0
3	CCC	8/15 (53%)	0.32	0 100 100	31, 35, 40, 43	0
3	FFF	8/15 (53%)	0.26	0 100 100	26, 28, 33, 37	0
All	All	859/900 (95%)	0.26	41 (4%) 30 29	13, 29, 50, 84	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	EEE	155	ILE	7.2
1	DDD	177	ASP	6.3
2	EEE	131	THR	5.7
2	EEE	197	TYR	5.3
1	DDD	210	VAL	4.6
2	EEE	130	LEU	3.9
2	EEE	184	LEU	3.8
2	EEE	185	THR	3.8
2	EEE	187	THR	3.5
1	AAA	57	ASN	3.5
1	DDD	176	SER	3.5
2	EEE	127	SER	3.5
2	EEE	195	ASN	3.4
2	EEE	132	SER	3.3
2	EEE	193	ARG	3.2
1	DDD	213	LYS	3.2
2	EEE	194	HIS	3.1
2	EEE	158	SER	3.0
1	DDD	211	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	EEE	145	TYR	3.0
1	AAA	54	LYS	2.9
2	EEE	191	TYR	2.8
1	AAA	58	HIS	2.7
2	EEE	135	ALA	2.6
2	EEE	160	ARG	2.6
2	EEE	188	LYS	2.5
2	BBB	1	ASP	2.5
2	BBB	82	ARG	2.4
2	EEE	196	SER	2.4
2	EEE	65	ASP	2.4
1	DDD	212	LYS	2.3
2	EEE	214	PHE	2.3
2	EEE	189	ASP	2.3
1	DDD	216	PRO	2.3
1	DDD	215	VAL	2.2
2	EEE	15	ILE	2.2
2	EEE	10	THR	2.2
2	EEE	111	LEU	2.1
1	AAA	195	GLU	2.1
2	EEE	46	GLY	2.1
2	EEE	61	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.