



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:25 am BST

PDB ID : 6TU5
Title : Influenza A/H7N9 polymerase core (apo)
Authors : Cusack, S.; Pflug, A.
Deposited on : 2020-01-02
Resolution : 3.33 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.

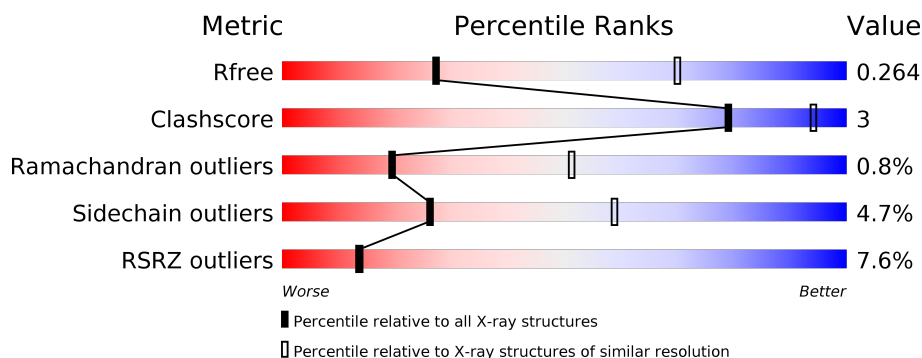
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

i

X-RAY DIFFRACTION

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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 ≥ 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	517	<div><div></div><div></div><div></div></div>	87%	11%
1	DDD	517	<div><div></div><div></div><div></div></div>	91%	8%
2	BBB	757	<div><div></div><div></div><div></div></div>	79%	11%
2	EEE	757	<div><div></div><div></div><div></div></div>	79%	10%
3	CCC	137	<div><div></div><div></div><div></div></div>	74%	12%
3	FFF	137	<div><div></div><div></div><div></div></div>	85%	6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21144 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	515	Total	C	N	O	S	0	0	0
			4142	2622	703	787	30			
1	DDD	514	Total	C	N	O	S	0	0	0
			4131	2616	699	786	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	200	MET	-	initiating methionine	UNP M9TI86
DDD	200	MET	-	initiating methionine	UNP M9TI86

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	685	Total	C	N	O	S	0	0	0
			5472	3455	942	1031	44			
2	EEE	675	Total	C	N	O	S	0	0	0
			5385	3401	924	1017	43			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	118	Total	C	N	O	S	0	0	0
			977	616	175	176	10			
3	FFF	125	Total	C	N	O	S	0	0	0
			1035	651	187	187	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	129	SER	-	linker	UNP X5F427
CCC	130	GLY	-	linker	UNP X5F427

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	131	SER	-	linker	UNP X5F427
CCC	132	GLU	-	expression tag	UNP X5F427
CCC	133	ASN	-	expression tag	UNP X5F427
CCC	134	LEU	-	expression tag	UNP X5F427
CCC	135	TYR	-	expression tag	UNP X5F427
CCC	136	PHE	-	expression tag	UNP X5F427
CCC	137	GLN	-	expression tag	UNP X5F427
FFF	129	SER	-	linker	UNP X5F427
FFF	130	GLY	-	linker	UNP X5F427
FFF	131	SER	-	linker	UNP X5F427
FFF	132	GLU	-	expression tag	UNP X5F427
FFF	133	ASN	-	expression tag	UNP X5F427
FFF	134	LEU	-	expression tag	UNP X5F427
FFF	135	TYR	-	expression tag	UNP X5F427
FFF	136	PHE	-	expression tag	UNP X5F427
FFF	137	GLN	-	expression tag	UNP X5F427

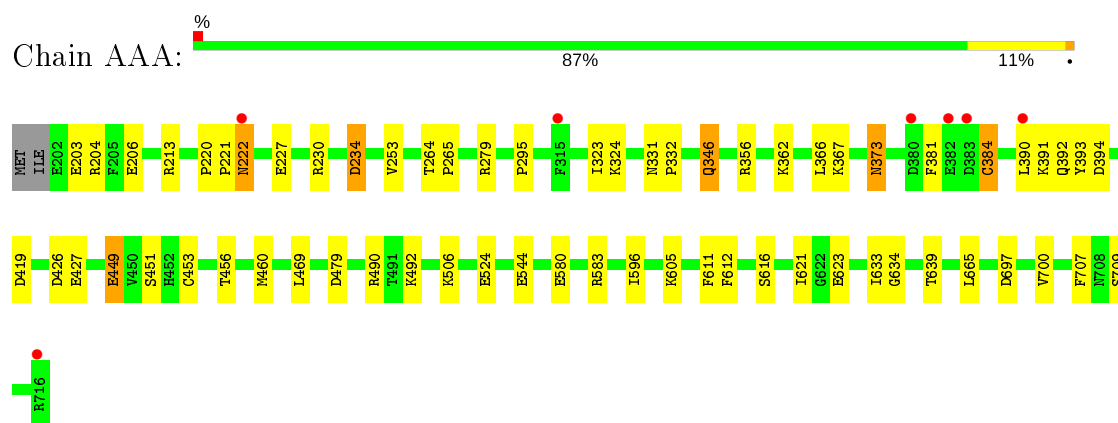
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	EEE	1	Total Mg 1 1	0	0
4	BBB	1	Total Mg 1 1	0	0

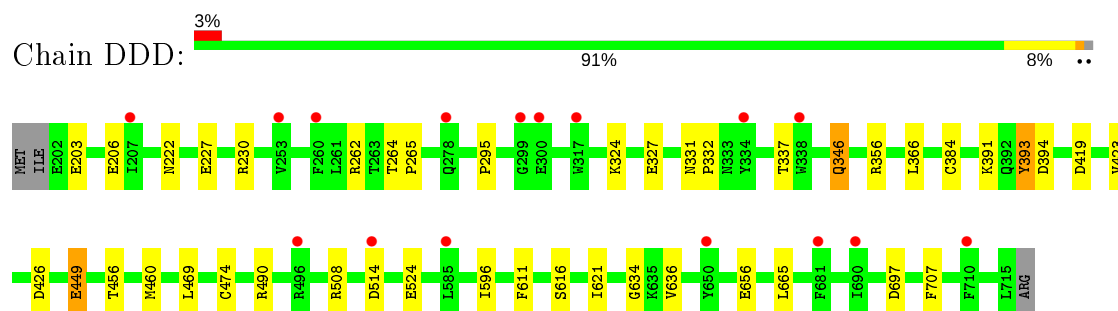
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

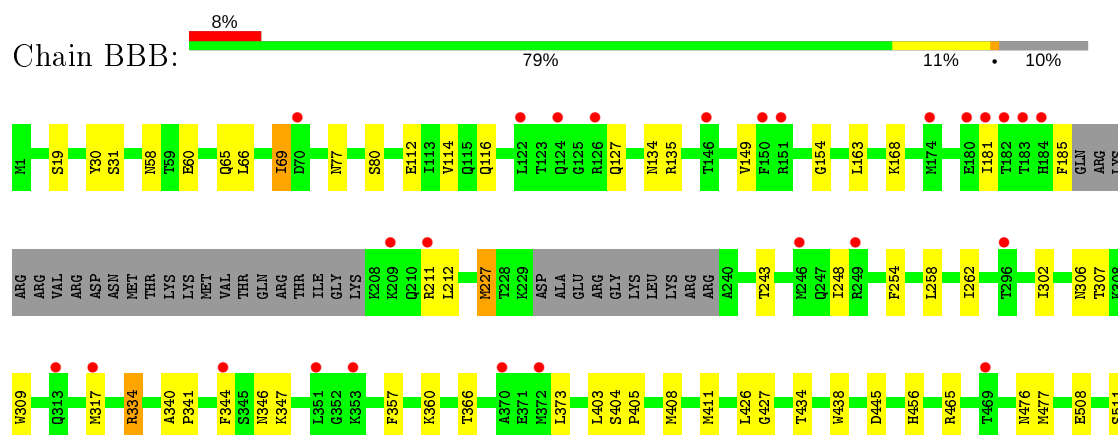
- Molecule 1: Polymerase acidic protein

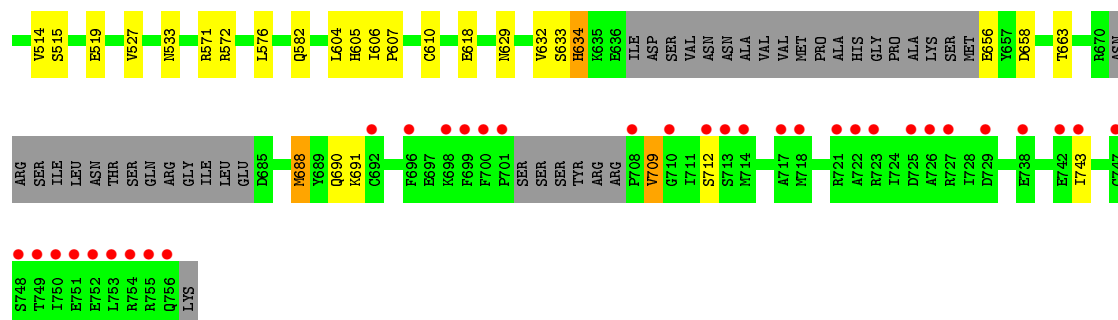


- Molecule 1: Polymerase acidic protein

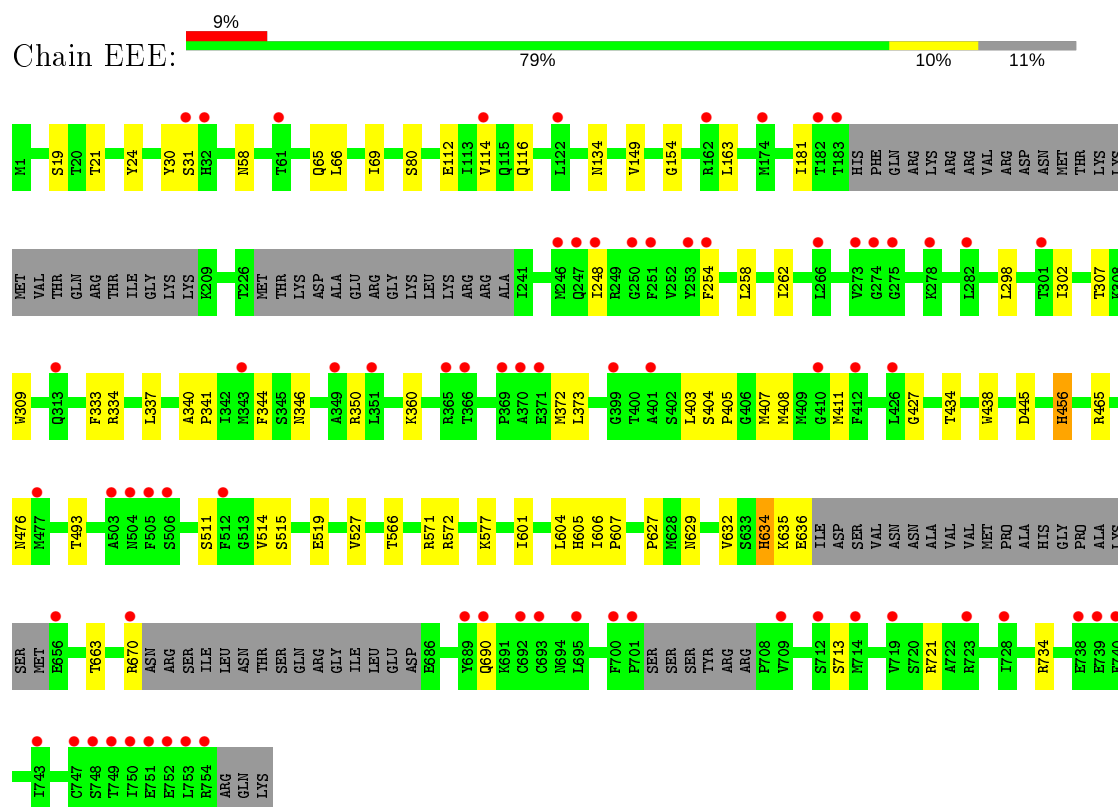


- Molecule 2: RNA-directed RNA polymerase catalytic subunit

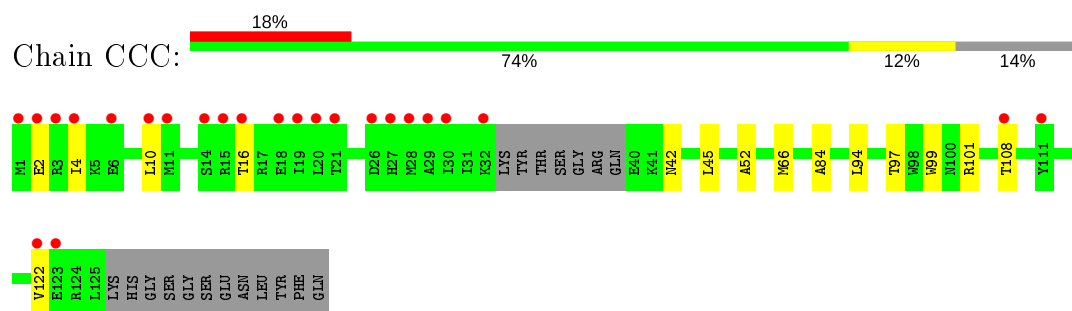




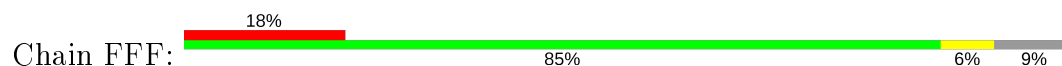
- Molecule 2: RNA-directed RNA polymerase catalytic subunit

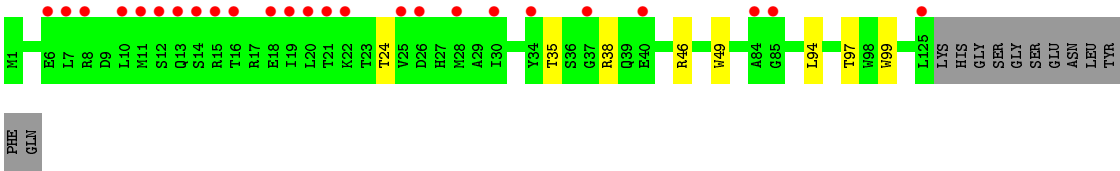


- Molecule 3: Polymerase basic protein 2



- Molecule 3: Polymerase basic protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.51Å 143.17Å 335.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	132.02 – 3.33 131.68 – 3.32	Depositor EDS
% Data completeness (in resolution range)	92.4 (132.02-3.33) 92.4 (131.68-3.32)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.204 , 0.268 0.205 , 0.264	Depositor DCC
R_{free} test set	2496 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	108.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21144	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.63	0/4231	0.73	0/5712
1	DDD	0.64	0/4220	0.72	0/5698
2	BBB	0.66	0/5580	0.72	0/7524
2	EEE	0.66	0/5491	0.72	0/7407
3	CCC	0.66	0/996	0.73	0/1340
3	FFF	0.66	0/1056	0.72	0/1421
All	All	0.65	0/21574	0.72	0/29102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4142	0	4109	29	0
1	DDD	4131	0	4096	15	0
2	BBB	5472	0	5436	45	0
2	EEE	5385	0	5348	38	0
3	CCC	977	0	1003	12	0
3	FFF	1035	0	1062	8	0
4	BBB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EEE	1	0	0	0	0
All	All	21144	0	21054	120	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 3.

All (120) 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:AAA:612:PHE:HA	1:AAA:633:ILE:HG21	1.64	0.78
2:BBB:572:ARG:HB3	2:BBB:576:LEU:HD13	1.74	0.69
2:EEE:519:GLU:OE2	2:EEE:572:ARG:NH1	2.27	0.68
2:BBB:519:GLU:OE2	2:BBB:572:ARG:NH1	2.26	0.67
2:EEE:629:ASN:HD21	2:EEE:632:VAL:HG23	1.59	0.67
2:EEE:635:LYS:CG	2:EEE:635:LYS:O	2.43	0.67
2:EEE:629:ASN:HD21	2:EEE:632:VAL:CG2	2.11	0.64
1:DDD:423:VAL:HG23	1:DDD:456:THR:CG2	2.28	0.64
2:BBB:306:ASN:HD22	2:BBB:477:MET:HA	1.63	0.63
1:DDD:656:GLU:HG3	2:EEE:24:TYR:HE2	1.63	0.63
2:BBB:576:LEU:HD12	3:CCC:97:THR:HG21	1.81	0.62
2:BBB:340:ALA:HB3	2:BBB:341:PRO:HD3	1.80	0.61
2:EEE:340:ALA:HB3	2:EEE:341:PRO:HD3	1.82	0.61
1:AAA:384:CYS:SG	1:AAA:384:CYS:O	2.59	0.61
2:EEE:663:THR:HG21	3:FFF:99:TRP:CD1	2.37	0.60
1:AAA:580:GLU:O	1:AAA:583:ARG:HG2	2.02	0.59
2:BBB:582:GLN:HE22	3:CCC:101:ARG:HA	1.69	0.58
1:DDD:384:CYS:O	1:DDD:384:CYS:SG	2.62	0.57
1:AAA:623:GLU:OE2	1:AAA:709:SER:OG	2.23	0.56
2:BBB:691:LYS:HE2	3:CCC:10:LEU:HD21	1.86	0.56
1:AAA:323:ILE:HG13	1:AAA:544:GLU:HB2	1.87	0.56
2:EEE:134:ASN:HD21	2:EEE:350:ARG:NH1	2.05	0.55
1:AAA:449:GLU:HG2	1:AAA:634:GLY:CA	2.37	0.55
1:DDD:346:GLN:N	1:DDD:346:GLN:HE21	2.05	0.55
2:BBB:227:MET:HE3	2:BBB:243:THR:HG23	1.90	0.54
2:EEE:629:ASN:ND2	2:EEE:632:VAL:HG23	2.22	0.54
1:AAA:392:GLN:HA	2:BBB:357:PHE:HA	1.88	0.54
2:EEE:627:PRO:HB2	2:EEE:635:LYS:HD2	1.88	0.53
1:AAA:373:ASN:N	1:AAA:373:ASN:HD22	2.05	0.53
2:EEE:635:LYS:O	2:EEE:635:LYS:HG3	2.08	0.53
2:EEE:427:GLY:HA3	2:EEE:438:TRP:CD1	2.44	0.52
2:BBB:58:ASN:HD22	2:BBB:65:GLN:NE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:427:GLY:HA3	2:BBB:438:TRP:CD1	2.44	0.52
1:AAA:453:CYS:O	1:AAA:456:THR:OG1	2.22	0.52
1:DDD:449:GLU:HG2	1:DDD:634:GLY:CA	2.40	0.52
1:AAA:449:GLU:HG2	1:AAA:634:GLY:HA3	1.92	0.51
2:EEE:114:VAL:HA	2:EEE:254:PHE:CE1	2.46	0.51
1:DDD:449:GLU:HG2	1:DDD:634:GLY:HA3	1.92	0.51
2:BBB:114:VAL:HA	2:BBB:254:PHE:CE1	2.47	0.50
2:EEE:58:ASN:HD22	2:EEE:65:GLN:NE2	2.09	0.50
1:AAA:596:ILE:HG12	1:AAA:611:PHE:CD2	2.47	0.50
1:AAA:346:GLN:N	1:AAA:346:GLN:HE21	2.10	0.50
2:BBB:743:ILE:HG23	3:CCC:4:ILE:HD13	1.95	0.49
2:EEE:634:HIS:O	2:EEE:636:GLU:HG3	2.13	0.48
2:EEE:258:LEU:O	2:EEE:262:ILE:HG12	2.14	0.48
2:BBB:258:LEU:O	2:BBB:262:ILE:HG12	2.13	0.48
2:BBB:404:SER:N	2:BBB:405:PRO:CD	2.77	0.48
2:BBB:605:HIS:CD2	2:BBB:606:ILE:HG13	2.48	0.48
2:BBB:606:ILE:HG22	2:BBB:607:PRO:O	2.14	0.47
2:BBB:227:MET:CE	2:BBB:243:THR:HG23	2.44	0.47
2:EEE:527:VAL:HG13	2:EEE:604:LEU:HD22	1.96	0.47
2:EEE:713:SER:HA	3:FFF:24:THR:HA	1.95	0.47
2:EEE:606:ILE:HG22	2:EEE:607:PRO:O	2.15	0.47
1:AAA:264:THR:N	1:AAA:265:PRO:CD	2.78	0.47
2:EEE:404:SER:N	2:EEE:405:PRO:CD	2.78	0.47
2:EEE:605:HIS:CD2	2:EEE:606:ILE:HG13	2.50	0.47
2:BBB:347:LYS:HE2	2:BBB:403:LEU:HD23	1.96	0.47
2:BBB:663:THR:HG21	3:CCC:99:TRP:CD1	2.50	0.46
2:EEE:572:ARG:HG2	3:FFF:94:LEU:HD23	1.97	0.46
2:BBB:227:MET:N	2:BBB:227:MET:SD	2.88	0.46
2:BBB:572:ARG:HG2	3:CCC:94:LEU:HD23	1.96	0.46
1:DDD:264:THR:N	1:DDD:265:PRO:CD	2.78	0.46
2:BBB:527:VAL:HG13	2:BBB:604:LEU:HD22	1.97	0.46
2:BBB:688:MET:HG3	3:CCC:16:THR:CG2	2.45	0.46
2:EEE:634:HIS:CG	2:EEE:635:LYS:N	2.84	0.46
1:AAA:621:ILE:HD11	1:AAA:639:THR:HG21	1.98	0.46
2:BBB:309:TRP:CG	2:BBB:445:ASP:HB3	2.51	0.45
1:AAA:362:LYS:O	1:AAA:367:LYS:HE2	2.17	0.45
1:DDD:665:LEU:HD23	1:DDD:707:PHE:CZ	2.52	0.45
1:AAA:665:LEU:HD23	1:AAA:707:PHE:CZ	2.51	0.45
1:DDD:337:THR:HG22	1:DDD:366:LEU:HD13	1.98	0.45
2:EEE:635:LYS:HG2	2:EEE:635:LYS:O	2.17	0.45
1:AAA:204:ARG:O	2:BBB:168:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:134:ASN:O	2:BBB:134:ASN:ND2	2.49	0.45
2:EEE:309:TRP:CG	2:EEE:445:ASP:HB3	2.52	0.44
2:EEE:670:ARG:HB2	3:FFF:38:ARG:NH2	2.33	0.44
1:AAA:220:PRO:CB	2:BBB:69:ILE:HD11	2.48	0.44
2:EEE:134:ASN:ND2	2:EEE:134:ASN:O	2.50	0.44
1:AAA:366:LEU:HD23	1:AAA:366:LEU:HA	1.84	0.44
3:CCC:42:ASN:OD1	3:CCC:45:LEU:HG	2.18	0.44
2:BBB:149:VAL:HG22	2:BBB:181:ILE:HD13	2.00	0.43
1:AAA:234:ASP:OD1	2:BBB:334:ARG:NH2	2.50	0.43
2:EEE:344:PHE:CZ	2:EEE:411:MET:HG2	2.52	0.43
2:BBB:65:GLN:HE22	2:BBB:346:ASN:HA	1.84	0.43
2:EEE:670:ARG:HB2	3:FFF:38:ARG:HH22	1.83	0.43
1:DDD:621:ILE:HG21	1:DDD:636:VAL:HG22	2.01	0.43
2:EEE:298:LEU:CD1	2:EEE:456:HIS:ND1	2.82	0.43
2:EEE:572:ARG:HH21	3:FFF:97:THR:HG1	1.66	0.43
2:EEE:670:ARG:O	3:FFF:46:ARG:NH2	2.52	0.43
1:AAA:697:ASP:HB3	1:AAA:700:VAL:HG12	2.01	0.43
3:CCC:115:TYR:HD1	3:CCC:118:TYR:CE1	2.37	0.42
1:DDD:474:CYS:HB2	3:FFF:49:TRP:CH2	2.54	0.42
2:EEE:58:ASN:ND2	2:EEE:346:ASN:OD1	2.51	0.42
2:BBB:58:ASN:ND2	2:BBB:346:ASN:OD1	2.52	0.42
2:EEE:149:VAL:HG22	2:EEE:181:ILE:HD13	2.01	0.42
2:EEE:65:GLN:HE22	2:EEE:346:ASN:HA	1.85	0.42
1:AAA:220:PRO:HB3	2:BBB:69:ILE:HD11	2.01	0.42
2:BBB:658:ASP:HB3	3:CCC:118:TYR:CD2	2.55	0.42
1:DDD:366:LEU:HD12	1:DDD:366:LEU:HA	1.86	0.42
2:BBB:629:ASN:HD21	2:BBB:632:VAL:HG23	1.84	0.42
2:EEE:333:PHE:CZ	2:EEE:337:LEU:HD11	2.55	0.42
2:EEE:566:THR:O	2:EEE:577:LYS:HE2	2.20	0.42
1:AAA:221:PRO:O	1:AAA:222:ASN:HB2	2.20	0.41
1:AAA:390:LEU:HD21	2:BBB:366:THR:HG21	2.02	0.41
2:BBB:344:PHE:CZ	2:BBB:411:MET:HG2	2.55	0.41
2:BBB:571:ARG:NH2	3:CCC:52:ALA:O	2.54	0.41
2:BBB:610:CYS:HB3	3:CCC:122:VAL:HG21	2.02	0.41
1:AAA:253:VAL:HA	2:BBB:77:ASN:HD21	1.86	0.41
1:DDD:331:ASN:N	1:DDD:332:PRO:CD	2.84	0.41
1:AAA:213:ARG:HE	2:BBB:60:GLU:CD	2.24	0.41
1:AAA:479:ASP:O	1:AAA:506:LYS:NZ	2.54	0.41
2:BBB:212:LEU:HA	2:BBB:212:LEU:HD23	1.97	0.41
2:BBB:127:GLN:OE1	2:BBB:227:MET:HB2	2.21	0.40
2:BBB:709:VAL:HG13	2:BBB:712:SER:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:331:ASN:N	1:AAA:332:PRO:CD	2.84	0.40
2:BBB:248:ILE:HD11	2:BBB:344:PHE:CD2	2.55	0.40
1:DDD:697:ASP:C	1:DDD:697:ASP:OD1	2.60	0.40
1:DDD:596:ILE:HG12	1:DDD:611:PHE:CD2	2.56	0.40
2:EEE:248:ILE:HD11	2:EEE:344:PHE:CD2	2.57	0.40
1:AAA:449:GLU:HG2	1:AAA:634:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

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	AAA	513/517 (99%)	478 (93%)	30 (6%)	5 (1%)	15	47
1	DDD	512/517 (99%)	474 (93%)	34 (7%)	4 (1%)	19	51
2	BBB	673/757 (89%)	621 (92%)	47 (7%)	5 (1%)	22	55
2	EEE	663/757 (88%)	608 (92%)	49 (7%)	6 (1%)	17	49
3	CCC	114/137 (83%)	105 (92%)	8 (7%)	1 (1%)	17	49
3	FFF	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
All	All	2598/2822 (92%)	2400 (92%)	177 (7%)	21 (1%)	19	51

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	EEE	634	HIS
1	AAA	222	ASN
1	AAA	394	ASP
3	CCC	84	ALA
1	DDD	222	ASN
1	DDD	394	ASP

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Mol	Chain	Res	Type
1	AAA	295	PRO
2	BBB	31	SER
1	DDD	295	PRO
2	EEE	31	SER
1	AAA	393	TYR
2	BBB	511	SER
1	DDD	393	TYR
1	AAA	451	SER
2	BBB	30	TYR
2	BBB	634	HIS
2	EEE	30	TYR
2	EEE	511	SER
2	EEE	601	ILE
2	BBB	154	GLY
2	EEE	154	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	AAA	462/464 (100%)	438 (95%)	24 (5%)	23	55
1	DDD	461/464 (99%)	440 (95%)	21 (5%)	27	60
2	BBB	604/668 (90%)	570 (94%)	34 (6%)	21	53
2	EEE	595/668 (89%)	567 (95%)	28 (5%)	26	59
3	CCC	109/125 (87%)	106 (97%)	3 (3%)	43	71
3	FFF	115/125 (92%)	114 (99%)	1 (1%)	78	88
All	All	2346/2514 (93%)	2235 (95%)	111 (5%)	26	59

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	203	GLU
1	AAA	206	GLU
1	AAA	227	GLU

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Mol	Chain	Res	Type
1	AAA	230	ARG
1	AAA	234	ASP
1	AAA	279	ARG
1	AAA	324	LYS
1	AAA	346	GLN
1	AAA	356	ARG
1	AAA	373	ASN
1	AAA	381	PHE
1	AAA	384	CYS
1	AAA	391	LYS
1	AAA	419	ASP
1	AAA	426	ASP
1	AAA	427	GLU
1	AAA	449	GLU
1	AAA	460	MET
1	AAA	469	LEU
1	AAA	490	ARG
1	AAA	492	LYS
1	AAA	524	GLU
1	AAA	605	LYS
1	AAA	616	SER
2	BBB	19	SER
2	BBB	66	LEU
2	BBB	69	ILE
2	BBB	80	SER
2	BBB	112	GLU
2	BBB	116	GLN
2	BBB	135	ARG
2	BBB	163	LEU
2	BBB	185	PHE
2	BBB	211	ARG
2	BBB	227	MET
2	BBB	302	ILE
2	BBB	307	THR
2	BBB	317	MET
2	BBB	334	ARG
2	BBB	360	LYS
2	BBB	373	LEU
2	BBB	408	MET
2	BBB	426	LEU
2	BBB	434	THR
2	BBB	456	HIS

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Mol	Chain	Res	Type
2	BBB	465	ARG
2	BBB	476	ASN
2	BBB	508	GLU
2	BBB	514	VAL
2	BBB	515	SER
2	BBB	533	ASN
2	BBB	618	GLU
2	BBB	633	SER
2	BBB	634	HIS
2	BBB	656	GLU
2	BBB	688	MET
2	BBB	690	GLN
2	BBB	709	VAL
3	CCC	2	GLU
3	CCC	66	MET
3	CCC	108	THR
1	DDD	203	GLU
1	DDD	206	GLU
1	DDD	227	GLU
1	DDD	230	ARG
1	DDD	262	ARG
1	DDD	324	LYS
1	DDD	327	GLU
1	DDD	346	GLN
1	DDD	356	ARG
1	DDD	391	LYS
1	DDD	393	TYR
1	DDD	419	ASP
1	DDD	426	ASP
1	DDD	449	GLU
1	DDD	460	MET
1	DDD	469	LEU
1	DDD	490	ARG
1	DDD	508	ARG
1	DDD	514	ASP
1	DDD	524	GLU
1	DDD	616	SER
2	EEE	19	SER
2	EEE	21	THR
2	EEE	66	LEU
2	EEE	69	ILE
2	EEE	80	SER

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Mol	Chain	Res	Type
2	EEE	112	GLU
2	EEE	116	GLN
2	EEE	163	LEU
2	EEE	302	ILE
2	EEE	307	THR
2	EEE	334	ARG
2	EEE	360	LYS
2	EEE	372	MET
2	EEE	373	LEU
2	EEE	403	LEU
2	EEE	407	MET
2	EEE	408	MET
2	EEE	434	THR
2	EEE	456	HIS
2	EEE	465	ARG
2	EEE	476	ASN
2	EEE	493	THR
2	EEE	514	VAL
2	EEE	515	SER
2	EEE	571	ARG
2	EEE	690	GLN
2	EEE	721	ARG
2	EEE	734	ARG
3	FFF	35	THR

Some 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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

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, 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	515/517 (99%)	0.40	7 (1%)	75 75	59, 88, 175, 266	0
1	DDD	514/517 (99%)	0.34	16 (3%)	49 48	85, 127, 183, 221	0
2	BBB	685/757 (90%)	0.62	59 (8%)	10 10	60, 118, 207, 239	0
2	EEE	675/757 (89%)	0.65	70 (10%)	6 6	80, 139, 205, 241	0
3	CCC	118/137 (86%)	0.94	24 (20%)	1 0	80, 151, 216, 241	0
3	FFF	125/137 (91%)	1.04	25 (20%)	1 0	86, 148, 217, 233	0
All	All	2632/2822 (93%)	0.56	201 (7%)	13 14	59, 123, 204, 266	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	750	ILE	7.6
2	BBB	755	ARG	7.4
2	BBB	751	GLU	6.5
1	AAA	383	ASP	5.9
2	BBB	756	GLN	5.9
2	EEE	274	GLY	5.8
2	EEE	504	ASN	5.8
2	BBB	701	PRO	5.7
3	FFF	13	GLN	5.7
3	FFF	12	SER	5.1
3	CCC	2	GLU	5.0
2	EEE	505	PHE	5.0
2	EEE	31	SER	4.9
2	EEE	273	VAL	4.8
1	AAA	382	GLU	4.6
3	CCC	16	THR	4.5
2	EEE	506	SER	4.4
2	EEE	750	ILE	4.3
3	FFF	8	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
2	EEE	122	LEU	4.1
2	BBB	699	PHE	4.1
2	BBB	718	MET	4.0
2	EEE	183	THR	4.0
2	EEE	246	MET	4.0
2	BBB	754	ARG	4.0
2	EEE	695	LEU	3.9
3	FFF	84	ALA	3.9
3	CCC	1	MET	3.9
2	EEE	248	ILE	3.8
3	FFF	37	GLY	3.8
2	BBB	712	SER	3.8
3	FFF	85	GLY	3.8
2	BBB	181	ILE	3.8
3	FFF	7	LEU	3.8
2	EEE	693	CYS	3.7
3	CCC	15	ARG	3.6
2	BBB	713	SER	3.6
2	EEE	752	GLU	3.6
2	BBB	753	LEU	3.6
2	BBB	700	PHE	3.5
3	FFF	11	MET	3.5
2	EEE	365	ARG	3.5
3	CCC	14	SER	3.4
2	EEE	749	THR	3.4
3	FFF	34	TYR	3.4
2	EEE	182	THR	3.4
2	BBB	749	THR	3.4
3	FFF	16	THR	3.4
2	EEE	410	GLY	3.3
2	BBB	692	CYS	3.3
3	CCC	111	TYR	3.3
2	BBB	725	ASP	3.3
3	FFF	14	SER	3.3
3	CCC	32	LYS	3.3
2	EEE	690	GLN	3.3
3	FFF	18	GLU	3.3
2	EEE	740	PHE	3.2
2	BBB	729	ASP	3.2
2	BBB	714	MET	3.2
2	BBB	182	THR	3.2
1	AAA	390	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	CCC	20	LEU	3.2
2	BBB	246	MET	3.1
2	EEE	738	GLU	3.1
3	FFF	40	GLU	3.1
2	EEE	753	LEU	3.1
2	EEE	754	ARG	3.0
3	CCC	10	LEU	3.0
3	CCC	27	HIS	3.0
2	EEE	343	MET	3.0
3	FFF	10	LEU	3.0
1	DDD	690	ILE	3.0
2	BBB	742	GLU	2.9
2	BBB	752	GLU	2.9
2	EEE	278	LYS	2.9
3	CCC	18	GLU	2.9
1	DDD	299	GLY	2.9
2	EEE	247	GLN	2.8
2	BBB	122	LEU	2.8
3	FFF	15	ARG	2.8
2	BBB	708	PRO	2.8
2	EEE	282	LEU	2.8
2	EEE	254	PHE	2.8
1	DDD	317	TRP	2.8
2	EEE	712	SER	2.8
3	CCC	29	ALA	2.8
1	AAA	315	PHE	2.8
2	BBB	747	CYS	2.8
2	BBB	184	HIS	2.8
3	FFF	20	LEU	2.8
2	BBB	722	ALA	2.8
2	BBB	209	LYS	2.8
2	EEE	61	THR	2.8
2	BBB	124	GLN	2.7
3	CCC	6	GLU	2.7
2	BBB	249	ARG	2.7
3	CCC	4	ILE	2.7
3	CCC	108	THR	2.7
2	EEE	701	PRO	2.7
3	CCC	122	VAL	2.7
3	FFF	125	LEU	2.7
2	EEE	32	HIS	2.6
2	EEE	719	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	FFF	21	THR	2.6
2	BBB	748	SER	2.6
2	EEE	371	GLU	2.6
2	BBB	723	ARG	2.6
2	BBB	70	ASP	2.6
2	EEE	512	PHE	2.5
2	EEE	401	ALA	2.5
1	DDD	650	TYR	2.5
2	BBB	726	ALA	2.5
2	EEE	751	GLU	2.5
2	EEE	275	GLY	2.5
3	CCC	21	THR	2.5
2	EEE	114	VAL	2.5
2	EEE	399	GLY	2.5
3	CCC	19	ILE	2.5
3	FFF	30	ILE	2.5
2	BBB	696	PHE	2.5
2	BBB	738	GLU	2.5
2	BBB	710	GLY	2.5
2	EEE	313	GLN	2.5
3	CCC	11	MET	2.5
1	DDD	496	ARG	2.5
2	EEE	728	ILE	2.5
1	DDD	514	ASP	2.4
3	FFF	25	VAL	2.4
2	BBB	717	ALA	2.4
2	BBB	698	LYS	2.4
2	EEE	747	CYS	2.4
1	AAA	716	ARG	2.4
2	BBB	353	LYS	2.4
1	DDD	300	GLU	2.4
2	EEE	692	CYS	2.4
2	BBB	721	ARG	2.4
2	EEE	253	TYR	2.4
2	EEE	366	THR	2.4
2	BBB	174	MET	2.4
2	BBB	344	PHE	2.3
2	EEE	477	MET	2.3
2	EEE	748	SER	2.3
2	BBB	296	THR	2.3
2	BBB	151	ARG	2.3
2	EEE	162	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	BBB	150	PHE	2.3
1	AAA	222	ASN	2.3
2	EEE	174	MET	2.3
3	FFF	26	ASP	2.3
3	FFF	22	LYS	2.3
3	CCC	3	ARG	2.3
1	DDD	207	ILE	2.3
2	EEE	670	ARG	2.3
2	BBB	370	ALA	2.3
2	EEE	349	ALA	2.3
1	DDD	681	PHE	2.3
1	AAA	380	ASP	2.2
2	EEE	301	THR	2.2
2	EEE	351	LEU	2.2
2	EEE	709	VAL	2.2
2	BBB	183	THR	2.2
2	BBB	469	THR	2.2
2	EEE	251	PHE	2.2
3	FFF	28	MET	2.2
2	BBB	727	ARG	2.2
2	EEE	714	MET	2.2
3	CCC	123	GLU	2.2
2	BBB	313	GLN	2.2
2	EEE	266	LEU	2.2
2	EEE	250	GLY	2.2
2	EEE	369	PRO	2.2
2	BBB	211	ARG	2.2
1	DDD	585	LEU	2.2
2	EEE	743	ILE	2.2
1	DDD	334	TYR	2.1
2	EEE	426	LEU	2.1
2	EEE	370	ALA	2.1
1	DDD	260	PHE	2.1
2	BBB	180	GLU	2.1
3	CCC	30	ILE	2.1
3	CCC	26	ASP	2.1
1	DDD	338	TRP	2.1
1	DDD	253	VAL	2.1
2	BBB	146	THR	2.1
2	BBB	317	MET	2.1
2	EEE	412	PHE	2.1
2	EEE	739	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	EEE	656	GLU	2.1
3	FFF	6	GLU	2.1
2	EEE	723	ARG	2.1
2	EEE	689	TYR	2.1
3	FFF	19	ILE	2.1
1	DDD	278	GLN	2.0
2	BBB	126	ARG	2.0
3	CCC	28	MET	2.0
2	EEE	503	ALA	2.0
2	BBB	351	LEU	2.0
2	BBB	743	ILE	2.0
2	EEE	700	PHE	2.0
2	BBB	372	MET	2.0
1	DDD	710	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	EEE	801	1/1	0.94	0.08	103,103,103,103	0
4	MG	BBB	801	1/1	0.96	0.15	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.