



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:06 PM UTC

PDB ID : 8QFY / pdb_00008qfy
Title : Crystal structure of high affinity TCR in complex with pHLA harbouring bacterial peptide
Authors : Pengelly, R.J.; Robinson, R.A.
Deposited on : 2023-09-05
Resolution : 2.33 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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

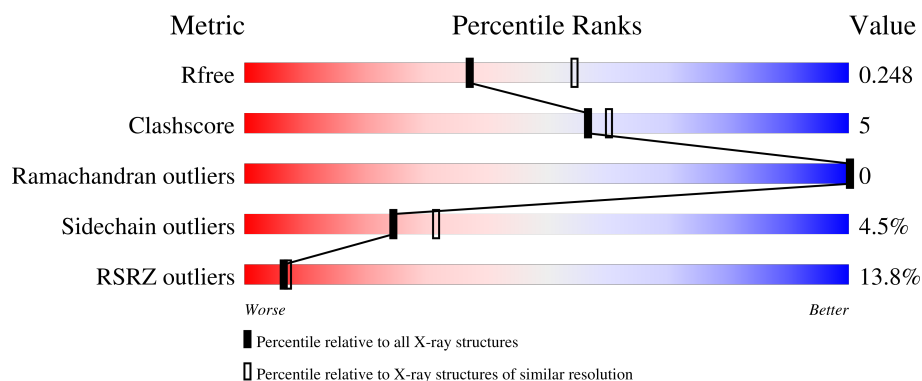
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	276	10% 82% 8% 9%
1	FFF	276	25% 83% 12% • •
2	BBB	100	21% 91% 9%
2	GGG	100	15% 87% 13%
3	CCC	9	78% 22%

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Mol	Chain	Length	Quality of chain
3	HHH	9	67% 22% 11%
4	DDD	197	10% 77% 16% •• 5%
4	III	197	13% 79% 15% • 5%
5	EEE	243	7% 85% 13% ••
5	JJJ	243	9% 90% 9% •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13151 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 I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	250	Total	C	N	O	S	0	1	0
			2038	1278	363	390	7			
1	FFF	267	Total	C	N	O	S	0	1	0
			2185	1371	390	417	7			

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	MET	-	initiating methionine	UNP P61769
GGG	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Peptide from inhA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	9	Total	C	N	O	0	0	0
			69	46	13	10			
3	HHH	9	Total	C	N	O	0	0	0
			69	46	13	10			

- Molecule 4 is a protein called T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	187	Total	C	N	O	S	0	2	0
			1484	917	254	304	9			

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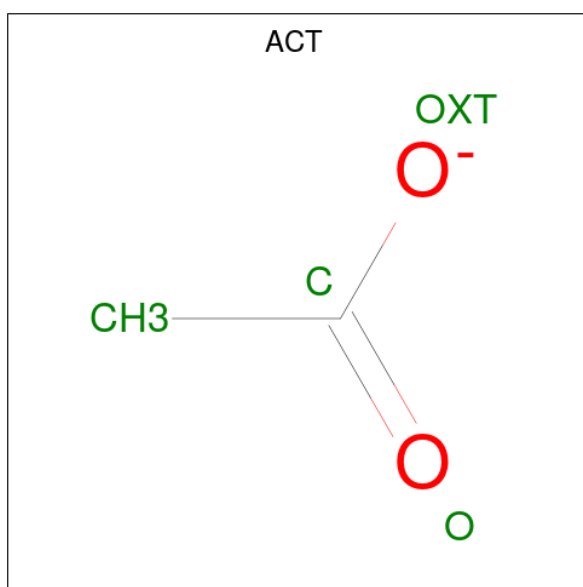
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	III	187	Total	C	N	O	S	0	0	0
			1471	909	251	302	9			

- Molecule 5 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	EEE	241	Total	C	N	O	S	0	0	0
			1936	1213	345	372	6			
5	JJJ	241	Total	C	N	O	S	0	0	0
			1936	1213	345	372	6			

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	FFF	1	Total	C	O	0	0
			4	2	2		
6	JJJ	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	43	Total	O	0	0
			43	43		
7	BBB	10	Total	O	0	0
			10	10		

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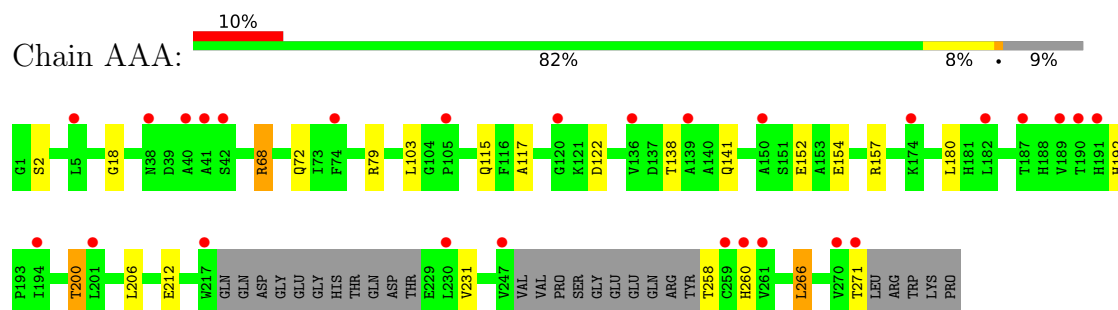
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	2	Total 2	O 2	0	0
7	DDD	38	Total 38	O 38	0	0
7	EEE	51	Total 51	O 51	0	0
7	FFF	63	Total 63	O 63	0	0
7	GGG	11	Total 11	O 11	0	0
7	HHH	6	Total 6	O 6	0	0
7	III	33	Total 33	O 33	0	0
7	JJJ	24	Total 24	O 24	0	0

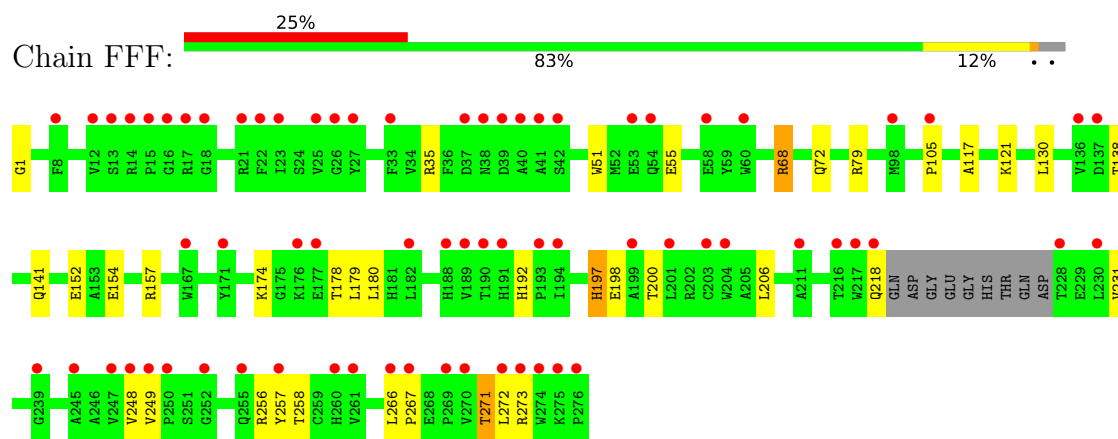
3 Residue-property plots [i](#)

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.

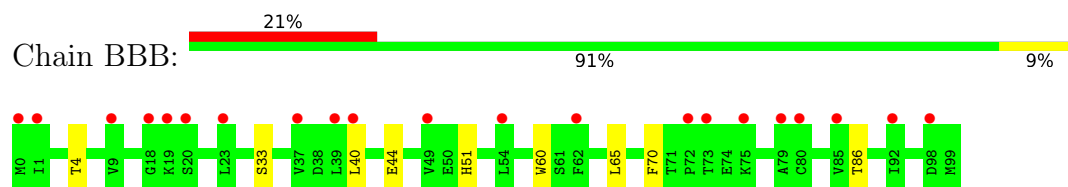
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 2: Beta-2-microglobulin

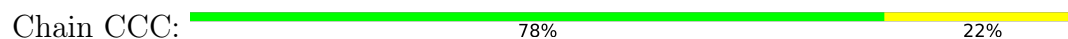


- Molecule 2: Beta-2-microglobulin





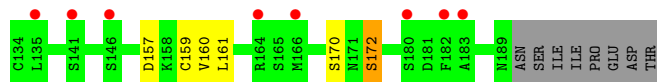
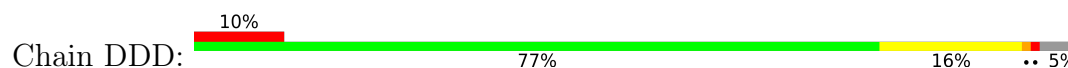
- Molecule 3: Peptide from inhA



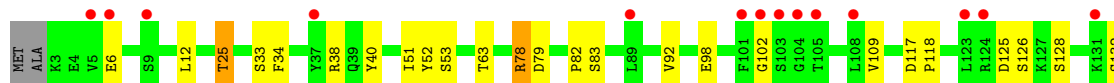
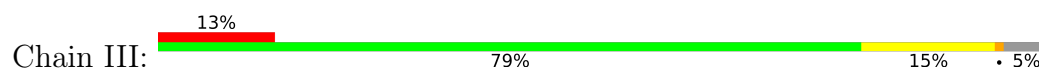
- Molecule 3: Peptide from inhA



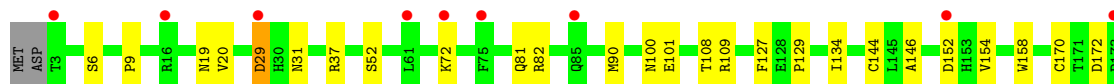
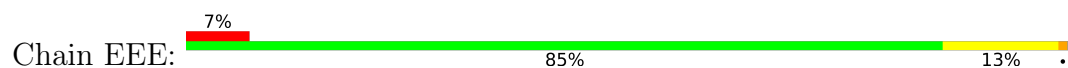
- Molecule 4: T-cell receptor alpha chain



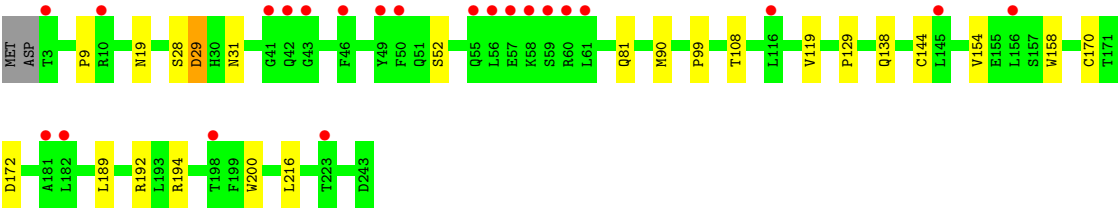
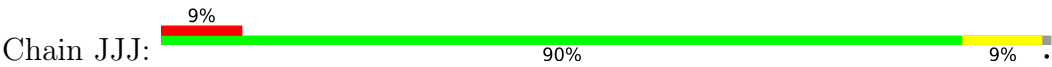
- Molecule 4: T-cell receptor alpha chain



- Molecule 5: T-cell receptor beta chain



- Molecule 5: T-cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	326.83Å 79.88Å 104.07Å 90.00° 96.89° 90.00°	Depositor
Resolution (Å)	82.90 – 2.33 82.90 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (82.90-2.33) 98.9 (82.90-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.242 , 0.289 (Not available) , 0.248	Depositor DCC
R_{free} test set	5685 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13151	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

5.1 Standard geometry

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

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	1.01	0/2097	1.33	0/2849
1	FFF	1.02	0/2250	1.33	0/3058
2	BBB	0.99	0/860	1.17	0/1162
2	GGG	0.99	0/860	1.19	0/1162
3	CCC	0.95	0/70	1.31	0/93
3	HHH	1.22	1/70 (1.4%)	1.64	1/93 (1.1%)
4	DDD	1.10	0/1518	1.28	3/2050 (0.1%)
4	III	1.09	0/1499	1.29	1/2025 (0.0%)
5	EEE	0.99	0/1987	1.30	0/2699
5	JJJ	0.97	0/1987	1.28	0/2699
All	All	1.02	1/13198 (0.0%)	1.29	5/17890 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	HHH	3	PRO	C-O	-5.66	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	HHH	7	PRO	CB-CA-C	-6.15	103.75	111.56
4	DDD	25	THR	CB-CA-C	5.41	120.06	109.35
4	DDD	125	ASP	CA-CB-CG	5.09	117.69	112.60
4	III	102	GLY	CA-C-O	-5.09	116.25	122.82
4	DDD	157	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2038	0	1896	17	0
1	FFF	2185	0	2041	30	0
2	BBB	837	0	803	4	0
2	GGG	837	0	803	7	0
3	CCC	69	0	85	2	0
3	HHH	69	0	85	4	0
4	DDD	1484	0	1410	20	0
4	III	1471	0	1393	23	0
5	EEE	1936	0	1843	18	0
5	JJJ	1936	0	1843	18	0
6	FFF	4	0	3	0	0
6	JJJ	4	0	3	0	0
7	AAA	43	0	0	2	0
7	BBB	10	0	0	0	0
7	CCC	2	0	0	0	0
7	DDD	38	0	0	0	0
7	EEE	51	0	0	1	0
7	FFF	63	0	0	9	0
7	GGG	11	0	0	0	0
7	HHH	6	0	0	0	0
7	III	33	0	0	1	0
7	JJJ	24	0	0	0	0
All	All	13151	0	12208	114	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 5.

All (114) 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:FFF:68:ARG:HH11	1:FFF:68:ARG:HG2	1.54	0.72
1:AAA:72:GLN:HG2	5:EEE:31:ASN:HB3	1.73	0.69
1:FFF:272:LEU:HD12	7:FFF:404:HOH:O	1.96	0.66
4:DDD:33:SER:HB3	4:DDD:52:TYR:CD1	2.31	0.65
4:III:161:LEU:HB3	5:JJJ:170:CYS:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:152:GLU:OE1	3:CCC:5:LYS:NZ	2.31	0.64
1:AAA:68:ARG:HG2	1:AAA:68:ARG:HH11	1.62	0.64
1:FFF:178:THR:HG23	7:FFF:419:HOH:O	1.98	0.63
4:III:33:SER:HB3	4:III:52:TYR:CD1	2.35	0.62
1:FFF:55:GLU:OE2	1:FFF:174:LYS:NZ	2.29	0.62
2:GGG:4:THR:HA	2:GGG:86:THR:HG21	1.82	0.62
3:HHH:5:LYS:HB2	5:JJJ:99:PRO:HG2	1.82	0.61
4:III:163:MET:HE3	5:JJJ:194:ARG:HD3	1.82	0.61
1:FFF:272:LEU:CD1	7:FFF:404:HOH:O	2.48	0.60
4:III:159:CYS:C	5:JJJ:170:CYS:SG	2.85	0.60
4:DDD:6:GLU:HB2	4:DDD:25:THR:HG22	1.82	0.60
4:DDD:63:THR:OG1	4:DDD:78:ARG:NH2	2.35	0.60
1:FFF:72:GLN:HG2	5:JJJ:31:ASN:HB3	1.84	0.59
1:AAA:271:THR:C	7:AAA:332:HOH:O	2.45	0.59
4:DDD:161:LEU:HB3	5:EEE:170:CYS:HB2	1.85	0.58
1:AAA:260:HIS:ND1	1:AAA:271:THR:HG22	2.21	0.56
1:FFF:117:ALA:HB2	2:GGG:60:TRP:CE2	2.40	0.56
2:BBB:4:THR:HA	2:BBB:86:THR:HG21	1.88	0.55
4:III:6:GLU:HB2	4:III:25:THR:HG22	1.88	0.55
1:FFF:192:HIS:HB2	1:FFF:200:THR:CG2	2.37	0.55
4:DDD:33:SER:HB3	4:DDD:52:TYR:HD1	1.72	0.54
5:EEE:172:ASP:HB2	5:EEE:189:LEU:HD12	1.89	0.54
4:DDD:159:CYS:C	5:EEE:170:CYS:SG	2.91	0.54
1:FFF:154:GLU:OE2	1:FFF:157:ARG:NH2	2.37	0.53
4:DDD:33:SER:HB3	4:DDD:52:TYR:CE1	2.44	0.53
4:III:163:MET:CE	5:JJJ:194:ARG:HG2	2.38	0.53
1:FFF:152:GLU:HG2	3:HHH:7:PRO:HB3	1.91	0.53
1:FFF:248:VAL:HG13	1:FFF:249:VAL:HG12	1.92	0.52
4:III:33:SER:HB3	4:III:52:TYR:HD1	1.74	0.52
1:AAA:2:SER:HB2	1:AAA:103:LEU:O	2.09	0.52
1:FFF:121:LYS:HE3	7:FFF:435:HOH:O	2.09	0.51
4:III:117:ASP:N	4:III:118:PRO:HD3	2.25	0.51
1:FFF:192:HIS:HB2	1:FFF:200:THR:HG22	1.92	0.51
1:AAA:154:GLU:OE2	1:AAA:157:ARG:NH2	2.40	0.50
1:FFF:256:ARG:HB2	7:FFF:430:HOH:O	2.09	0.50
1:FFF:267:PRO:HG3	7:FFF:460:HOH:O	2.12	0.50
1:FFF:152:GLU:OE1	3:HHH:5:LYS:NZ	2.40	0.50
5:JJJ:172:ASP:HB2	5:JJJ:189:LEU:HD12	1.93	0.49
4:DDD:160:VAL:C	5:EEE:170:CYS:SG	2.96	0.49
1:AAA:18:GLY:HA2	2:GGG:89:GLN:HB3	1.94	0.48
1:AAA:258:THR:HA	7:AAA:323:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:III:163:MET:HE1	5:JJJ:194:ARG:HG2	1.95	0.48
4:DDD:82:PRO:HA	4:DDD:109:VAL:HB	1.96	0.47
2:GGG:51:HIS:HA	2:GGG:65:LEU:O	2.15	0.47
5:EEE:241:ARG:HD3	7:EEE:333:HOH:O	2.14	0.47
1:AAA:117:ALA:HB2	2:BBB:60:TRP:CE2	2.49	0.47
1:FFF:266:LEU:HD12	1:FFF:266:LEU:O	2.15	0.46
4:III:33:SER:HB3	4:III:52:TYR:CE1	2.50	0.46
4:III:82:PRO:HA	4:III:109:VAL:HB	1.98	0.46
4:III:157:ASP:N	7:III:203:HOH:O	2.48	0.46
1:FFF:138:THR:N	7:FFF:406:HOH:O	2.48	0.46
2:GGG:0:MET:HE3	2:GGG:0:MET:HB2	1.89	0.46
4:DDD:34:PHE:HB2	4:DDD:51:ILE:HG23	1.98	0.45
4:III:34:PHE:CD2	4:III:92:VAL:HG13	2.51	0.45
4:III:34:PHE:HB2	4:III:51:ILE:HG23	1.98	0.45
1:FFF:258:THR:CG2	1:FFF:271:THR:HG23	2.47	0.45
1:FFF:68:ARG:HG2	1:FFF:68:ARG:NH1	2.27	0.45
1:FFF:138:THR:O	1:FFF:141:GLN:HB2	2.17	0.45
4:DDD:117:ASP:N	4:DDD:118:PRO:HD3	2.32	0.45
1:FFF:79:ARG:NH2	5:JJJ:29:ASP:OD2	2.50	0.45
5:EEE:19:ASN:OD1	5:EEE:81:GLN:HA	2.17	0.44
1:AAA:68:ARG:HG2	1:AAA:68:ARG:NH1	2.30	0.44
4:DDD:4:GLU:HG2	4:DDD:27:SER:OG	2.16	0.44
4:III:163:MET:CE	5:JJJ:194:ARG:CG	2.95	0.44
1:AAA:79:ARG:NH2	5:EEE:29:ASP:OD2	2.43	0.44
1:AAA:212:GLU:HA	1:AAA:212:GLU:OE1	2.16	0.44
4:DDD:160:VAL:N	5:EEE:170:CYS:SG	2.91	0.44
2:GGG:40:LEU:HA	2:GGG:44:GLU:O	2.18	0.44
4:DDD:172:SER:HB2	5:EEE:192:ARG:HE	1.83	0.44
1:FFF:197:HIS:NE2	1:FFF:198:GLU:HG3	2.33	0.44
4:DDD:133:VAL:HG13	5:EEE:127:PHE:CE2	2.53	0.44
5:JJJ:129:PRO:HD2	5:JJJ:200:TRP:CZ2	2.53	0.44
1:AAA:138:THR:O	1:AAA:141:GLN:HB2	2.18	0.43
4:III:160:VAL:N	5:JJJ:170:CYS:SG	2.91	0.43
1:AAA:152:GLU:HG2	3:CCC:7:PRO:HB3	2.00	0.43
5:JJJ:119:VAL:HG11	5:JJJ:216:LEU:HD13	2.00	0.43
4:DDD:38:ARG:HD3	4:DDD:40:TYR:CZ	2.54	0.43
1:FFF:197:HIS:CD2	7:FFF:449:HOH:O	2.71	0.43
4:III:12:LEU:C	4:III:12:LEU:HD23	2.43	0.43
2:BBB:40:LEU:HA	2:BBB:44:GLU:O	2.18	0.43
2:BBB:51:HIS:HA	2:BBB:65:LEU:O	2.19	0.43
3:HHH:5:LYS:HB2	5:JJJ:99:PRO:CG	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:EEE:9:PRO:O	5:EEE:108:THR:HG23	2.18	0.43
1:FFF:198:GLU:OE2	1:FFF:249:VAL:HG23	2.18	0.43
5:JJJ:9:PRO:O	5:JJJ:108:THR:HG23	2.18	0.43
5:EEE:129:PRO:HD2	5:EEE:200:TRP:CZ2	2.54	0.42
1:AAA:192:HIS:HB2	1:AAA:200:THR:HG22	2.01	0.42
1:AAA:266:LEU:O	1:AAA:266:LEU:HD12	2.19	0.42
4:III:12:LEU:C	4:III:12:LEU:CD2	2.92	0.42
5:JJJ:19:ASN:OD1	5:JJJ:81:GLN:HA	2.20	0.42
2:GGG:16:GLU:O	2:GGG:19:LYS:HG2	2.20	0.42
4:DDD:93:MET:HE1	5:EEE:100:ASN:O	2.20	0.42
1:FFF:1:GLY:HA3	1:FFF:105:PRO:HA	2.01	0.42
5:EEE:134:ILE:HG23	5:EEE:197:ALA:HB1	2.02	0.41
1:FFF:178:THR:CG2	7:FFF:419:HOH:O	2.64	0.41
1:FFF:51:TRP:CZ2	1:FFF:179:LEU:HD11	2.55	0.41
4:III:163:MET:CE	5:JJJ:194:ARG:HD3	2.48	0.41
4:III:38:ARG:HD3	4:III:40:TYR:CZ	2.56	0.41
1:FFF:55:GLU:OE2	1:FFF:174:LYS:CE	2.67	0.41
5:EEE:146:ALA:O	5:EEE:188:ALA:HA	2.21	0.41
4:III:117:ASP:O	4:III:118:PRO:C	2.64	0.41
4:III:125:ASP:HB3	4:III:128:SER:O	2.21	0.41
5:JJJ:144:CYS:HB2	5:JJJ:158:TRP:CZ2	2.56	0.41
5:EEE:144:CYS:HB2	5:EEE:158:TRP:CZ2	2.56	0.41
1:FFF:257:TYR:O	1:FFF:273:ARG:HB2	2.22	0.41
4:DDD:56:ASP:HB3	4:DDD:65:GLN:NE2	2.36	0.40
4:DDD:125:ASP:HB3	4:DDD:128:SER:O	2.21	0.40
4:DDD:159:CYS:HB3	5:EEE:192:ARG:NH2	2.36	0.40
4:III:63:THR:OG1	4:III:78:ARG:NH2	2.47	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	245/276 (89%)	236 (96%)	9 (4%)	0	100	100
1	FFF	264/276 (96%)	252 (96%)	12 (4%)	0	100	100
2	BBB	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
2	GGG	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
3	CCC	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	HHH	7/9 (78%)	7 (100%)	0	0	100	100
4	DDD	187/197 (95%)	175 (94%)	12 (6%)	0	100	100
4	III	185/197 (94%)	170 (92%)	15 (8%)	0	100	100
5	EEE	239/243 (98%)	225 (94%)	14 (6%)	0	100	100
5	JJJ	239/243 (98%)	228 (95%)	11 (5%)	0	100	100
All	All	1569/1650 (95%)	1482 (94%)	87 (6%)	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	215/237 (91%)	207 (96%)	8 (4%)	30	39
1	FFF	231/237 (98%)	222 (96%)	9 (4%)	28	37
2	BBB	95/95 (100%)	93 (98%)	2 (2%)	47	60
2	GGG	95/95 (100%)	93 (98%)	2 (2%)	47	60
3	CCC	7/7 (100%)	7 (100%)	0	100	100
3	HHH	7/7 (100%)	7 (100%)	0	100	100
4	DDD	170/177 (96%)	159 (94%)	11 (6%)	15	17
4	III	168/177 (95%)	158 (94%)	10 (6%)	17	20
5	EEE	212/214 (99%)	197 (93%)	15 (7%)	13	14
5	JJJ	212/214 (99%)	205 (97%)	7 (3%)	33	43
All	All	1412/1460 (97%)	1348 (96%)	64 (4%)	24	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	68	ARG
1	AAA	115	GLN
1	AAA	122	ASP
1	AAA	180	LEU
1	AAA	200	THR
1	AAA	206	LEU
1	AAA	231	VAL
1	AAA	266	LEU
2	BBB	33	SER
2	BBB	70	PHE
4	DDD	25	THR
4	DDD	50	SER
4	DDD	53	SER
4	DDD	79[A]	ASP
4	DDD	79[B]	ASP
4	DDD	83	SER
4	DDD	98	GLU
4	DDD	127	LYS
4	DDD	132	SER
4	DDD	170	SER
4	DDD	172	SER
5	EEE	6	SER
5	EEE	20	VAL
5	EEE	29	ASP
5	EEE	37	ARG
5	EEE	52	SER
5	EEE	72	LYS
5	EEE	82	ARG
5	EEE	90	MET
5	EEE	101	GLU
5	EEE	109	ARG
5	EEE	152	ASP
5	EEE	154	VAL
5	EEE	183	ASN
5	EEE	192	ARG
5	EEE	221	GLU
1	FFF	35	ARG
1	FFF	68	ARG
1	FFF	130	LEU
1	FFF	180	LEU
1	FFF	197	HIS
1	FFF	206	LEU

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Mol	Chain	Res	Type
1	FFF	218	GLN
1	FFF	231	VAL
1	FFF	271	THR
2	GGG	33	SER
2	GGG	70	PHE
4	III	25	THR
4	III	53	SER
4	III	78	ARG
4	III	79	ASP
4	III	83	SER
4	III	98	GLU
4	III	126	SER
4	III	132	SER
4	III	170	SER
4	III	172	SER
5	JJJ	28	SER
5	JJJ	29	ASP
5	JJJ	52	SER
5	JJJ	90	MET
5	JJJ	138	GLN
5	JJJ	154	VAL
5	JJJ	192	ARG

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ACT	FFF	301	-	3,3,3	1.24	0	3,3,3	0.87	0
6	ACT	JJJ	301	-	3,3,3	1.13	0	3,3,3	0.71	0

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](#)

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	250/276 (90%)	0.91	27 (10%)	11 12	49, 83, 126, 166	1 (0%)
1	FFF	267/276 (96%)	1.44	70 (26%)	1 1	34, 71, 153, 198	1 (0%)
2	BBB	100/100 (100%)	1.31	21 (21%)	2 3	68, 106, 138, 157	0
2	GGG	100/100 (100%)	1.14	15 (15%)	5 6	52, 75, 109, 129	0
3	CCC	9/9 (100%)	0.64	0	100 100	46, 60, 76, 77	0
3	HHH	9/9 (100%)	0.04	0	100 100	43, 47, 57, 61	0
4	DDD	187/197 (94%)	0.73	20 (10%)	11 13	32, 68, 132, 156	3 (1%)
4	III	187/197 (94%)	0.91	26 (13%)	6 7	39, 66, 141, 162	1 (0%)
5	EEE	241/243 (99%)	0.57	18 (7%)	20 24	39, 61, 95, 135	0
5	JJJ	241/243 (99%)	0.88	22 (9%)	15 18	35, 83, 123, 150	0
All	All	1591/1650 (96%)	0.95	219 (13%)	6 7	32, 75, 133, 198	6 (0%)

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	248	VAL	7.4
1	FFF	17	ARG	6.7
5	JJJ	60	ARG	6.6
1	FFF	16	GLY	6.5
1	FFF	272	LEU	6.3
1	FFF	39	ASP	6.0
1	FFF	21	ARG	5.7
4	DDD	129	SER	5.2
1	AAA	270	VAL	5.1
1	FFF	249	VAL	5.1
1	FFF	38	ASN	5.0
1	FFF	54	GLN	4.9
1	AAA	247	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	FFF	41	ALA	4.6
1	FFF	201	LEU	4.5
1	FFF	228	THR	4.4
1	FFF	27	TYR	4.3
4	DDD	120	VAL	4.2
1	FFF	274	TRP	4.1
2	GGG	43	GLY	4.0
1	AAA	150	ALA	4.0
1	AAA	201	LEU	4.0
1	FFF	58	GLU	4.0
2	GGG	14	PRO	3.9
4	III	166	MET	3.9
1	FFF	14	ARG	3.9
4	III	182	PHE	3.8
1	FFF	18	GLY	3.8
1	FFF	182	LEU	3.8
1	FFF	261	VAL	3.8
2	BBB	19	LYS	3.7
4	DDD	166	MET	3.7
1	FFF	22	PHE	3.7
4	DDD	127	LYS	3.7
1	FFF	42	SER	3.7
5	EEE	72	LYS	3.7
4	III	102	GLY	3.7
1	FFF	267	PRO	3.6
1	FFF	190	THR	3.5
2	GGG	85	VAL	3.5
1	AAA	38	ASN	3.5
1	FFF	177	GLU	3.5
1	FFF	189	VAL	3.5
1	FFF	276	PRO	3.4
1	FFF	266	LEU	3.4
4	III	104	GLY	3.4
2	BBB	98	ASP	3.4
2	GGG	83	ASN	3.4
1	AAA	217	TRP	3.3
5	EEE	182	LEU	3.3
1	FFF	191	HIS	3.3
1	FFF	23	ILE	3.3
1	AAA	271	THR	3.3
4	III	124	ARG	3.3
1	FFF	275	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
4	DDD	131	LYS	3.3
5	JJJ	223	THR	3.2
1	FFF	40	ALA	3.2
4	DDD	124	ARG	3.2
4	III	103	SER	3.2
1	FFF	12	VAL	3.2
1	FFF	270	VAL	3.2
4	III	145	VAL	3.2
1	FFF	98	MET	3.2
1	AAA	174	LYS	3.2
2	GGG	87	LEU	3.2
1	AAA	42	SER	3.1
5	JJJ	43	GLY	3.1
1	FFF	247	VAL	3.1
1	FFF	230	LEU	3.1
1	AAA	189	VAL	3.1
2	BBB	37	VAL	3.1
1	FFF	13	SER	3.0
4	III	189	ASN	3.0
5	JJJ	57	GLU	3.0
5	EEE	181	ALA	3.0
1	FFF	216	THR	3.0
5	EEE	75	PHE	2.9
1	AAA	74	PHE	2.9
4	III	101	PHE	2.9
2	GGG	1	ILE	2.9
5	EEE	223	THR	2.9
5	JJJ	49	TYR	2.9
1	FFF	194	ILE	2.9
1	FFF	218	GLN	2.9
5	JJJ	61	LEU	2.9
2	BBB	75	LYS	2.8
4	DDD	180	SER	2.8
5	EEE	29	ASP	2.9
5	JJJ	55	GLN	2.8
5	EEE	176	LEU	2.8
1	FFF	188	HIS	2.8
5	JJJ	182	LEU	2.8
1	FFF	136	VAL	2.8
1	FFF	60	TRP	2.8
5	EEE	241	ARG	2.8
4	III	9	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	FFF	252	GLY	2.8
5	JJJ	58	LYS	2.8
1	FFF	25	VAL	2.8
1	AAA	194	ILE	2.7
5	EEE	3	THR	2.7
4	III	123	LEU	2.7
5	JJJ	56	LEU	2.7
2	GGG	37	VAL	2.7
1	FFF	269	PRO	2.7
1	FFF	203	CYS	2.7
2	GGG	81	ARG	2.7
4	DDD	130	ASP	2.7
4	DDD	141	SER	2.7
5	EEE	174	GLN	2.7
4	III	6	GLU	2.7
2	BBB	18	GLY	2.7
5	JJJ	46	PHE	2.6
2	BBB	9	VAL	2.6
4	DDD	164[A]	ARG	2.6
4	III	184	CYS	2.6
1	AAA	261	VAL	2.6
1	FFF	53	GLU	2.6
1	AAA	40	ALA	2.6
1	AAA	187	THR	2.6
4	III	37	TYR	2.6
2	BBB	39	LEU	2.6
2	GGG	15	ALA	2.6
1	FFF	204	TRP	2.6
1	FFF	250	PRO	2.6
5	EEE	61	LEU	2.5
1	AAA	139	ALA	2.5
4	III	131	LYS	2.5
2	BBB	49	VAL	2.5
5	JJJ	42	GLN	2.5
4	DDD	8	ASN	2.5
4	III	171	ASN	2.5
1	FFF	26	GLY	2.5
1	FFF	8	PHE	2.5
5	JJJ	59	SER	2.5
2	BBB	0	MET	2.5
2	BBB	85	VAL	2.4
4	III	108	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
5	EEE	173	PRO	2.4
5	JJJ	41	GLY	2.4
2	GGG	73	THR	2.4
1	AAA	41	ALA	2.4
1	FFF	105	PRO	2.4
1	AAA	230	LEU	2.4
4	III	135	LEU	2.4
5	JJJ	116	LEU	2.4
1	FFF	217	TRP	2.4
1	FFF	211	ALA	2.4
4	DDD	183	ALA	2.4
1	AAA	136	VAL	2.4
2	BBB	1	ILE	2.4
1	AAA	191	HIS	2.4
1	FFF	193	PRO	2.3
4	III	185	ALA	2.3
5	JJJ	3	THR	2.3
4	DDD	9	SER	2.3
4	III	164	ARG	2.3
4	III	89	LEU	2.3
5	JJJ	145	LEU	2.3
5	EEE	180	PRO	2.3
4	III	105	THR	2.3
5	JJJ	198	THR	2.3
4	DDD	128	SER	2.3
1	FFF	33	PHE	2.3
2	BBB	40	LEU	2.3
2	GGG	40	LEU	2.3
1	FFF	171	TYR	2.3
4	DDD	182	PHE	2.3
1	AAA	5	LEU	2.3
1	FFF	176	LYS	2.3
1	FFF	37	ASP	2.3
5	EEE	175	PRO	2.3
1	FFF	257	TYR	2.3
2	BBB	79	ALA	2.3
2	BBB	20	SER	2.3
4	III	149	LYS	2.3
1	AAA	182	LEU	2.2
2	BBB	54	LEU	2.2
2	GGG	27	VAL	2.3
1	FFF	239	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	FFF	199	ALA	2.2
2	GGG	82	VAL	2.2
5	EEE	152	ASP	2.2
1	FFF	245	ALA	2.2
4	DDD	135	LEU	2.2
5	EEE	183	ASN	2.2
1	FFF	260	HIS	2.2
4	DDD	3	LYS	2.2
4	III	5	VAL	2.2
1	AAA	105	PRO	2.2
1	AAA	259	CYS	2.2
2	BBB	73	THR	2.2
4	DDD	118	PRO	2.1
5	JJJ	50	PHE	2.1
5	EEE	85	GLN	2.1
4	DDD	146	SER	2.1
2	BBB	23	LEU	2.1
4	DDD	123	LEU	2.1
5	JJJ	156	LEU	2.1
1	AAA	260	HIS	2.1
1	FFF	167	TRP	2.1
4	III	188	PHE	2.1
5	JJJ	181	ALA	2.1
2	BBB	62	PHE	2.1
4	III	176	TRP	2.1
1	AAA	120	GLY	2.1
1	FFF	273	ARG	2.1
2	GGG	97	ARG	2.1
5	EEE	16	ARG	2.1
2	BBB	80	CYS	2.1
1	FFF	255	GLN	2.1
1	FFF	15	PRO	2.1
2	BBB	72	PRO	2.1
1	FFF	137	ASP	2.0
2	GGG	34	ASP	2.0
1	AAA	190	THR	2.0
2	BBB	92	ILE	2.0
5	JJJ	10	ARG	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](#)

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($\text{\AA}^2$)	Q<0.9
6	ACT	FFF	301	4/4	0.56	0.20	70,73,73,84	0
6	ACT	JJJ	301	4/4	0.71	0.16	94,95,99,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.