



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:21 PM UTC

PDB ID : 7PDX / pdb_00007pdx
Title : Crystal structure of parent MAGE-A10 TCR (728)
Authors : Simister, P.C.; Border, E.C.; Vieira, J.F.; Pumphrey, N.J.
Deposited on : 2021-08-09
Resolution : 2.27 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

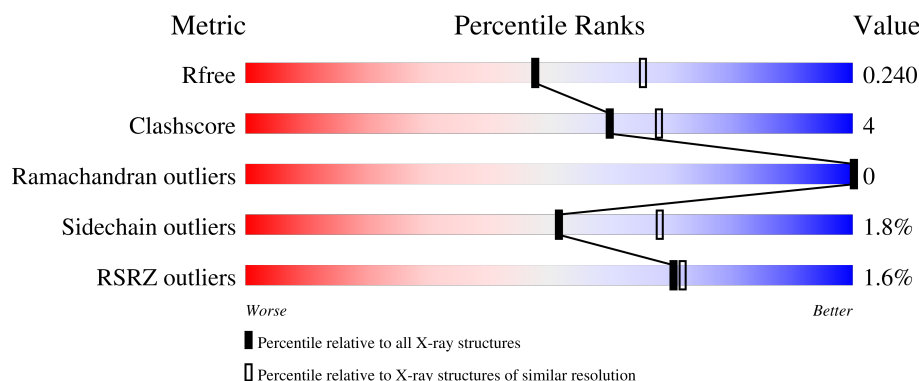
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

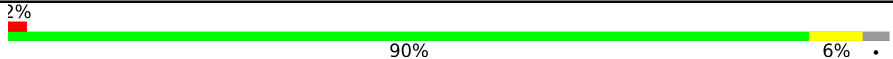
The reported resolution of this entry is 2.27 Å.

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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	206	
1	CCC	206	
2	BBB	241	
2	DDD	241	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13438 atoms, of which 6377 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 T-cell receptor alpha chain (TRAV/TRAC).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	CCC	201	Total	C	H	N	O	S	59	0	0
			2957	947	1430	257	315	8			
1	AAA	200	Total	C	H	N	O	S	60	0	0
			2925	940	1413	251	313	8			

- Molecule 2 is a protein called T-cell receptor beta chain (TRBV/TRBC).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	DDD	237	Total	C	H	N	O	S	66	1	0
			3648	1186	1780	320	353	9			
2	BBB	237	Total	C	H	N	O	S	68	0	0
			3602	1173	1754	315	351	9			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DDD	1	Total	Cl	0	0
			1	1		
3	BBB	1	Total	Cl	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	O	P	0	0
			5	4	1		

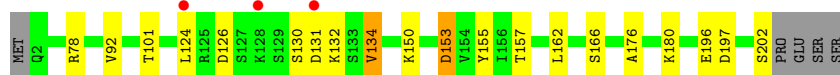
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	CCC	75	Total	O	0	0
			75	75		
5	DDD	85	Total	O	0	0
			85	85		
5	AAA	66	Total	O	0	0
			66	66		
5	BBB	73	Total	O	0	0
			73	73		

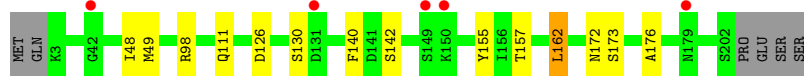
3 Residue-property plots [i](#)

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.

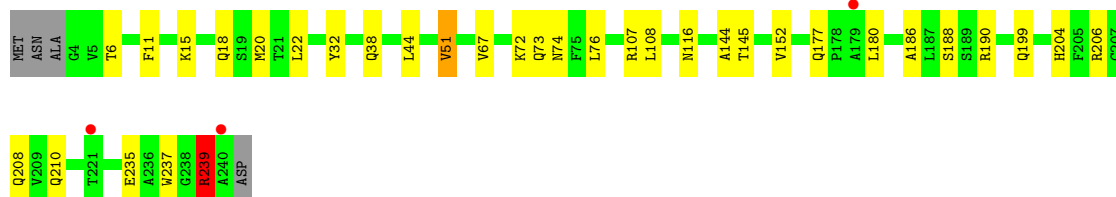
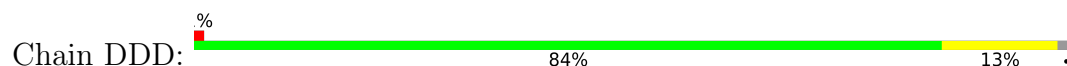
- Molecule 1: T-cell receptor alpha chain (TRAV/TRAC)



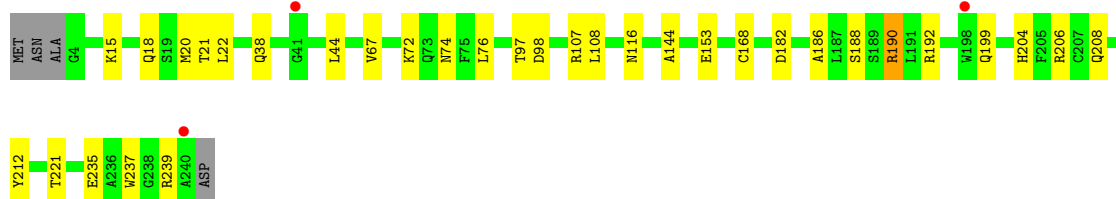
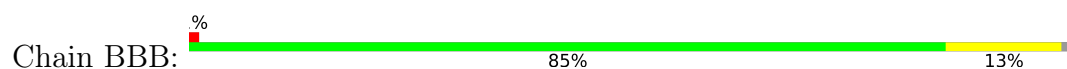
- Molecule 1: T-cell receptor alpha chain (TRAV/TRAC)



- Molecule 2: T-cell receptor beta chain (TRBV/TRBC)



- Molecule 2: T-cell receptor beta chain (TRBV/TRBC)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.93Å 59.17Å 86.02Å 101.94° 105.87° 104.69°	Depositor
Resolution (Å)	79.01 – 2.27 79.01 – 2.27	Depositor EDS
% Data completeness (in resolution range)	86.2 (79.01-2.27) 62.3 (79.01-2.27)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.252 0.190 , 0.240	Depositor DCC
R_{free} test set	1875 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 42.2	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	13438	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% 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: CL, PO4

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	1.04	1/1543 (0.1%)	1.35	4/2096 (0.2%)
1	CCC	1.05	0/1558	1.34	3/2115 (0.1%)
2	BBB	1.03	0/1900	1.28	0/2594
2	DDD	1.01	0/1920	1.30	1/2617 (0.0%)
All	All	1.03	1/6921 (0.0%)	1.32	8/9422 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	172	ASN	C-O	5.13	1.30	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	162	LEU	N-CA-CB	-5.83	101.31	110.69
1	CCC	162	LEU	N-CA-CB	-5.54	101.76	110.69
1	AAA	140	PHE	CA-C-N	5.50	128.51	120.71
1	AAA	140	PHE	C-N-CA	5.50	128.51	120.71
1	CCC	150	LYS	N-CA-C	-5.39	106.71	113.28
1	AAA	126	ASP	CA-CB-CG	5.38	117.97	112.60
2	DDD	239	ARG	CA-C-O	-5.18	115.73	121.33
1	CCC	153	ASP	CA-CB-CG	5.17	117.77	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	1512	1413	1390	8	0
1	CCC	1527	1430	1409	10	0
2	BBB	1848	1754	1727	20	1
2	DDD	1868	1780	1755	23	1
3	BBB	1	0	0	0	0
3	DDD	1	0	0	0	0
4	BBB	5	0	0	1	0
5	AAA	66	0	0	2	0
5	BBB	73	0	0	0	0
5	CCC	75	0	0	2	0
5	DDD	85	0	0	5	0
All	All	7061	6377	6281	56	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 4.

All (56) 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:DDD:20:MET:HE3	2:DDD:22:LEU:HD11	1.60	0.83
2:DDD:20:MET:HE2	2:DDD:108:LEU:HD22	1.62	0.81
2:BBB:20:MET:HE3	2:BBB:22:LEU:HD11	1.64	0.80
2:BBB:20:MET:HE2	2:BBB:108:LEU:HD22	1.69	0.74
2:BBB:97:THR:HG23	2:BBB:98:ASP:H	1.54	0.71
2:DDD:206:ARG:NH2	2:DDD:208:GLN:OE1	2.24	0.70
2:BBB:206:ARG:NH2	2:BBB:208:GLN:OE1	2.26	0.68
2:DDD:11:PHE:CE2	2:DDD:107[B]:ARG:HG3	2.33	0.63
1:AAA:173:SER:OG	2:BBB:190:ARG:HD2	2.02	0.60
2:DDD:6:THR:HB	5:DDD:466:HOH:O	2.03	0.59
2:DDD:38:GLN:HB2	2:DDD:44:LEU:HD23	1.85	0.58
1:AAA:48:ILE:HG22	1:AAA:49:MET:HG2	1.87	0.57
2:BBB:21:THR:CG2	2:BBB:76:LEU:HD22	2.35	0.56
2:DDD:107[A]:ARG:HD3	5:DDD:462:HOH:O	2.05	0.56
2:BBB:20:MET:CE	2:BBB:108:LEU:HD22	2.33	0.56
2:DDD:177:GLN:OE1	2:DDD:180:LEU:HD12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:196:GLU:O	1:CCC:197:ASP:CB	2.54	0.55
2:DDD:20:MET:CE	2:DDD:108:LEU:HD22	2.35	0.54
1:CCC:132:LYS:HE2	2:DDD:145:THR:HG21	1.90	0.54
2:BBB:38:GLN:HB2	2:BBB:44:LEU:HD23	1.92	0.51
1:CCC:124:LEU:HB2	1:CCC:134:VAL:HG22	1.91	0.51
2:BBB:199:GLN:HA	2:BBB:239:ARG:O	2.12	0.50
1:CCC:153:ASP:HB2	1:CCC:180:LYS:HD2	1.92	0.50
2:BBB:116:ASN:ND2	2:BBB:182:ASP:OD2	2.44	0.50
2:DDD:199:GLN:HA	2:DDD:239:ARG:O	2.12	0.49
1:AAA:162:LEU:HD21	2:BBB:192:ARG:HB3	1.95	0.49
2:DDD:107[A]:ARG:CD	5:DDD:462:HOH:O	2.61	0.48
2:BBB:206:ARG:HG3	2:BBB:235:GLU:HB3	1.96	0.47
1:CCC:155:TYR:O	1:CCC:176:ALA:HA	2.15	0.47
1:AAA:157:THR:HG21	2:BBB:188:SER:OG	2.15	0.47
2:BBB:15:LYS:H	2:BBB:18:GLN:NE2	2.13	0.47
2:DDD:206:ARG:HG3	2:DDD:235:GLU:HB3	1.97	0.46
1:CCC:126:ASP:OD2	1:CCC:130:SER:HB3	2.15	0.46
1:AAA:155:TYR:O	1:AAA:176:ALA:HA	2.15	0.46
2:DDD:32:TYR:HE1	2:DDD:51:VAL:HG22	1.80	0.46
2:BBB:67:VAL:HA	2:BBB:76:LEU:O	2.16	0.46
1:CCC:92:VAL:O	1:CCC:101:THR:HG22	2.16	0.45
2:DDD:67:VAL:HA	2:DDD:76:LEU:O	2.15	0.45
2:BBB:204:HIS:HB2	2:BBB:237:TRP:CZ3	2.52	0.45
2:DDD:73:GLN:HB3	5:DDD:463:HOH:O	2.16	0.44
2:DDD:144:ALA:O	2:DDD:186:ALA:HA	2.19	0.43
2:DDD:204:HIS:HB2	2:DDD:237:TRP:CZ3	2.54	0.43
2:BBB:144:ALA:O	2:BBB:186:ALA:HA	2.19	0.43
2:BBB:153:GLU:OE1	2:BBB:212:TYR:OH	2.28	0.43
2:DDD:15:LYS:H	2:DDD:18:GLN:NE2	2.17	0.42
2:DDD:116:ASN:ND2	5:DDD:413:HOH:O	2.52	0.42
1:AAA:162:LEU:HB2	5:AAA:309:HOH:O	2.19	0.42
2:BBB:204:HIS:CE1	4:BBB:301:PO4:O3	2.71	0.42
2:DDD:22:LEU:N	2:DDD:22:LEU:HD12	2.35	0.42
1:CCC:202:SER:N	5:CCC:310:HOH:O	2.52	0.42
1:AAA:98:ARG:HB3	5:AAA:348:HOH:O	2.19	0.41
1:CCC:157:THR:HG21	2:DDD:188:SER:OG	2.20	0.41
1:AAA:111:GLN:HB3	1:AAA:142:SER:HB3	2.03	0.41
1:CCC:78:ARG:NE	5:CCC:313:HOH:O	2.54	0.40
2:DDD:152:VAL:HA	2:DDD:210:GLN:O	2.21	0.40
2:BBB:22:LEU:HD12	2:BBB:22:LEU:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DDD:74:ASN:OD1	2:BBB:74:ASN:OD1[1_556]	1.76	0.44

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	198/206 (96%)	191 (96%)	7 (4%)	0	100	100
1	CCC	199/206 (97%)	195 (98%)	4 (2%)	0	100	100
2	BBB	235/241 (98%)	226 (96%)	9 (4%)	0	100	100
2	DDD	236/241 (98%)	229 (97%)	7 (3%)	0	100	100
All	All	868/894 (97%)	841 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	166/183 (91%)	165 (99%)	1 (1%)	78	87
1	CCC	168/183 (92%)	165 (98%)	3 (2%)	51	68
2	BBB	194/208 (93%)	189 (97%)	5 (3%)	40	56
2	DDD	196/208 (94%)	192 (98%)	4 (2%)	48	65
All	All	724/782 (93%)	711 (98%)	13 (2%)	51	68

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	131	ASP
1	CCC	134	VAL
1	CCC	166	SER
2	DDD	51	VAL
2	DDD	72	LYS
2	DDD	190	ARG
2	DDD	239	ARG
1	AAA	130	SER
2	BBB	72	LYS
2	BBB	107	ARG
2	BBB	168	CYS
2	BBB	190	ARG
2	BBB	221	THR

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
4	PO4	BBB	301	-	4,4,4	1.02	0	6,6,6	0.73	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	301	PO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	200/206 (97%)	0.27	5 (2%) 58 60	17, 34, 64, 87	0
1	CCC	201/206 (97%)	0.22	3 (1%) 72 73	17, 31, 57, 69	0
2	BBB	237/241 (98%)	0.25	3 (1%) 75 76	20, 34, 57, 79	0
2	DDD	237/241 (98%)	0.15	3 (1%) 75 76	12, 32, 56, 81	1 (0%)
All	All	875/894 (97%)	0.22	14 (1%) 70 72	12, 33, 58, 87	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	240	ALA	3.7
2	DDD	240	ALA	3.6
1	AAA	131	ASP	3.2
2	DDD	221	THR	2.9
1	AAA	149	SER	2.3
1	AAA	179	ASN	2.3
2	BBB	198	TRP	2.2
1	CCC	128	LYS	2.2
1	CCC	131	ASP	2.1
2	DDD	179	ALA	2.1
1	AAA	42	GLY	2.1
2	BBB	41	GLY	2.1
1	AAA	150	LYS	2.0
1	CCC	124	LEU	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 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
3	CL	BBB	302	1/1	0.95	0.23	48,48,48,48	0
3	CL	DDD	301	1/1	0.96	0.14	47,47,47,47	0
4	PO4	BBB	301	5/5	0.98	0.05	28,31,34,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.