



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:42 PM GMT

PDB ID : 1BZQ
Title : COMPLEX OF A DROMEDARY SINGLE-DOMAIN VHH ANTIBODY
FRAGMENT WITH RNASE A
Authors : Decanniere, K.; Desmyter, A.; Gahrudhi, M.; Lauwereys, M.; Muyldermans,
S.; Wyns, L.
Deposited on : 1998-11-03
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

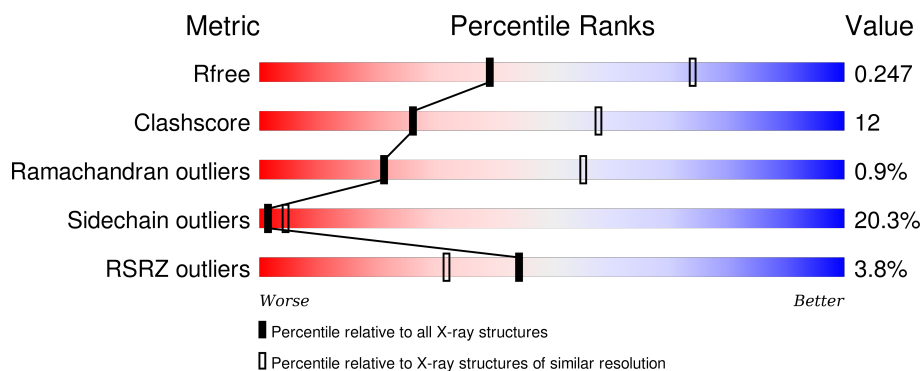
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	A	124	
1	B	124	
1	C	124	
1	D	124	
2	K	124	

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Mol	Chain	Length	Quality of chain
2	L	124	 4% 66% 24% 9% •
2	M	124	 5% 60% 33% 5% •
2	N	124	 4% 69% 21% 8% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7564 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 PROTEIN (RNASE A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			951	575	171	193	12			
1	B	124	Total	C	N	O	S	0	0	0
			951	575	171	193	12			
1	C	124	Total	C	N	O	S	0	0	0
			951	575	171	193	12			
1	D	124	Total	C	N	O	S	0	0	0
			951	575	171	193	12			

- Molecule 2 is a protein called PROTEIN (ANTIBODY CAB-RN05).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	124	Total	C	N	O	S	0	0	0
			935	579	167	184	5			
2	L	124	Total	C	N	O	S	0	0	0
			935	579	167	184	5			
2	M	124	Total	C	N	O	S	0	0	0
			935	579	167	184	5			
2	N	124	Total	C	N	O	S	0	0	0
			935	579	167	184	5			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

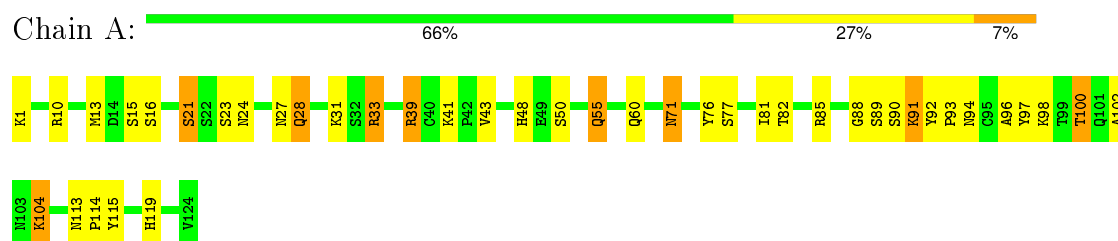


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

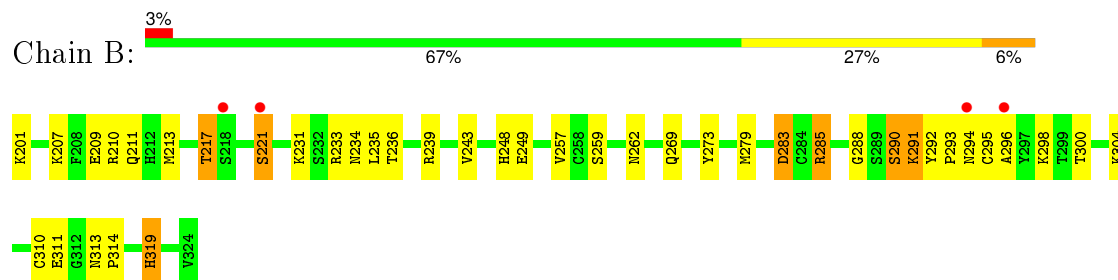
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

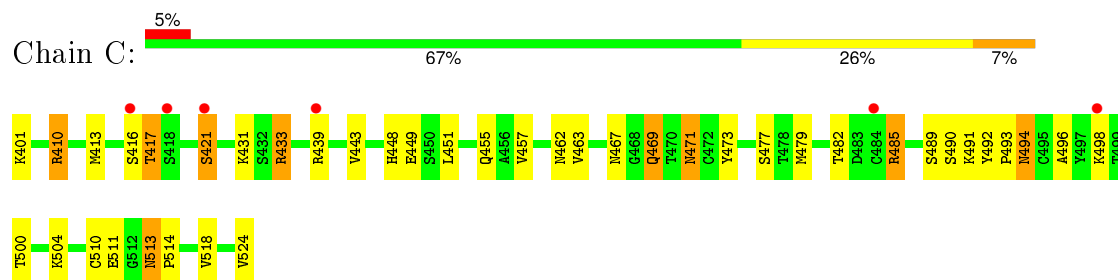
• Molecule 1: PROTEIN (RNASE A)



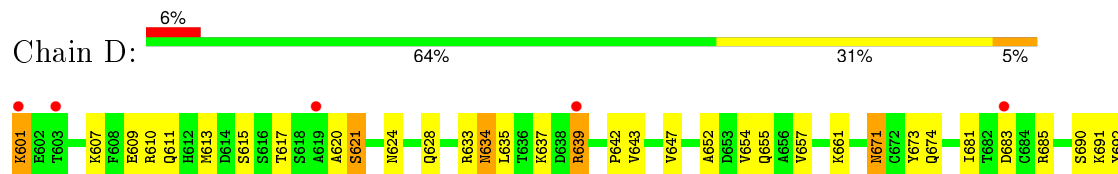
• Molecule 1: PROTEIN (RNASE A)

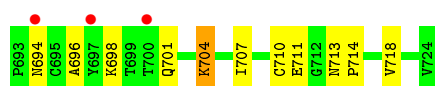


• Molecule 1: PROTEIN (RNASE A)

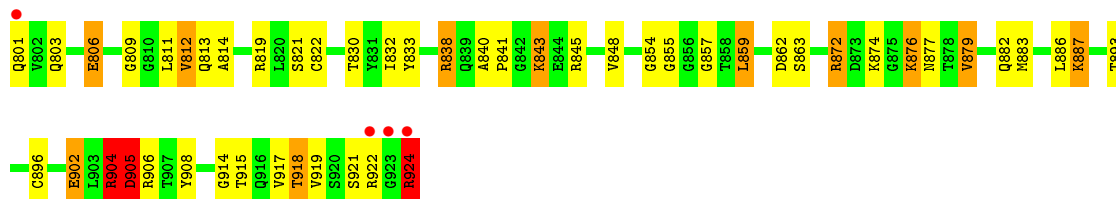


• Molecule 1: PROTEIN (RNASE A)

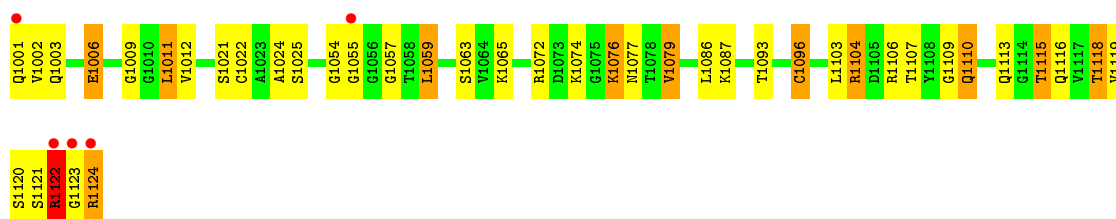




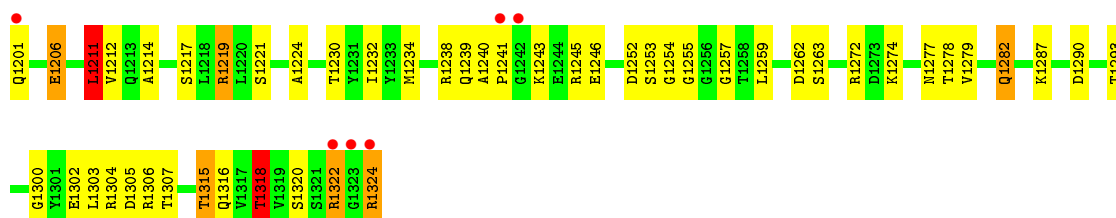
• Molecule 2: PROTEIN (ANTIBODY CAB-RN05)



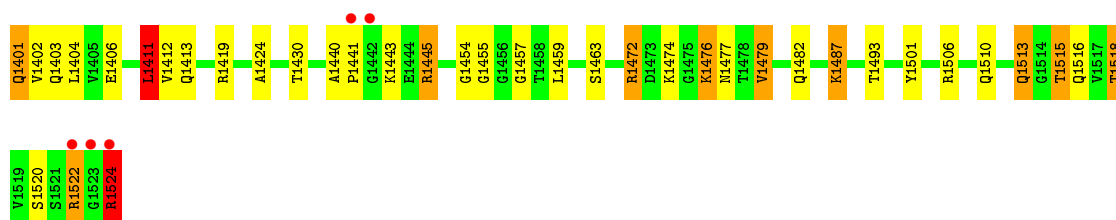
• Molecule 2: PROTEIN (ANTIBODY CAB-RN05)



• Molecule 2: PROTEIN (ANTIBODY CAB-RN05)



• Molecule 2: PROTEIN (ANTIBODY CAB-RN05)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.52Å 66.82Å 69.34Å 91.43° 117.34° 97.33°	Depositor
Resolution (Å)	20.00 – 2.80 14.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.80) 96.1 (14.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.282 0.197 , 0.247	Depositor DCC
R_{free} test set	1312 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.844	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25413 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7564	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	A	0.39	0/967	1.00	2/1304 (0.2%)
1	B	0.39	0/967	1.01	2/1304 (0.2%)
1	C	0.37	0/967	0.99	2/1304 (0.2%)
1	D	0.39	0/967	0.98	0/1304
2	K	0.45	0/952	1.27	9/1281 (0.7%)
2	L	0.45	0/952	1.16	3/1281 (0.2%)
2	M	0.43	0/952	1.20	6/1281 (0.5%)
2	N	0.44	0/952	1.18	8/1281 (0.6%)
All	All	0.42	0/7676	1.10	32/10340 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	872	ARG	NE-CZ-NH2	-10.53	115.04	120.30
2	K	904	ARG	CD-NE-CZ	10.08	137.72	123.60
2	K	872	ARG	NE-CZ-NH1	10.00	125.30	120.30
2	M	1219	ARG	NE-CZ-NH2	-9.84	115.38	120.30
2	K	904	ARG	NE-CZ-NH1	8.70	124.65	120.30
2	N	1445	ARG	CD-NE-CZ	8.29	135.21	123.60
2	K	838	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	N	1472	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	N	1524	ARG	CD-NE-CZ	7.67	134.34	123.60
2	M	1252	ASP	CB-CG-OD1	7.01	124.61	118.30
2	M	1318	THR	N-CA-CB	6.65	122.93	110.30
1	A	39	ARG	CA-CB-CG	6.58	127.88	113.40
1	C	433	ARG	NE-CZ-NH2	-6.37	117.12	120.30
2	N	1472	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	283	ASP	CB-CA-C	6.22	122.83	110.40
2	L	1122	ARG	NE-CZ-NH1	6.06	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1411	LEU	CA-CB-CG	5.95	128.98	115.30
2	M	1211	LEU	CA-CB-CG	5.90	128.87	115.30
2	K	857	GLY	N-CA-C	-5.87	98.43	113.10
2	K	908	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	C	410	ARG	NE-CZ-NH1	-5.77	117.41	120.30
2	N	1524	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	55	GLN	CA-CB-CG	5.59	125.69	113.40
2	L	1057	GLY	N-CA-C	-5.58	99.15	113.10
2	L	1122	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	K	924	ARG	CD-NE-CZ	5.45	131.24	123.60
2	M	1304	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	M	1257	GLY	N-CA-C	-5.37	99.68	113.10
2	K	905	ASP	CB-CG-OD1	-5.35	113.49	118.30
2	N	1457	GLY	N-CA-C	-5.20	100.09	113.10
1	B	283	ASP	CA-CB-CG	5.07	124.56	113.40
2	N	1515	THR	N-CA-CB	5.06	119.92	110.30

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	A	951	0	905	27	0
1	B	951	0	902	24	0
1	C	951	0	902	27	0
1	D	951	0	902	31	0
2	K	935	0	895	31	0
2	L	935	0	895	17	0
2	M	935	0	895	24	0
2	N	935	0	895	17	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
All	All	7564	0	7191	182	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 12.

All (182) 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:A:27:ASN:HD21	1:A:97:TYR:H	1.11	0.95
1:D:624:ASN:HD22	1:D:628:GLN:HE21	0.95	0.93
1:A:24:ASN:HD22	1:A:28:GLN:NE2	1.72	0.88
1:D:624:ASN:HD22	1:D:628:GLN:NE2	1.71	0.88
1:D:624:ASN:ND2	1:D:628:GLN:HE21	1.77	0.83
1:D:671:ASN:HD22	1:D:671:ASN:H	1.32	0.77
2:L:1059:LEU:HD23	2:L:1103:LEU:HG	1.66	0.77
2:L:1072:ARG:HD3	2:L:1079:VAL:HG13	1.67	0.77
2:M:1259:LEU:HD22	2:M:1302:GLU:HG2	1.69	0.75
2:N:1472:ARG:HD3	2:N:1479:VAL:HG13	1.71	0.73
1:A:24:ASN:HD22	1:A:28:GLN:HE21	1.35	0.73
1:C:471:ASN:HD22	1:C:471:ASN:H	1.37	0.73
1:A:71:ASN:HD22	1:A:71:ASN:H	1.37	0.72
1:D:639:ARG:HB2	1:D:639:ARG:HH11	1.54	0.72
2:K:814:ALA:HB3	2:K:922:ARG:HG3	1.71	0.72
1:A:27:ASN:ND2	1:A:97:TYR:H	1.87	0.69
2:L:1011:LEU:HD13	2:L:1118:THR:OG1	1.91	0.69
1:C:513:ASN:HA	1:C:514:PRO:C	2.12	0.69
2:L:1076:LYS:HD3	2:L:1077:ASN:H	1.58	0.68
1:B:217:THR:HG23	1:B:248:HIS:HD1	1.57	0.68
1:B:243:VAL:HG12	1:B:285:ARG:HG3	1.78	0.65
2:L:1006:GLU:OE1	2:L:1096:CYS:HB3	1.97	0.64
1:D:713:ASN:HA	1:D:714:PRO:C	2.18	0.64
1:B:291:LYS:NZ	1:B:291:LYS:HB2	2.12	0.63
1:C:469:GLN:HE21	1:C:471:ASN:HD21	1.47	0.63
2:K:876:LYS:HD3	2:K:877:ASN:H	1.62	0.63
1:B:290:SER:HB2	1:B:296:ALA:H	1.62	0.62
1:C:511:GLU:HG2	1:C:518:VAL:HG21	1.82	0.62
2:M:1211:LEU:HD22	2:M:1318:THR:HG23	1.82	0.61
1:A:10:ARG:O	1:A:33:ARG:HD3	1.99	0.61
2:M:1238:ARG:NH1	2:M:1290:ASP:HA	2.15	0.60
1:D:620:ALA:H	1:D:701:GLN:NE2	1.99	0.60
2:M:1282:GLN:HE21	2:M:1282:GLN:HA	1.65	0.59
1:C:448:HIS:HE2	1:C:482:THR:HG1	1.50	0.59
1:B:291:LYS:NZ	1:D:642:PRO:HB3	2.18	0.59
2:L:1076:LYS:HD3	2:L:1077:ASN:N	2.17	0.58
1:A:91:LYS:HD2	1:C:524:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1122:ARG:H	2:L:1122:ARG:HD3	1.68	0.58
2:M:1238:ARG:HH12	2:M:1290:ASP:HA	1.68	0.58
1:B:291:LYS:HZ2	1:B:291:LYS:HB2	1.67	0.58
1:B:217:THR:HG23	1:B:248:HIS:ND1	2.18	0.57
1:D:674:GLN:HG3	1:D:707:ILE:HG12	1.86	0.57
2:M:1254:GLY:O	2:M:1255:GLY:C	2.42	0.57
2:K:822:CYS:HB3	2:K:879:VAL:HG23	1.85	0.57
2:N:1476:LYS:HA	2:N:1476:LYS:HE2	1.85	0.57
2:L:1054:GLY:O	2:L:1055:GLY:C	2.43	0.57
1:A:60:GLN:HG2	1:A:76:TYR:CE2	2.40	0.56
2:K:854:GLY:O	2:K:855:GLY:C	2.42	0.56
2:M:1259:LEU:HD23	2:M:1303:LEU:HD12	1.87	0.56
2:L:1022:CYS:HB3	2:L:1079:VAL:HG23	1.85	0.56
1:A:27:ASN:HD21	1:A:97:TYR:N	1.94	0.56
2:N:1476:LYS:HD3	2:N:1477:ASN:H	1.70	0.56
2:K:876:LYS:HD3	2:K:877:ASN:N	2.20	0.56
2:N:1522:ARG:H	2:N:1522:ARG:HD3	1.71	0.56
2:L:1123:GLY:O	2:L:1124:ARG:NE	2.38	0.56
1:D:710:CYS:O	1:D:711:GLU:HB3	2.06	0.55
1:B:292:TYR:CD1	1:B:293:PRO:HA	2.40	0.55
2:N:1454:GLY:O	2:N:1455:GLY:C	2.43	0.55
1:B:207:LYS:HG2	1:B:211:GLN:NE2	2.21	0.55
2:K:886:LEU:HB3	2:K:919:VAL:HG21	1.89	0.55
2:L:1104:ARG:HB3	2:L:1107:THR:HG23	1.88	0.55
2:K:819:ARG:HH11	2:K:882:GLN:HE21	1.54	0.55
1:C:471:ASN:ND2	1:C:471:ASN:H	2.05	0.54
2:K:876:LYS:CD	2:K:877:ASN:H	2.20	0.54
1:A:48:HIS:HE2	1:A:82:THR:HG1	1.55	0.54
2:K:809:GLY:HA3	2:K:915:THR:HG22	1.90	0.54
1:D:611:GLN:HG2	1:D:635:LEU:HD21	1.89	0.54
2:N:1513:GLN:HE21	2:N:1513:GLN:HA	1.73	0.54
2:L:1024:ALA:HB3	2:L:1077:ASN:HB3	1.89	0.54
1:A:24:ASN:HB3	1:A:28:GLN:HE22	1.72	0.53
1:B:210:ARG:O	1:B:233:ARG:HD3	2.08	0.53
1:D:681:ILE:HD11	1:D:704:LYS:HG3	1.90	0.53
2:M:1282:GLN:NE2	2:M:1282:GLN:HA	2.23	0.53
2:M:1206:GLU:HG3	2:M:1315:THR:OG1	2.08	0.53
1:D:639:ARG:HB2	1:D:639:ARG:NH1	2.23	0.53
2:K:819:ARG:HH11	2:K:882:GLN:NE2	2.06	0.53
1:A:91:LYS:NZ	1:C:524:VAL:HG21	2.24	0.53
2:M:1239:GLN:HE21	2:M:1245:ARG:HB2	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:876:LYS:CE	2:K:877:ASN:H	2.23	0.52
1:D:601:LYS:HA	1:D:601:LYS:NZ	2.25	0.52
2:K:872:ARG:HD3	2:K:879:VAL:HG13	1.91	0.52
1:A:81:ILE:HD11	1:A:104:LYS:HG2	1.92	0.52
2:N:1476:LYS:HD3	2:N:1477:ASN:N	2.26	0.51
2:K:806:GLU:OE1	2:K:896:CYS:HB3	2.09	0.51
2:M:1240:ALA:HB1	2:M:1241:PRO:HD2	1.92	0.51
1:A:91:LYS:HD2	1:C:524:VAL:CG2	2.39	0.51
2:K:811:LEU:HD13	2:K:918:THR:HG23	1.91	0.51
1:C:492:TYR:CD1	1:C:493:PRO:HA	2.45	0.51
1:D:671:ASN:H	1:D:671:ASN:ND2	2.04	0.51
1:B:211:GLN:HG2	1:B:235:LEU:HD21	1.93	0.51
2:K:904:ARG:HH11	2:K:904:ARG:HG2	1.75	0.51
1:B:291:LYS:HZ3	1:D:642:PRO:HB3	1.75	0.50
1:A:113:ASN:HA	1:A:114:PRO:C	2.31	0.50
2:L:1009:GLY:HA3	2:L:1115:THR:HG22	1.93	0.50
2:K:887:LYS:HB3	2:K:887:LYS:HZ2	1.76	0.50
1:C:449:GLU:HG3	1:C:479:MET:HG2	1.93	0.49
2:K:811:LEU:HD13	2:K:918:THR:OG1	2.11	0.49
1:A:115:TYR:CD2	2:L:1109:GLY:HA3	2.47	0.49
2:N:1402:VAL:HG13	2:N:1510:GLN:NE2	2.27	0.49
2:M:1214:ALA:HB3	2:M:1322:ARG:HG3	1.95	0.49
1:B:262:ASN:HB2	1:B:273:TYR:CE2	2.48	0.49
1:C:413:MET:CE	1:C:451:LEU:HA	2.42	0.49
2:N:1401:GLN:HE21	2:N:1401:GLN:N	2.11	0.49
1:C:410:ARG:O	1:C:433:ARG:HD3	2.13	0.48
2:K:845:ARG:NH1	2:K:905:ASP:OD2	2.46	0.48
1:C:467:ASN:OD1	1:C:469:GLN:HG3	2.14	0.48
1:D:607:LYS:HG2	1:D:611:GLN:HE21	1.78	0.48
2:N:1419:ARG:HD2	2:N:1482:GLN:NE2	2.28	0.48
2:M:1224:ALA:HB3	2:M:1277:ASN:HB3	1.96	0.48
2:L:1002:VAL:HG13	2:L:1110:GLN:NE2	2.28	0.48
1:D:711:GLU:HG2	1:D:718:VAL:HG21	1.95	0.48
2:M:1234:MET:SD	2:M:1272:ARG:NH1	2.87	0.48
1:B:313:ASN:HA	1:B:314:PRO:C	2.33	0.48
1:C:462:ASN:OD1	2:M:1232:ILE:HD12	2.14	0.47
1:D:657:VAL:O	1:D:673:TYR:HB3	2.15	0.47
1:B:319:HIS:ND1	3:B:2002:PO4:O3	2.48	0.47
1:D:620:ALA:H	1:D:701:GLN:HE22	1.61	0.47
2:M:1245:ARG:NE	2:M:1305:ASP:OD2	2.47	0.47
2:K:887:LYS:HB3	2:K:887:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MET:O	1:A:33:ARG:NH1	2.48	0.47
2:K:859:LEU:HD22	2:K:902:GLU:HG2	1.97	0.46
2:K:832:ILE:O	2:K:872:ARG:NH2	2.48	0.46
1:C:462:ASN:CG	2:M:1232:ILE:HD12	2.36	0.46
1:C:417:THR:HG23	1:C:448:HIS:ND1	2.30	0.46
2:K:806:GLU:OE2	2:K:914:GLY:N	2.48	0.46
2:N:1424:ALA:HB3	2:N:1477:ASN:HB3	1.98	0.46
1:B:236:THR:HB	1:B:295:CYS:SG	2.56	0.46
1:A:88:GLY:HA3	1:C:463:VAL:HG12	1.97	0.45
1:B:269:GLN:HG2	2:N:1501:TYR:CD2	2.51	0.45
1:B:288:GLY:O	1:D:642:PRO:HG3	2.16	0.45
2:M:1219:ARG:HG3	2:M:1282:GLN:HE21	1.79	0.45
1:C:457:VAL:O	1:C:473:TYR:HB3	2.16	0.45
1:D:639:ARG:HA	1:D:692:TYR:CD1	2.52	0.45
1:B:257:VAL:O	1:B:273:TYR:HB3	2.17	0.45
1:A:102:ALA:HB1	1:A:104:LYS:HD3	1.99	0.45
2:N:1411:LEU:HD13	2:N:1518:THR:OG1	2.16	0.45
1:A:91:LYS:HZ2	1:C:524:VAL:HG21	1.82	0.45
2:K:883:MET:HE2	2:K:886:LEU:HD21	2.00	0.44
2:K:883:MET:HE1	2:K:917:VAL:HG11	1.99	0.44
2:K:906:ARG:HG2	2:K:906:ARG:HH11	1.83	0.44
1:B:310:CYS:O	1:B:311:GLU:HB3	2.16	0.44
1:A:90:SER:CB	1:A:96:ALA:H	2.31	0.44
2:L:1086:LEU:HB3	2:L:1119:VAL:HG21	1.98	0.44
2:M:1253:SER:HB3	2:M:1272:ARG:NH2	2.32	0.44
1:C:510:CYS:O	1:C:511:GLU:HB3	2.18	0.44
2:K:838:ARG:HG2	2:K:848:VAL:CG2	2.48	0.43
1:B:249:GLU:HG3	1:B:279:MET:SD	2.58	0.43
1:A:91:LYS:HZ3	1:C:524:VAL:HG11	1.83	0.43
1:A:100:THR:HG21	2:M:1255:GLY:N	2.34	0.43
2:M:1239:GLN:HG3	2:M:1245:ARG:N	2.34	0.43
2:K:924:ARG:HA	2:K:924:ARG:HD3	1.81	0.43
1:C:443:VAL:HG12	1:C:485:ARG:HG3	2.00	0.43
1:D:610:ARG:O	1:D:633:ARG:HD3	2.17	0.43
1:A:81:ILE:HD11	1:A:104:LYS:CG	2.48	0.43
1:D:652:ALA:HA	1:D:655:GLN:HG2	2.01	0.43
1:B:292:TYR:HA	1:B:293:PRO:HA	1.77	0.43
1:D:607:LYS:CG	1:D:611:GLN:HE21	2.31	0.43
1:C:494:ASN:ND2	2:K:862:ASP:OD1	2.52	0.43
1:A:41:LYS:HE2	1:A:43:VAL:O	2.19	0.43
1:A:92:TYR:CD1	1:A:93:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:ARG:O	1:D:634:ASN:HB2	2.18	0.42
2:N:1440:ALA:HB1	2:N:1441:PRO:HD2	2.00	0.42
1:D:681:ILE:HD11	1:D:704:LYS:CG	2.49	0.42
2:K:859:LEU:CD2	2:K:902:GLU:HG2	2.50	0.42
2:L:1124:ARG:HD3	2:L:1124:ARG:HA	1.84	0.42
1:B:269:GLN:HG2	2:N:1501:TYR:CE2	2.54	0.42
1:C:413:MET:HE2	1:C:451:LEU:HA	2.01	0.42
1:D:624:ASN:HB3	1:D:628:GLN:NE2	2.35	0.42
1:D:690:SER:HB2	1:D:696:ALA:HB3	2.01	0.42
2:N:1487:LYS:HZ2	2:N:1487:LYS:HB3	1.85	0.42
2:M:1272:ARG:HD2	2:M:1278:THR:O	2.20	0.41
2:M:1300:GLY:HA2	2:M:1307:THR:O	2.20	0.41
1:A:90:SER:HB2	1:A:96:ALA:H	1.85	0.41
2:K:840:ALA:HB1	2:K:841:PRO:HD2	2.00	0.41
2:K:812:VAL:HG22	2:K:813:GLN:H	1.86	0.41
1:D:609:GLU:HA	1:D:613:MET:HG2	2.02	0.41
1:C:490:SER:HB2	1:C:496:ALA:HB3	2.03	0.41
1:B:209:GLU:HA	1:B:213:MET:HG2	2.03	0.41
1:C:490:SER:CB	1:C:496:ALA:H	2.34	0.41
2:M:1324:ARG:HA	2:M:1324:ARG:HD3	1.87	0.40
2:N:1524:ARG:HD3	2:N:1524:ARG:HA	1.85	0.40
1:D:647:VAL:HG11	1:D:654:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/124 (98%)	110 (90%)	10 (8%)	2 (2%)	12	38
1	B	122/124 (98%)	110 (90%)	11 (9%)	1 (1%)	24	58
1	C	122/124 (98%)	110 (90%)	10 (8%)	2 (2%)	12	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	122/124 (98%)	109 (89%)	12 (10%)	1 (1%)	24	58
2	K	122/124 (98%)	113 (93%)	8 (7%)	1 (1%)	24	58
2	L	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
2	M	122/124 (98%)	112 (92%)	9 (7%)	1 (1%)	24	58
2	N	122/124 (98%)	112 (92%)	9 (7%)	1 (1%)	24	58
All	All	976/992 (98%)	890 (91%)	77 (8%)	9 (1%)	21	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	1243	LYS
2	N	1443	LYS
1	A	21	SER
1	C	421	SER
1	D	621	SER
2	K	843	LYS
1	B	221	SER
1	C	416	SER
1	A	16	SER

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	A	109/109 (100%)	89 (82%)	20 (18%)	2	6
1	B	109/109 (100%)	93 (85%)	16 (15%)	4	11
1	C	109/109 (100%)	92 (84%)	17 (16%)	3	9
1	D	109/109 (100%)	93 (85%)	16 (15%)	4	11
2	K	92/92 (100%)	71 (77%)	21 (23%)	1	3
2	L	92/92 (100%)	65 (71%)	27 (29%)	0	1
2	M	92/92 (100%)	70 (76%)	22 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	92/92 (100%)	68 (74%)	24 (26%)	0	1
All	All	804/804 (100%)	641 (80%)	163 (20%)	1	4

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	15	SER
1	A	21	SER
1	A	23	SER
1	A	28	GLN
1	A	31	LYS
1	A	33	ARG
1	A	39	ARG
1	A	50	SER
1	A	55	GLN
1	A	71	ASN
1	A	77	SER
1	A	85	ARG
1	A	89	SER
1	A	91	LYS
1	A	94	ASN
1	A	98	LYS
1	A	100	THR
1	A	104	LYS
1	A	119	HIS
1	B	201	LYS
1	B	217	THR
1	B	221	SER
1	B	231	LYS
1	B	234	ASN
1	B	239	ARG
1	B	259	SER
1	B	283	ASP
1	B	285	ARG
1	B	290	SER
1	B	291	LYS
1	B	294	ASN
1	B	298	LYS
1	B	300	THR
1	B	304	LYS
1	B	319	HIS

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Mol	Chain	Res	Type
1	C	401	LYS
1	C	417	THR
1	C	421	SER
1	C	431	LYS
1	C	439	ARG
1	C	455	GLN
1	C	469	GLN
1	C	471	ASN
1	C	477	SER
1	C	485	ARG
1	C	489	SER
1	C	491	LYS
1	C	494	ASN
1	C	498	LYS
1	C	500	THR
1	C	504	LYS
1	C	513	ASN
1	D	601	LYS
1	D	615	SER
1	D	617	THR
1	D	621	SER
1	D	634	ASN
1	D	637	LYS
1	D	639	ARG
1	D	643	VAL
1	D	661	LYS
1	D	671	ASN
1	D	683	ASP
1	D	685	ARG
1	D	691	LYS
1	D	694	ASN
1	D	698	LYS
1	D	704	LYS
2	K	801	GLN
2	K	803	GLN
2	K	806	GLU
2	K	812	VAL
2	K	821	SER
2	K	830	THR
2	K	833	TYR
2	K	843	LYS
2	K	859	LEU

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Mol	Chain	Res	Type
2	K	863	SER
2	K	874	LYS
2	K	876	LYS
2	K	879	VAL
2	K	887	LYS
2	K	893	THR
2	K	902	GLU
2	K	904	ARG
2	K	905	ASP
2	K	918	THR
2	K	921	SER
2	K	924	ARG
2	L	1001	GLN
2	L	1003	GLN
2	L	1006	GLU
2	L	1011	LEU
2	L	1012	VAL
2	L	1021	SER
2	L	1025	SER
2	L	1059	LEU
2	L	1063	SER
2	L	1065	LYS
2	L	1074	LYS
2	L	1076	LYS
2	L	1079	VAL
2	L	1087	LYS
2	L	1093	THR
2	L	1096	CYS
2	L	1104	ARG
2	L	1106	ARG
2	L	1110	GLN
2	L	1113	GLN
2	L	1115	THR
2	L	1116	GLN
2	L	1118	THR
2	L	1120	SER
2	L	1121	SER
2	L	1122	ARG
2	L	1124	ARG
2	M	1201	GLN
2	M	1206	GLU
2	M	1211	LEU

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Mol	Chain	Res	Type
2	M	1212	VAL
2	M	1217	SER
2	M	1221	SER
2	M	1230	THR
2	M	1246	GLU
2	M	1262	ASP
2	M	1263	SER
2	M	1274	LYS
2	M	1279	VAL
2	M	1282	GLN
2	M	1287	LYS
2	M	1293	THR
2	M	1306	ARG
2	M	1315	THR
2	M	1316	GLN
2	M	1318	THR
2	M	1320	SER
2	M	1322	ARG
2	M	1324	ARG
2	N	1401	GLN
2	N	1403	GLN
2	N	1404	LEU
2	N	1406	GLU
2	N	1411	LEU
2	N	1412	VAL
2	N	1413	GLN
2	N	1430	THR
2	N	1445	ARG
2	N	1459	LEU
2	N	1463	SER
2	N	1474	LYS
2	N	1476	LYS
2	N	1479	VAL
2	N	1487	LYS
2	N	1493	THR
2	N	1506	ARG
2	N	1513	GLN
2	N	1515	THR
2	N	1516	GLN
2	N	1518	THR
2	N	1520	SER
2	N	1522	ARG

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Mol	Chain	Res	Type
2	N	1524	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	28	GLN
1	A	69	GLN
1	A	71	ASN
1	A	94	ASN
1	A	101	GLN
1	B	211	GLN
1	B	228	GLN
1	B	294	ASN
1	B	301	GLN
1	C	411	GLN
1	C	471	ASN
1	C	501	GLN
1	D	628	GLN
1	D	655	GLN
1	D	669	GLN
1	D	671	ASN
1	D	701	GLN
2	K	839	GLN
2	K	882	GLN
2	L	1001	GLN
2	L	1110	GLN
2	M	1201	GLN
2	M	1213	GLN
2	M	1239	GLN
2	M	1282	GLN
2	N	1413	GLN
2	N	1482	GLN
2	N	1510	GLN
2	N	1513	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	PO4	A	2001	-	4,4,4	0.66	0	6,6,6	0.27	0
3	PO4	B	2002	-	4,4,4	0.81	0	6,6,6	0.27	0
3	PO4	C	2003	-	4,4,4	0.67	0	6,6,6	0.28	0
3	PO4	D	2004	-	4,4,4	0.69	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2002	-	-	0/0/0/0	0/0/0/0
3	PO4	C	2003	-	-	0/0/0/0	0/0/0/0
3	PO4	D	2004	-	-	0/0/0/0	0/0/0/0

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
3	B	2002	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 ⓘ

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	A	124/124 (100%)	0.01	0	100	100	12, 30, 46, 48	0
1	B	124/124 (100%)	0.11	4 (3%)	51	39	12, 31, 46, 48	0
1	C	124/124 (100%)	0.04	6 (4%)	34	23	12, 31, 46, 48	0
1	D	124/124 (100%)	0.20	8 (6%)	22	13	12, 31, 46, 48	0
2	K	124/124 (100%)	-0.24	4 (3%)	51	39	12, 21, 36, 59	0
2	L	124/124 (100%)	-0.20	5 (4%)	42	30	12, 21, 36, 59	0
2	M	124/124 (100%)	-0.23	6 (4%)	34	23	12, 21, 36, 59	0
2	N	124/124 (100%)	-0.19	5 (4%)	42	30	12, 21, 36, 59	0
All	All	992/992 (100%)	-0.06	38 (3%)	44	32	12, 25, 46, 59	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	1124	ARG	6.4
2	K	924	ARG	6.2
2	N	1524	ARG	6.0
2	M	1324	ARG	5.7
2	M	1323	GLY	5.6
2	N	1523	GLY	5.4
2	L	1123	GLY	4.6
2	K	923	GLY	3.9
1	D	601	LYS	3.8
1	B	218	SER	3.3
2	K	801	GLN	3.3
2	M	1322	ARG	3.3
2	L	1122	ARG	3.1
1	C	418	SER	3.1
2	L	1001	GLN	3.1
2	N	1522	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	M	1242	GLY	3.0
1	D	683	ASP	2.9
1	C	439	ARG	2.9
2	M	1201	GLN	2.9
2	K	922	ARG	2.9
1	D	619	ALA	2.7
1	B	294	ASN	2.7
2	N	1442	GLY	2.7
1	D	697	TYR	2.6
1	C	416	SER	2.6
1	C	484	CYS	2.5
1	D	639	ARG	2.5
2	M	1241	PRO	2.4
1	C	421	SER	2.4
1	B	296	ALA	2.3
2	L	1055	GLY	2.3
1	B	221	SER	2.2
1	D	694	ASN	2.2
1	D	603	THR	2.2
2	N	1441	PRO	2.2
1	D	700	THR	2.1
1	C	498	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	B	2002	5/5	0.96	0.15	0.13	37,37,38,38	0
3	PO4	C	2003	5/5	0.95	0.14	-0.33	47,47,48,48	0
3	PO4	D	2004	5/5	0.95	0.16	-0.69	38,38,39,39	0
3	PO4	A	2001	5/5	0.96	0.12	-1.55	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.