Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:15 AM EDT

PDB ID	:	7KF1
Title	:	Crystal structure of bH1 Fab variant (CDR H3 loop design 14_0130) in complex with VEGF
Authors	:	Shi, R.; Picard, M.-E.; Manenda, M.S.
Deposited on	:	2020-10-13
Resolution	:	2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

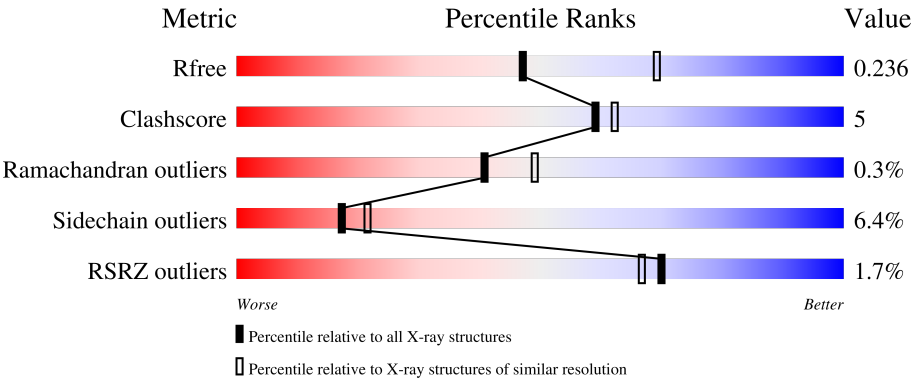
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	81% 9% 9%
1	D	237	79% 11% 9%
1	G	237	77% 11% 8%
1	H	237	80% 13% 5%
2	B	218	5% 86% 12%

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Mol	Chain	Length	Quality of chain
2	E	218	86% 12%
2	I	218	87% 11%
2	L	218	88% 11%
3	C	116	7% 65% 16% 19%
3	F	116	74% 7% 18%
3	J	116	4% 71% 10% 19%
3	V	116	2% 66% 15% 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17155 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 anti-VEGF-A Fab bH1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	225	Total	C	N	O	S	0	0	0
			1684	1066	281	330	7			
1	A	215	Total	C	N	O	S	0	0	0
			1615	1028	269	312	6			
1	D	216	Total	C	N	O	S	0	0	0
			1626	1035	271	314	6			
1	G	217	Total	C	N	O	S	0	0	0
			1632	1038	272	316	6			

- Molecule 2 is a protein called anti-VEGF-A Fab bH1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1679	1056	280	338	5			
2	B	216	Total	C	N	O	S	0	0	0
			1670	1051	279	335	5			
2	E	217	Total	C	N	O	S	0	0	0
			1679	1056	280	338	5			
2	I	217	Total	C	N	O	S	0	1	0
			1685	1060	280	340	5			

- Molecule 3 is a protein called Isoform L-VEGF206 of Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	95	Total	C	N	O	S	0	0	0
			770	483	129	145	13			
3	C	94	Total	C	N	O	S	0	0	0
			761	478	128	142	13			
3	F	95	Total	C	N	O	S	0	0	0
			770	483	129	145	13			
3	J	94	Total	C	N	O	S	0	0	0
			761	478	128	142	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	111	HIS	-	expression tag	UNP P15692-14
V	112	HIS	-	expression tag	UNP P15692-14
V	113	HIS	-	expression tag	UNP P15692-14
V	114	HIS	-	expression tag	UNP P15692-14
V	115	HIS	-	expression tag	UNP P15692-14
V	116	HIS	-	expression tag	UNP P15692-14
C	111	HIS	-	expression tag	UNP P15692-14
C	112	HIS	-	expression tag	UNP P15692-14
C	113	HIS	-	expression tag	UNP P15692-14
C	114	HIS	-	expression tag	UNP P15692-14
C	115	HIS	-	expression tag	UNP P15692-14
C	116	HIS	-	expression tag	UNP P15692-14
F	111	HIS	-	expression tag	UNP P15692-14
F	112	HIS	-	expression tag	UNP P15692-14
F	113	HIS	-	expression tag	UNP P15692-14
F	114	HIS	-	expression tag	UNP P15692-14
F	115	HIS	-	expression tag	UNP P15692-14
F	116	HIS	-	expression tag	UNP P15692-14
J	111	HIS	-	expression tag	UNP P15692-14
J	112	HIS	-	expression tag	UNP P15692-14
J	113	HIS	-	expression tag	UNP P15692-14
J	114	HIS	-	expression tag	UNP P15692-14
J	115	HIS	-	expression tag	UNP P15692-14
J	116	HIS	-	expression tag	UNP P15692-14

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	3	Total Cl 3 3	0	0
4	L	1	Total Cl 1 1	0	0
4	A	3	Total Cl 3 3	0	0
4	D	3	Total Cl 3 3	0	0
4	G	2	Total Cl 2 2	0	0

- Molecule 5 is water.

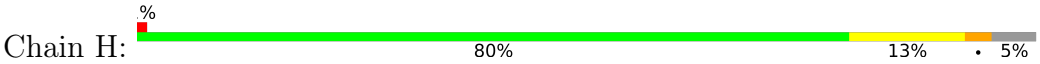
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	131	Total O 131 131	0	0
5	L	173	Total O 173 173	0	0
5	V	30	Total O 30 30	0	0
5	A	55	Total O 55 55	0	0
5	B	70	Total O 70 70	0	0
5	C	5	Total O 5 5	0	0
5	D	110	Total O 110 110	0	0
5	E	94	Total O 94 94	0	0
5	F	8	Total O 8 8	0	0
5	G	36	Total O 36 36	0	0
5	I	87	Total O 87 87	0	0
5	J	12	Total O 12 12	0	0

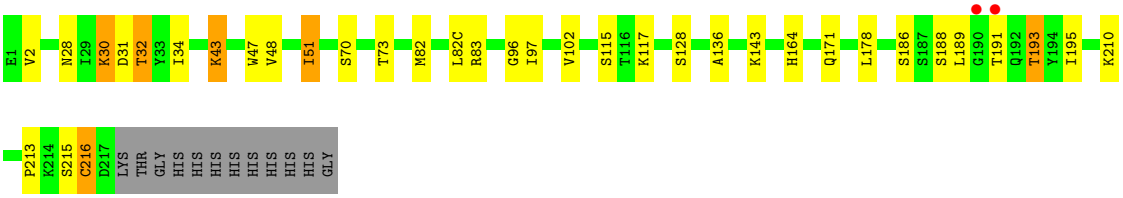
3 Residue-property plots (i)

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: anti-VEGF-A Fab bH1 heavy chain

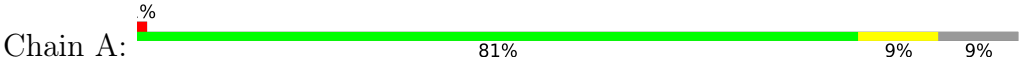
Chain H:

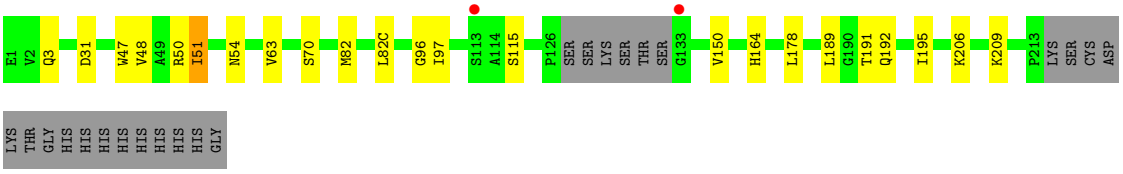




• Molecule 1: anti-VEGF-A Fab bH1 heavy chain

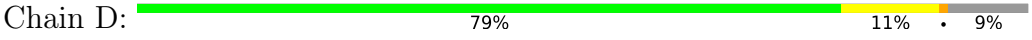
Chain A:

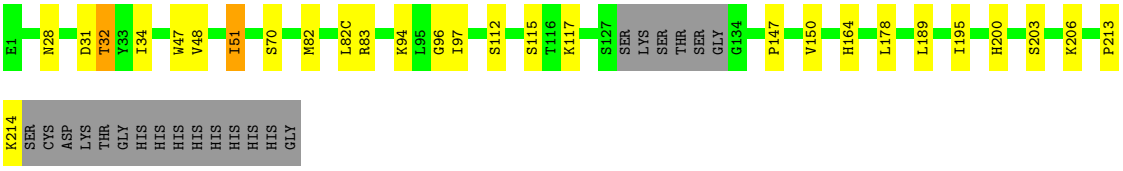




• Molecule 1: anti-VEGF-A Fab bH1 heavy chain

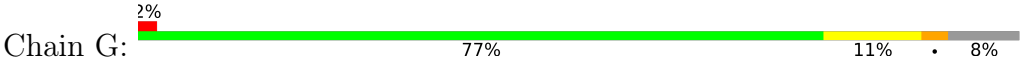
Chain D:

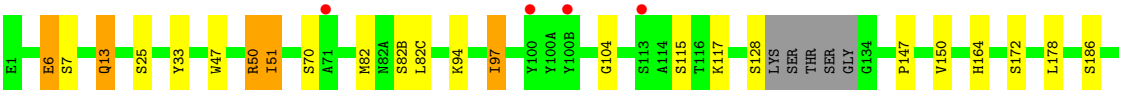




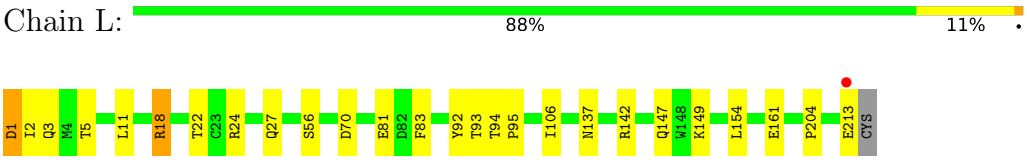
• Molecule 1: anti-VEGF-A Fab bH1 heavy chain

Chain G:

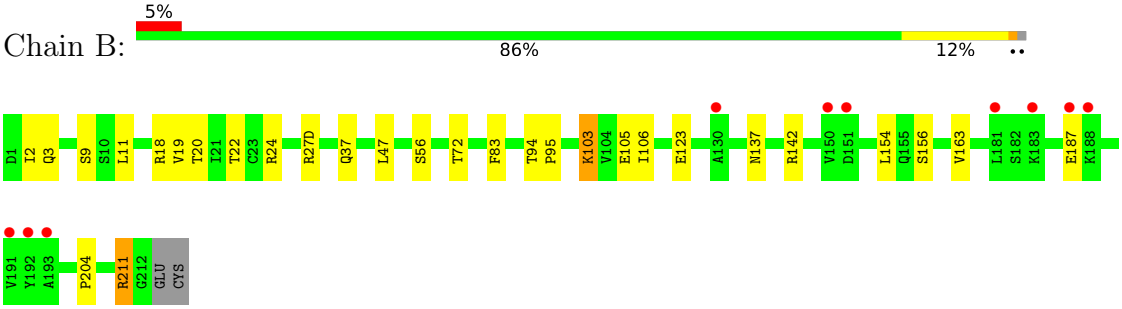




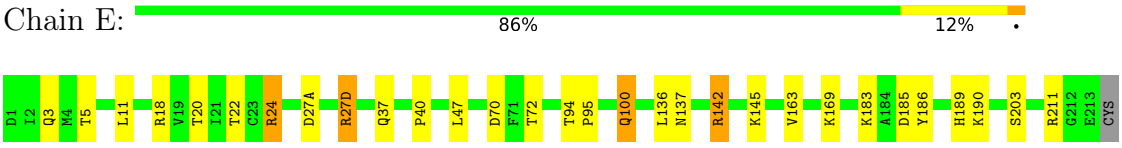
• Molecule 2: anti-VEGF-A Fab bH1 light chain



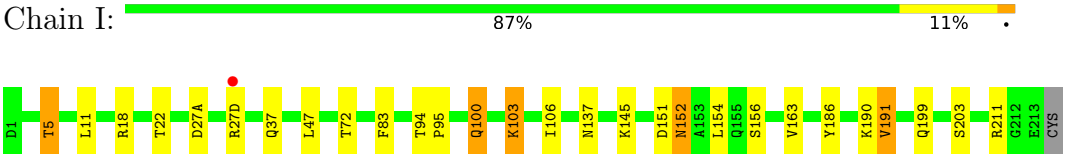
• Molecule 2: anti-VEGF-A Fab bH1 light chain



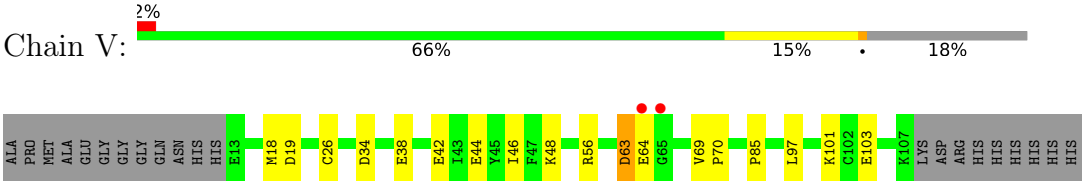
• Molecule 2: anti-VEGF-A Fab bH1 light chain



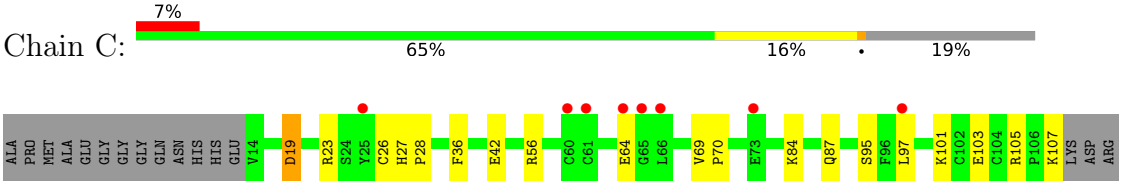
• Molecule 2: anti-VEGF-A Fab bH1 light chain



• Molecule 3: Isoform L-VEGF206 of Vascular endothelial growth factor A

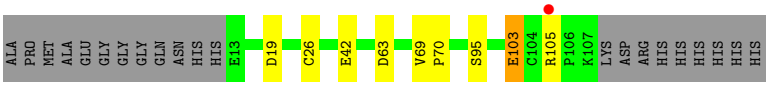


• Molecule 3: Isoform L-VEGF206 of Vascular endothelial growth factor A



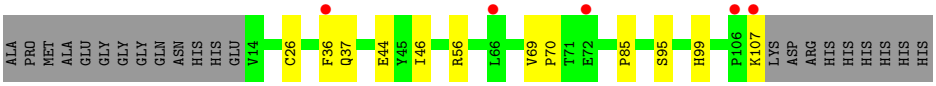
• Molecule 3: Isoform L-VEGF206 of Vascular endothelial growth factor A

Chain F:



• Molecule 3: Isoform L-VEGF206 of Vascular endothelial growth factor A

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	194.17Å 100.75Å 153.51Å 90.00° 91.69° 90.00°	Depositor
Resolution (Å)	48.57 – 2.45 48.52 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.57-2.45) 98.6 (48.52-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.189 , 0.232 0.194 , 0.236	Depositor DCC
R_{free} test set	5376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17155	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1331e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.56	0/1655	0.71	0/2257
1	D	0.55	0/1666	0.74	0/2271
1	G	0.55	0/1672	0.74	0/2279
1	H	0.72	0/1725	0.77	0/2351
2	B	0.56	0/1711	0.71	0/2327
2	E	0.61	0/1720	0.74	0/2339
2	I	0.56	0/1729	0.72	0/2351
2	L	0.62	0/1720	0.72	0/2339
3	C	0.48	0/779	0.67	0/1050
3	F	0.46	0/788	0.68	1/1062 (0.1%)
3	J	0.47	0/779	0.66	0/1050
3	V	0.57	0/788	0.78	1/1062 (0.1%)
All	All	0.58	0/16732	0.73	2/22738 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	I	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	19	ASP	CB-CA-C	5.47	121.35	110.40
3	V	63	ASP	CB-CG-OD1	5.37	123.13	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	27(D)	ARG	Sidechain
2	I	27(D)	ARG	Sidechain

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	A	1615	0	1586	15	0
1	D	1626	0	1601	16	0
1	G	1632	0	1606	20	0
1	H	1684	0	1654	23	0
2	B	1670	0	1619	24	0
2	E	1679	0	1625	21	0
2	I	1685	0	1631	28	0
2	L	1679	0	1625	20	0
3	C	761	0	728	6	0
3	F	770	0	734	3	0
3	J	761	0	728	4	0
3	V	770	0	734	4	0
4	A	3	0	0	0	0
4	D	3	0	0	0	0
4	G	2	0	0	0	0
4	H	3	0	0	0	0
4	L	1	0	0	0	0
5	A	55	0	0	0	0
5	B	70	0	0	2	0
5	C	5	0	0	0	0
5	D	110	0	0	0	0
5	E	94	0	0	2	0
5	F	8	0	0	1	0
5	G	36	0	0	0	0
5	H	131	0	0	3	0
5	I	87	0	0	3	0
5	J	12	0	0	1	0
5	L	173	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	30	0	0	0	0
All	All	17155	0	15871	151	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 (151) 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:G:50:ARG:NH2	2:I:94:THR:HG21	1.76	0.99
1:H:216:CYS:HB2	2:L:213:GLU:HB3	1.45	0.98
1:G:13:GLN:HE21	1:G:13:GLN:H	1.08	0.97
2:B:24:ARG:HH12	2:I:18:ARG:HH11	1.03	0.95
2:E:142:ARG:HH11	2:E:142:ARG:HG2	1.32	0.91
3:F:63:ASP:HB3	5:F:203:HOH:O	1.73	0.86
2:B:24:ARG:HH12	2:I:18:ARG:NH1	1.71	0.86
1:G:6:GLU:OE2	1:G:104:GLY:HA3	1.77	0.84
2:B:24:ARG:NH1	2:I:18:ARG:HH11	1.79	0.80
1:G:13:GLN:H	1:G:13:GLN:NE2	1.79	0.80
1:G:13:GLN:HE21	1:G:13:GLN:N	1.87	0.72
2:E:142:ARG:HH11	2:E:142:ARG:CG	2.04	0.71
1:A:191:THR:CG2	1:D:206:LYS:O	2.38	0.70
1:A:195:ILE:CD1	1:D:195:ILE:HD11	2.21	0.69
2:E:189:HIS:O	2:E:211:ARG:NH1	2.26	0.68
2:B:19:VAL:HA	5:B:346:HOH:O	1.95	0.67
1:A:191:THR:HG22	1:D:206:LYS:O	1.94	0.67
1:A:209:LYS:NZ	2:B:123:GLU:OE2	2.27	0.66
2:I:94:THR:HG23	2:I:95:PRO:HA	1.77	0.66
2:I:151:ASP:HA	2:I:191:VAL:HG13	1.77	0.66
1:A:195:ILE:HD11	1:D:195:ILE:HD11	1.77	0.65
3:J:56:ARG:HD2	5:J:210:HOH:O	1.94	0.65
2:B:142:ARG:HG2	2:B:142:ARG:HH11	1.64	0.62
3:V:38:GLU:CD	3:V:56:ARG:HH12	2.03	0.62
2:L:149:LYS:HG2	2:L:154:LEU:HD22	1.83	0.61
1:A:164:HIS:CD2	2:B:137:ASN:HD21	2.19	0.61
1:H:216:CYS:HB2	2:L:213:GLU:CB	2.28	0.61
3:C:56:ARG:NH2	3:C:97:LEU:O	2.34	0.61
1:H:193:THR:HG21	5:H:406:HOH:O	2.00	0.60
2:L:2:ILE:HD11	2:L:92:TYR:HD2	1.66	0.60
1:D:31:ASP:O	1:D:97:ILE:HD13	2.02	0.60
2:L:161:GLU:HG3	5:L:447:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:HIS:CD2	2:E:137:ASN:HD21	2.19	0.60
3:V:56:ARG:NH2	3:V:97:LEU:O	2.33	0.59
2:B:154:LEU:HD22	2:I:156:SER:HB2	1.84	0.59
1:H:136:ALA:HA	5:H:419:HOH:O	2.02	0.59
1:H:28:ASN:HD22	1:H:30:LYS:HD2	1.69	0.58
2:L:18:ARG:HB3	2:E:22:THR:HG21	1.83	0.58
1:H:31:ASP:O	1:H:97:ILE:HD13	2.03	0.58
2:L:81:GLU:HG3	5:L:427:HOH:O	2.04	0.58
2:B:18:ARG:HB3	2:I:22:THR:HG21	1.85	0.57
1:H:51:ILE:HD13	1:H:70:SER:HA	1.86	0.57
2:E:100:GLN:NE2	5:E:303:HOH:O	2.37	0.57
1:G:164:HIS:CD2	2:I:137:ASN:HD21	2.23	0.57
1:A:31:ASP:O	1:A:97:ILE:HD13	2.05	0.56
1:H:164:HIS:CD2	2:L:137:ASN:HD21	2.24	0.56
1:H:82:MET:HB3	1:H:82(C):LEU:HD21	1.88	0.55
1:A:51:ILE:HD13	1:A:70:SER:HA	1.87	0.55
1:G:33:TYR:CE2	1:G:97:ILE:HD12	2.42	0.54
2:B:27(D):ARG:HG2	5:B:326:HOH:O	2.08	0.54
2:L:142:ARG:HH11	2:L:142:ARG:HG2	1.72	0.54
1:H:28:ASN:ND2	1:H:30:LYS:HD2	2.23	0.54
1:G:195:ILE:HD13	1:G:210:LYS:HA	1.90	0.54
1:G:214:LYS:N	1:G:214:LYS:HD3	2.23	0.53
2:I:211:ARG:HB3	2:I:211:ARG:HH11	1.71	0.53
1:H:178:LEU:C	1:H:178:LEU:HD12	2.29	0.53
1:A:178:LEU:C	1:A:178:LEU:HD12	2.29	0.53
1:G:178:LEU:C	1:G:178:LEU:HD12	2.28	0.53
2:I:94:THR:CG2	2:I:95:PRO:HA	2.37	0.53
1:D:178:LEU:C	1:D:178:LEU:HD12	2.30	0.52
1:A:209:LYS:HZ1	2:B:123:GLU:CD	2.11	0.52
2:B:22:THR:HG21	2:I:18:ARG:HB3	1.92	0.52
3:C:69:VAL:HB	3:C:70:PRO:HD2	1.91	0.52
1:D:51:ILE:HD13	1:D:70:SER:HA	1.91	0.52
2:I:186:TYR:CE2	2:I:211:ARG:HD2	2.45	0.52
1:H:195:ILE:HD13	1:H:210:LYS:HA	1.91	0.52
3:V:69:VAL:HB	3:V:70:PRO:HD2	1.91	0.51
2:B:156:SER:HB2	2:I:154:LEU:CD2	2.41	0.51
3:J:69:VAL:HB	3:J:70:PRO:HD2	1.92	0.51
2:E:20:THR:HG23	2:E:72:THR:HG23	1.93	0.50
1:H:32:THR:HG21	1:H:34:ILE:HD11	1.94	0.50
1:A:96:GLY:C	1:A:97:ILE:HD12	2.32	0.50
1:D:164:HIS:HD2	2:E:137:ASN:HD21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:69:VAL:HB	3:F:70:PRO:HD2	1.93	0.50
1:H:47:TRP:CZ2	2:L:95:PRO:HB3	2.47	0.49
1:D:96:GLY:C	1:D:97:ILE:HD12	2.33	0.49
1:H:96:GLY:C	1:H:97:ILE:HD12	2.33	0.49
1:H:195:ILE:CD1	1:H:210:LYS:HB2	2.42	0.49
2:E:40:PRO:O	5:E:301:HOH:O	2.20	0.48
2:L:83:PHE:HB2	2:L:106:ILE:HD13	1.96	0.48
1:G:164:HIS:HD2	2:I:137:ASN:HD21	1.61	0.48
2:L:2:ILE:HD12	2:L:93:THR:OG1	2.13	0.48
2:B:83:PHE:HB2	2:B:106:ILE:HD13	1.95	0.48
2:L:22:THR:HG21	2:E:18:ARG:HB3	1.96	0.47
1:A:82:MET:HB3	1:A:82(C):LEU:HD21	1.97	0.47
2:I:5:THR:HA	2:I:100:GLN:HE22	1.78	0.47
1:H:143:LYS:NZ	1:H:171:GLN:OE1	2.47	0.47
2:I:151:ASP:O	2:I:152:ASN:ND2	2.47	0.47
2:I:100:GLN:HE21	2:I:100:GLN:H	1.61	0.47
2:B:211:ARG:HH11	2:B:211:ARG:HB2	1.79	0.47
1:D:32:THR:HG21	1:D:34:ILE:HD11	1.97	0.46
1:H:43:LYS:NZ	5:H:410:HOH:O	2.47	0.46
3:V:46:ILE:HD12	3:V:85:PRO:HG3	1.96	0.46
1:A:48:VAL:HG13	1:A:63:VAL:HG21	1.98	0.46
2:B:20:THR:HG23	2:B:72:THR:HG23	1.98	0.46
1:D:82:MET:HB3	1:D:82(C):LEU:HD21	1.97	0.46
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.97	0.46
1:H:2:VAL:CG1	1:H:102:VAL:HG21	2.46	0.45
2:L:94:THR:HA	2:L:95:PRO:C	2.36	0.45
2:E:142:ARG:HG2	2:E:142:ARG:NH1	2.14	0.45
1:G:212:GLU:HB2	1:G:213:PRO:HD2	1.99	0.45
3:C:103:GLU:OE2	3:C:105:ARG:NH2	2.45	0.45
2:L:2:ILE:CD1	2:L:92:TYR:HD2	2.28	0.45
1:D:213:PRO:O	1:D:214:LYS:HB3	2.16	0.45
2:B:156:SER:HB2	2:I:154:LEU:HD22	1.99	0.45
2:I:37:GLN:HB2	2:I:47:LEU:HD11	1.98	0.45
2:B:94:THR:HA	2:B:95:PRO:C	2.37	0.45
1:A:164:HIS:HD2	2:B:137:ASN:HD21	1.62	0.45
1:G:50:ARG:HH21	2:I:94:THR:HG21	1.74	0.45
2:I:83:PHE:HE1	2:I:103:LYS:HE2	1.81	0.44
2:E:186:TYR:CE2	2:E:211:ARG:HD2	2.52	0.44
1:H:216:CYS:CB	2:L:213:GLU:HB3	2.31	0.44
1:G:82:MET:HB3	1:G:82(C):LEU:HD21	1.99	0.44
2:E:94:THR:HA	2:E:95:PRO:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.00	0.44
2:B:11:LEU:HD12	2:B:11:LEU:C	2.38	0.43
2:E:24:ARG:HD3	2:E:70:ASP:OD1	2.17	0.43
1:A:47:TRP:CH2	2:B:95:PRO:HB3	2.53	0.43
3:C:19:ASP:O	3:C:23:ARG:HG3	2.18	0.43
1:G:47:TRP:CZ3	2:I:95:PRO:HB3	2.54	0.43
1:G:51:ILE:HD13	1:G:70:SER:HA	1.99	0.43
1:D:147:PRO:O	1:D:200:HIS:HE1	2.02	0.43
1:D:47:TRP:CZ2	2:E:95:PRO:HB3	2.54	0.43
1:D:200:HIS:HD2	1:D:203:SER:OG	2.02	0.43
2:E:11:LEU:C	2:E:11:LEU:HD12	2.39	0.42
2:I:83:PHE:HB2	2:I:106:ILE:HD13	2.01	0.42
2:I:100:GLN:H	2:I:100:GLN:NE2	2.18	0.42
2:E:211:ARG:NH1	2:E:211:ARG:HB3	2.35	0.42
1:G:33:TYR:CD1	1:G:50:ARG:HD2	2.54	0.42
1:H:30:LYS:H	1:H:30:LYS:CE	2.32	0.42
3:C:84:LYS:HB3	3:C:87:GLN:HB2	2.01	0.42
2:L:1:ASP:HB2	5:L:555:HOH:O	2.20	0.42
1:G:147:PRO:O	1:G:200:HIS:HE1	2.03	0.42
2:L:24:ARG:HG3	2:L:70:ASP:OD1	2.20	0.41
2:B:103:LYS:HE3	2:B:103:LYS:HB2	1.94	0.41
3:F:103:GLU:HB3	3:F:105:ARG:NH1	2.36	0.41
1:H:189:LEU:HD13	1:H:213:PRO:HG2	2.02	0.41
3:J:46:ILE:HD12	3:J:85:PRO:HG3	2.03	0.41
2:B:9:SER:HB2	5:I:355:HOH:O	2.20	0.41
3:C:27:HIS:HB2	3:C:28:PRO:HD2	2.01	0.41
1:G:189:LEU:HD12	1:G:189:LEU:HA	1.93	0.41
2:I:18:ARG:NH2	5:I:310:HOH:O	2.53	0.41
2:L:11:LEU:HD12	2:L:11:LEU:C	2.41	0.41
1:G:200:HIS:HD2	1:G:203:SER:OG	2.04	0.41
1:H:30:LYS:NZ	1:H:73:THR:O	2.48	0.41
2:L:18:ARG:HD3	2:E:24:ARG:NH1	2.35	0.40
3:J:56:ARG:HD3	3:J:99:HIS:CE1	2.56	0.40
2:I:11:LEU:HD12	2:I:11:LEU:C	2.41	0.40
2:E:142:ARG:CG	2:E:142:ARG:NH1	2.72	0.40
2:E:136:LEU:HD12	2:E:136:LEU:N	2.37	0.40
2:I:72:THR:HG22	5:I:311:HOH:O	2.21	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	A	211/237 (89%)	209 (99%)	2 (1%)	0	100	100
1	D	212/237 (90%)	210 (99%)	2 (1%)	0	100	100
1	G	213/237 (90%)	208 (98%)	5 (2%)	0	100	100
1	H	223/237 (94%)	218 (98%)	3 (1%)	2 (1%)	17	19
2	B	214/218 (98%)	206 (96%)	8 (4%)	0	100	100
2	E	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
2	I	216/218 (99%)	208 (96%)	7 (3%)	1 (0%)	29	34
2	L	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
3	C	92/116 (79%)	90 (98%)	1 (1%)	1 (1%)	14	14
3	F	93/116 (80%)	91 (98%)	1 (1%)	1 (1%)	14	14
3	J	92/116 (79%)	88 (96%)	3 (3%)	1 (1%)	14	14
3	V	93/116 (80%)	89 (96%)	3 (3%)	1 (1%)	14	14
All	All	2089/2284 (92%)	2035 (97%)	47 (2%)	7 (0%)	41	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	152	ASN
1	H	216	CYS
1	H	215	SER
3	V	26	CYS
3	C	26	CYS
3	F	26	CYS
3	J	26	CYS

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	A	176/196 (90%)	167 (95%)	9 (5%)	24	31
1	D	178/196 (91%)	167 (94%)	11 (6%)	18	23
1	G	179/196 (91%)	160 (89%)	19 (11%)	6	6
1	H	186/196 (95%)	173 (93%)	13 (7%)	15	18
2	B	190/192 (99%)	181 (95%)	9 (5%)	26	34
2	E	191/192 (100%)	177 (93%)	14 (7%)	14	16
2	I	192/192 (100%)	182 (95%)	10 (5%)	23	30
2	L	191/192 (100%)	183 (96%)	8 (4%)	30	39
3	C	89/106 (84%)	82 (92%)	7 (8%)	12	14
3	F	90/106 (85%)	87 (97%)	3 (3%)	38	49
3	J	89/106 (84%)	84 (94%)	5 (6%)	21	27
3	V	90/106 (85%)	80 (89%)	10 (11%)	6	5
All	All	1841/1976 (93%)	1723 (94%)	118 (6%)	17	21

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30	LYS
1	H	32	THR
1	H	43	LYS
1	H	48	VAL
1	H	51	ILE
1	H	83	ARG
1	H	115	SER
1	H	117	LYS
1	H	128	SER
1	H	186	SER
1	H	188	SER
1	H	191	THR
1	H	193	THR
2	L	1	ASP

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Mol	Chain	Res	Type
2	L	3	GLN
2	L	5	THR
2	L	18	ARG
2	L	27	GLN
2	L	56	SER
2	L	147	GLN
2	L	204	PRO
3	V	18	MET
3	V	19	ASP
3	V	34	ASP
3	V	42	GLU
3	V	44	GLU
3	V	48	LYS
3	V	63	ASP
3	V	64	GLU
3	V	101	LYS
3	V	103	GLU
1	A	3	GLN
1	A	50	ARG
1	A	51	ILE
1	A	54	ASN
1	A	115	SER
1	A	150	VAL
1	A	189	LEU
1	A	192	GLN
1	A	206	LYS
2	B	2	ILE
2	B	3	GLN
2	B	56	SER
2	B	103	LYS
2	B	105	GLU
2	B	163	VAL
2	B	187	GLU
2	B	204	PRO
2	B	211	ARG
3	C	19	ASP
3	C	36	PHE
3	C	42	GLU
3	C	64	GLU
3	C	95	SER
3	C	101	LYS
3	C	107	LYS

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Mol	Chain	Res	Type
1	D	28	ASN
1	D	32	THR
1	D	48	VAL
1	D	51	ILE
1	D	83	ARG
1	D	94	LYS
1	D	112	SER
1	D	115	SER
1	D	117	LYS
1	D	150	VAL
1	D	189	LEU
2	E	3	GLN
2	E	5	THR
2	E	24	ARG
2	E	27(A)	ASP
2	E	27(D)	ARG
2	E	100	GLN
2	E	142	ARG
2	E	145	LYS
2	E	163	VAL
2	E	169	LYS
2	E	183	LYS
2	E	185	ASP
2	E	190	LYS
2	E	203	SER
3	F	42	GLU
3	F	95	SER
3	F	103	GLU
1	G	6	GLU
1	G	7	SER
1	G	13	GLN
1	G	25	SER
1	G	50	ARG
1	G	51	ILE
1	G	82(B)	SER
1	G	94	LYS
1	G	97	ILE
1	G	115	SER
1	G	117	LYS
1	G	128	SER
1	G	150	VAL
1	G	172	SER

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Mol	Chain	Res	Type
1	G	186	SER
1	G	189	LEU
1	G	192	GLN
1	G	201	LYS
1	G	214	LYS
2	I	5	THR
2	I	27(A)	ASP
2	I	100	GLN
2	I	103	LYS
2	I	145	LYS
2	I	163	VAL
2	I	190	LYS
2	I	191	VAL
2	I	199	GLN
2	I	203	SER
3	J	36	PHE
3	J	37	GLN
3	J	44	GLU
3	J	95	SER
3	J	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	28	ASN
2	L	124	GLN
2	L	137	ASN
3	V	37	GLN
3	V	75	ASN
1	A	3	GLN
2	B	137	ASN
2	B	189	HIS
3	C	37	GLN
3	C	75	ASN
3	C	100	ASN
1	D	3	GLN
1	D	200	HIS
2	E	137	ASN
3	F	75	ASN
3	F	100	ASN
1	G	3	GLN

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Mol	Chain	Res	Type
1	G	13	GLN
1	G	200	HIS
2	I	100	GLN
2	I	137	ASN
2	I	189	HIS
2	I	199	GLN
3	J	37	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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 (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	215/237 (90%)	-0.07	2 (0%) 84 85	32, 53, 73, 94	0
1	D	216/237 (91%)	-0.32	0 100 100	25, 40, 64, 85	0
1	G	217/237 (91%)	0.16	4 (1%) 68 65	29, 59, 86, 107	0
1	H	225/237 (94%)	-0.27	2 (0%) 84 85	19, 33, 65, 108	0
2	B	216/218 (99%)	0.16	10 (4%) 32 30	24, 47, 91, 106	0
2	E	217/218 (99%)	-0.25	0 100 100	20, 35, 62, 91	0
2	I	217/218 (99%)	-0.07	1 (0%) 91 92	24, 41, 76, 99	0
2	L	217/218 (99%)	-0.23	1 (0%) 91 92	16, 28, 51, 98	0
3	C	94/116 (81%)	0.69	8 (8%) 10 8	46, 73, 108, 119	0
3	F	95/116 (81%)	0.21	1 (1%) 80 80	33, 60, 96, 107	0
3	J	94/116 (81%)	0.28	5 (5%) 26 23	43, 62, 101, 119	0
3	V	95/116 (81%)	-0.13	2 (2%) 63 60	24, 42, 77, 106	0
All	All	2118/2284 (92%)	-0.05	36 (1%) 70 67	16, 44, 85, 119	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	65	GLY	5.6
2	B	191	VAL	3.7
2	B	192	TYR	3.5
2	B	188	LYS	3.5
2	B	130	ALA	3.3
3	J	107	LYS	3.3
1	G	71	ALA	3.0
3	C	73	GLU	3.0
3	C	66	LEU	2.9
2	B	183	LYS	2.7
1	G	100	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	213	GLU	2.6
3	C	60	CYS	2.6
3	J	106	PRO	2.5
1	G	113	SER	2.4
3	V	64	GLU	2.4
3	J	72	GLU	2.4
2	B	181	LEU	2.4
3	J	66	LEU	2.4
2	B	187	GLU	2.3
3	C	61	CYS	2.3
3	J	36	PHE	2.3
3	F	105	ARG	2.3
3	C	97	LEU	2.2
1	H	190	GLY	2.2
1	H	191	THR	2.2
1	A	113	SER	2.2
2	B	151	ASP	2.2
1	A	133	GLY	2.1
2	B	150	VAL	2.1
3	C	65	GLY	2.1
3	C	25	TYR	2.1
1	G	100(B)	TYR	2.1
2	I	27(D)	ARG	2.1
2	B	193	ALA	2.0
3	C	64	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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(Å^2)	Q<0.9
4	CL	G	302	1/1	0.91	0.10	59,59,59,59	0
4	CL	G	301	1/1	0.95	0.19	44,44,44,44	0
4	CL	H	302	1/1	0.97	0.11	31,31,31,31	0
4	CL	A	303	1/1	0.97	0.07	54,54,54,54	0
4	CL	L	301	1/1	0.98	0.08	42,42,42,42	0
4	CL	D	302	1/1	0.98	0.08	42,42,42,42	0
4	CL	H	303	1/1	0.99	0.09	34,34,34,34	0
4	CL	H	301	1/1	0.99	0.12	22,22,22,22	0
4	CL	D	303	1/1	0.99	0.08	46,46,46,46	0
4	CL	A	301	1/1	0.99	0.07	34,34,34,34	0
4	CL	A	302	1/1	0.99	0.07	55,55,55,55	0
4	CL	D	301	1/1	1.00	0.12	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.