



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:23 PM GMT

PDB ID : 2B2X  
Title : VLA1 RdeltaH I-domain complexed with a quadruple mutant of the AQC2 Fab  
Authors : Clark, L.A.; Boriack-Sjodin, P.A.; Eldredge, J.; Fitch, C.; Friedman, B.; Hanf, K.J.; Jarpe, M.; Liparoto, S.F.; Li, Y.; Lugovskoy, A.  
Deposited on : 2005-09-19  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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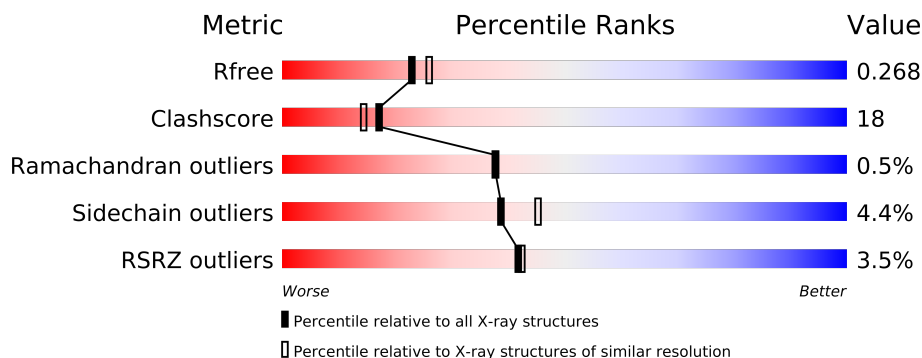
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	223	
1	B	223	
2	H	226	
2	I	226	
3	L	213	
3	M	213	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9537 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Integrin alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1490	940	258	288	4			
1	B	176	Total	C	N	O	S	0	0	0
			1397	884	240	270	3			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	CLONING ARTIFACT	UNP P18614
A	126	SER	-	CLONING ARTIFACT	UNP P18614
A	217	VAL	GLY	ENGINEERED	UNP P18614
A	218	GLN	ARG	ENGINEERED	UNP P18614
A	219	ARG	GLN	ENGINEERED	UNP P18614
A	222	ARG	LEU	ENGINEERED	UNP P18614
A	341	LEU	-	CLONING ARTIFACT	UNP P18614
A	342	GLU	-	CLONING ARTIFACT	UNP P18614
A	343	ARG	-	CLONING ARTIFACT	UNP P18614
A	344	PRO	-	CLONING ARTIFACT	UNP P18614
A	345	HIS	-	CLONING ARTIFACT	UNP P18614
A	346	ARG	-	CLONING ARTIFACT	UNP P18614
A	347	ASP	-	CLONING ARTIFACT	UNP P18614
B	125	GLY	-	CLONING ARTIFACT	UNP P18614
B	126	SER	-	CLONING ARTIFACT	UNP P18614
B	217	VAL	GLY	ENGINEERED	UNP P18614
B	218	GLN	ARG	ENGINEERED	UNP P18614
B	219	ARG	GLN	ENGINEERED	UNP P18614
B	222	ARG	LEU	ENGINEERED	UNP P18614
B	341	LEU	-	CLONING ARTIFACT	UNP P18614
B	342	GLU	-	CLONING ARTIFACT	UNP P18614
B	343	ARG	-	CLONING ARTIFACT	UNP P18614
B	344	PRO	-	CLONING ARTIFACT	UNP P18614
B	345	HIS	-	CLONING ARTIFACT	UNP P18614
B	346	ARG	-	CLONING ARTIFACT	UNP P18614

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Chain	Residue	Modelled	Actual	Comment	Reference
B	347	ASP	-	CLONING ARTIFACT	UNP P18614

- Molecule 2 is a protein called Antibody AQC2 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1575	1000	260	308	7			
2	I	210	Total	C	N	O	S	0	0	0
			1575	1000	260	308	7			

- Molecule 3 is a protein called Antibody AQC2 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1636	1026	274	330	6			
3	M	210	Total	C	N	O	S	0	0	0
			1636	1026	274	330	6			

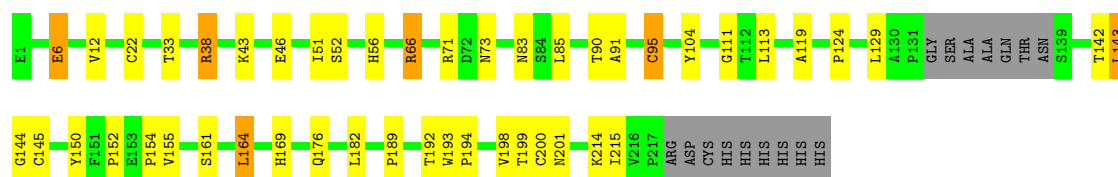
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

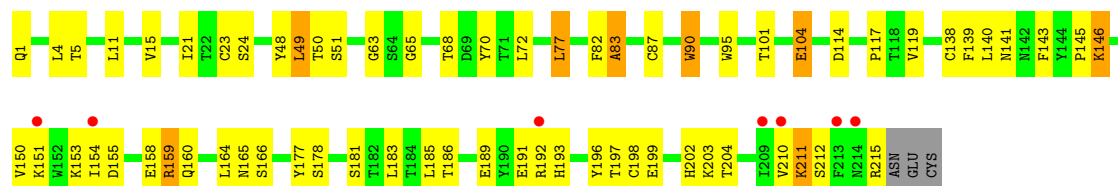
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	5	Total	O	0	0
			5	5		
5	H	73	Total	O	0	0
			73	73		
5	I	77	Total	O	0	0
			77	77		
5	L	30	Total	O	0	0
			30	30		
5	M	28	Total	O	0	0
			28	28		





### • Molecule 3: Antibody AQC2 Fab

Chain L:



### • Molecule 3: Antibody AQC2 Fab

Chain M:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.12Å 43.68Å 153.88Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	35.00 – 2.20 49.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (35.00-2.20) 94.3 (49.75-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.20Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.238 , 0.272 0.236 , 0.268	Depositor DCC
$R_{free}$ test set	3380 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 66552 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 36.80 % 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 4.7301e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.28	0/1510	0.56	0/2036
1	B	0.27	0/1414	0.55	0/1903
2	H	0.39	0/1616	0.71	0/2208
2	I	0.37	0/1616	0.70	0/2208
3	L	0.35	0/1680	0.63	0/2288
3	M	0.33	0/1680	0.61	0/2288
All	All	0.34	0/9516	0.63	0/12931

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1490	0	1497	67	0
1	B	1397	0	1395	75	0
2	H	1575	0	1537	39	0
2	I	1575	0	1537	38	0
3	L	1636	0	1561	53	0
3	M	1636	0	1561	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	13	0	0	0	0
5	B	5	0	0	0	0
5	H	73	0	0	0	0
5	I	77	0	0	1	0
5	L	30	0	0	1	0
5	M	28	0	0	0	0
All	All	9537	0	9088	315	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (315) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:191:GLU:HA	3:L:215:ARG:HH12	1.25	0.98
1:B:234:ARG:HH11	1:B:234:ARG:HB3	1.27	0.97
2:H:161:SER:H	2:H:201:ASN:HD21	1.00	0.95
2:I:161:SER:H	2:I:201:ASN:HD21	1.08	0.94
3:M:6:GLN:H	3:M:99:GLN:NE2	1.64	0.94
3:M:6:GLN:N	3:M:99:GLN:HE22	1.69	0.91
3:M:23:CYS:HG	3:M:87:CYS:HG	1.03	0.91
1:B:286:LEU:HD11	1:B:317:ASN:HD21	1.36	0.89
2:H:140:MET:HG2	2:H:189:PRO:HA	1.55	0.89
1:B:224:THR:H	1:B:261:HIS:CD2	1.92	0.87
3:L:23:CYS:HG	3:L:87:CYS:HG	0.94	0.85
3:L:138:CYS:HG	3:L:198:CYS:HG	1.00	0.85
2:I:38:ARG:HD2	2:I:46:GLU:OE1	1.79	0.83
3:M:6:GLN:H	3:M:99:GLN:HE22	0.84	0.82
2:H:161:SER:H	2:H:201:ASN:ND2	1.78	0.81
1:B:224:THR:H	1:B:261:HIS:HD2	1.30	0.79
3:M:138:CYS:HG	3:M:198:CYS:HG	0.82	0.79
3:L:159:ARG:HG3	3:L:159:ARG:HH11	1.48	0.79
2:I:161:SER:H	2:I:201:ASN:ND2	1.82	0.76
1:A:224:THR:H	1:A:261:HIS:CD2	2.03	0.76
1:B:174:LYS:NZ	1:B:175:ARG:HH12	1.83	0.76
1:A:224:THR:H	1:A:261:HIS:HD2	1.32	0.76
1:A:181:LYS:HE2	1:A:181:LYS:HA	1.68	0.75
1:A:234:ARG:HE	1:A:272:ASP:HB3	1.50	0.75
1:A:157:ASN:HB3	2:H:33:THR:HG21	1.69	0.75
1:A:195:THR:HG21	1:A:219:ARG:HE	1.51	0.74
2:H:38:ARG:HD2	2:H:46:GLU:OE1	1.88	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:71:ARG:HD3	2:H:73:ASN:HD21	1.56	0.71
1:A:327:ILE:HG22	1:A:331:LEU:HB2	1.72	0.71
3:M:159:ARG:HD2	3:M:161:ASN:OD1	1.91	0.71
3:L:191:GLU:HA	3:L:215:ARG:NH1	2.05	0.70
2:H:22:CYS:HG	2:H:95:CYS:CB	2.04	0.69
1:B:234:ARG:NH1	1:B:234:ARG:HB3	2.07	0.68
1:B:251:VAL:HG11	1:B:335:ILE:HD11	1.74	0.68
3:L:104:GLU:HG3	3:L:177:TYR:OH	1.92	0.68
1:B:166:ILE:HD11	1:B:216:ILE:O	1.93	0.68
2:H:161:SER:N	2:H:201:ASN:HD21	1.84	0.68
1:B:266:LEU:O	1:B:270:ILE:HG12	1.95	0.67
2:H:145:CYS:CB	2:H:200:CYS:HG	2.07	0.67
2:I:145:CYS:HG	2:I:200:CYS:CB	2.08	0.66
1:B:252:MET:HG2	1:B:254:ILE:HD11	1.77	0.66
1:A:171:ASP:OD2	1:A:328:VAL:HG21	1.96	0.66
2:I:176:GLN:OE1	3:M:164:LEU:HD11	1.96	0.65
3:L:153:LYS:HB3	3:L:197:THR:HG23	1.78	0.65
1:A:236:GLU:O	1:A:242:ARG:HD2	1.97	0.65
2:H:189:PRO:HG2	2:H:192:THR:OG1	1.97	0.65
3:M:104:GLU:HG2	3:M:105:ILE:N	2.09	0.65
2:I:71:ARG:HD3	2:I:73:ASN:HD21	1.61	0.64
1:B:174:LYS:HZ1	1:B:175:ARG:HH12	1.45	0.64
3:M:153:LYS:HB3	3:M:197:THR:HG22	1.80	0.64
3:L:146:LYS:HB3	3:L:177:TYR:CD2	2.32	0.64
3:L:5:THR:HG23	5:L:226:HOH:O	1.97	0.63
1:A:192:GLU:HG3	1:A:221:GLY:HA2	1.81	0.63
2:I:22:CYS:HG	2:I:95:CYS:HG	1.06	0.63
3:L:21:ILE:HD12	3:L:101:THR:HG21	1.80	0.62
1:B:157:ASN:ND2	1:B:221:GLY:H	1.97	0.62
3:L:154:ILE:O	3:L:154:ILE:HG13	1.98	0.62
3:L:141:ASN:HD22	3:L:178:SER:HB3	1.63	0.62
2:I:71:ARG:HD3	2:I:73:ASN:ND2	2.15	0.62
1:B:313:LYS:HZ3	1:B:334:ARG:HD3	1.64	0.62
1:A:249:LYS:CE	1:A:279:GLN:HG2	2.30	0.62
1:B:236:GLU:O	1:B:242:ARG:HD2	2.00	0.62
2:I:22:CYS:HG	2:I:95:CYS:CB	2.13	0.62
1:B:289:TYR:CB	1:B:296:THR:HG22	2.29	0.62
1:A:195:THR:HG21	1:A:219:ARG:NE	2.15	0.61
1:B:254:ILE:HD12	1:B:254:ILE:N	2.16	0.61
1:B:207:GLU:HG3	1:B:208:GLU:N	2.15	0.61
2:H:71:ARG:HD3	2:H:73:ASN:ND2	2.14	0.60
1:B:312:GLU:HG3	1:B:313:LYS:HG2	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:182:LEU:HD12	2:H:182:LEU:C	2.21	0.60
2:H:71:ARG:CD	2:H:73:ASN:HD21	2.15	0.60
2:I:182:LEU:C	2:I:182:LEU:HD12	2.22	0.60
1:A:153:LEU:HD21	1:A:169:LEU:HD11	1.85	0.59
1:A:266:LEU:O	1:A:270:ILE:HG12	2.02	0.59
3:L:159:ARG:HG3	3:L:159:ARG:NH1	2.16	0.59
1:B:263:ASN:HB3	3:M:30:ASN:HD22	1.66	0.59
1:A:318:VAL:HG13	1:A:327:ILE:HD11	1.84	0.59
1:B:192:GLU:HG3	1:B:221:GLY:HA2	1.84	0.59
1:B:331:LEU:HD23	1:B:331:LEU:O	2.02	0.59
1:A:147:LEU:HA	1:A:248:VAL:HG12	1.85	0.59
1:B:203:TYR:HD2	1:B:208:GLU:HG2	1.68	0.58
2:I:6:GLU:HG3	2:I:111:GLY:CA	2.33	0.58
1:B:157:ASN:HB3	2:I:33:THR:HG21	1.84	0.58
2:I:199:THR:HG22	2:I:214:LYS:HA	1.86	0.57
1:B:147:LEU:HD12	1:B:147:LEU:O	2.04	0.57
3:L:146:LYS:HB3	3:L:177:TYR:CG	2.40	0.57
2:H:33:THR:HB	2:H:52:SER:HA	1.84	0.57
1:B:211:VAL:O	1:B:215:LYS:HE2	2.04	0.57
1:B:154:ASP:O	1:B:159:ILE:HG13	2.04	0.57
3:M:24:SER:HA	3:M:68:THR:O	2.04	0.56
2:I:189:PRO:O	2:I:192:THR:HB	2.04	0.56
1:B:230:ILE:HG23	1:B:252:MET:SD	2.45	0.56
1:A:147:LEU:HA	1:A:248:VAL:CG1	2.35	0.56
3:M:140:LEU:N	3:M:140:LEU:HD12	2.19	0.56
1:A:205:SER:OG	1:A:207:GLU:HG2	2.05	0.56
1:A:162:TRP:HB2	1:A:218:GLN:NE2	2.19	0.56
3:M:151:LYS:HD3	3:M:158:GLU:OE1	2.05	0.56
1:B:232:THR:O	1:B:236:GLU:HB2	2.05	0.56
1:A:149:ILE:O	1:A:185:VAL:HA	2.05	0.56
1:B:211:VAL:HG12	1:B:215:LYS:HE2	1.86	0.56
1:A:199:ASN:HB3	1:A:242:ARG:O	2.05	0.56
1:A:195:THR:CG2	1:A:219:ARG:HE	2.19	0.55
1:A:180:PRO:HD3	1:A:204:SER:HB2	1.88	0.55
3:M:153:LYS:HG2	3:M:157:SER:N	2.22	0.55
3:L:82:PHE:O	3:L:83:ALA:HB2	2.05	0.55
3:M:163:VAL:O	3:M:164:LEU:HD23	2.07	0.55
3:M:79:PRO:HA	3:M:105:ILE:HG21	1.89	0.55
3:L:145:PRO:HG2	3:L:203:LYS:NZ	2.21	0.55
2:I:6:GLU:OE2	2:I:95:CYS:N	2.40	0.54
1:B:151:ILE:HB	1:B:187:ILE:CD1	2.37	0.54
3:L:140:LEU:HD12	3:L:140:LEU:N	2.23	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:119:VAL:HG23	3:L:211:LYS:HD3	1.90	0.54
1:A:286:LEU:HD11	1:A:317:ASN:HD21	1.73	0.54
2:I:90:THR:O	2:I:91:ALA:HB2	2.09	0.53
3:M:136:VAL:CG1	3:M:183:LEU:HB3	2.37	0.53
1:B:174:LYS:HZ3	1:B:175:ARG:HH12	1.56	0.53
3:L:165:ASN:HD22	3:L:181:SER:HA	1.73	0.53
2:H:141:VAL:HG23	2:H:190:SER:HA	1.89	0.53
2:I:199:THR:HG22	2:I:214:LYS:HG3	1.90	0.53
1:B:289:TYR:HB2	1:B:296:THR:HG22	1.90	0.53
3:M:192:ARG:HA	3:M:192:ARG:NE	2.23	0.53
1:B:251:VAL:HG22	1:B:279:GLN:HB2	1.91	0.53
3:M:104:GLU:HG3	3:M:177:TYR:OH	2.08	0.53
3:L:153:LYS:HB3	3:L:197:THR:CG2	2.39	0.53
3:M:154:ILE:O	3:M:154:ILE:HG13	2.09	0.52
3:L:199:GLU:HG2	3:L:210:VAL:HG22	1.90	0.52
1:B:234:ARG:CB	1:B:234:ARG:HH11	2.12	0.52
1:A:146:GLN:O	1:A:146:GLN:HG3	2.08	0.52
1:B:181:LYS:HE2	1:B:181:LYS:HA	1.92	0.52
1:A:234:ARG:NE	1:A:272:ASP:HB3	2.21	0.52
2:I:71:ARG:CD	2:I:73:ASN:HD21	2.23	0.52
3:L:117:PRO:HB3	3:L:143:PHE:HB3	1.92	0.51
1:B:165:VAL:O	1:B:168:PHE:HB3	2.09	0.51
2:H:50:VAL:HG12	2:H:58:TYR:HB2	1.93	0.51
3:L:49:LEU:O	3:L:50:THR:HB	2.10	0.50
1:A:328:VAL:HG23	1:A:329:LYS:N	2.26	0.50
3:M:197:THR:OG1	3:M:212:SER:HB3	2.11	0.50
1:B:174:LYS:O	1:B:174:LYS:HG3	2.12	0.50
3:L:186:THR:OG1	3:L:189:GLU:HG3	2.12	0.50
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.42	0.50
1:B:151:ILE:HG22	1:B:153:LEU:HD12	1.94	0.50
3:M:136:VAL:HG12	3:M:183:LEU:HB3	1.94	0.50
3:L:65:GLY:HA3	3:L:70:TYR:HA	1.93	0.49
2:H:33:THR:CB	2:H:52:SER:HA	2.41	0.49
2:H:90:THR:O	2:H:91:ALA:HB2	2.12	0.49
3:M:99:GLN:H	3:M:99:GLN:NE2	2.09	0.49
3:M:119:VAL:HA	3:M:139:PHE:O	2.13	0.49
1:A:265:ARG:O	1:A:269:VAL:HG23	2.12	0.49
1:B:202:LYS:HG3	1:B:203:TYR:CE1	2.48	0.49
1:B:207:GLU:HG3	1:B:208:GLU:H	1.74	0.49
3:L:202:HIS:CE1	3:L:204:THR:HG23	2.48	0.49
1:A:259:GLU:HG3	1:A:289:TYR:OH	2.12	0.49
1:B:283:ILE:HD11	1:B:331:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:171:ASP:OD2	1:B:328:VAL:HG21	2.12	0.49
3:L:139:PHE:C	3:L:140:LEU:HD12	2.33	0.49
1:A:150:VAL:HA	1:A:186:GLY:O	2.13	0.49
3:L:119:VAL:CG2	3:L:211:LYS:HD3	2.43	0.48
3:L:189:GLU:O	3:L:192:ARG:HB3	2.14	0.48
3:M:13:ALA:HB3	3:M:77:LEU:HD12	1.96	0.48
1:A:157:ASN:ND2	1:A:221:GLY:H	2.12	0.48
1:B:265:ARG:O	1:B:269:VAL:HG23	2.12	0.48
1:A:289:TYR:CB	1:A:296:THR:HG22	2.43	0.48
2:I:12:VAL:HG11	2:I:85:LEU:HD13	1.95	0.48
2:I:143:LEU:HD23	2:I:198:VAL:HG11	1.95	0.48
1:B:252:MET:HG2	1:B:254:ILE:CD1	2.43	0.48
3:M:128:GLN:HG2	3:M:133:GLY:O	2.14	0.48
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.96	0.48
2:H:192:THR:O	2:H:196:GLU:HB2	2.13	0.48
1:A:230:ILE:HG23	1:A:252:MET:SD	2.54	0.48
3:M:119:VAL:HG12	3:M:140:LEU:HG	1.95	0.47
2:I:143:LEU:HG	2:I:215:ILE:HG21	1.95	0.47
3:M:153:LYS:HB3	3:M:197:THR:CG2	2.43	0.47
1:B:286:LEU:HD11	1:B:317:ASN:ND2	2.16	0.47
1:B:235:LYS:O	1:B:236:GLU:HG3	2.15	0.47
3:L:183:LEU:HD11	3:L:185:LEU:HD21	1.96	0.47
3:M:105:ILE:HG12	3:M:105:ILE:O	2.13	0.47
1:B:171:ASP:HB3	1:B:328:VAL:HG21	1.97	0.47
3:L:11:LEU:HD12	3:L:11:LEU:C	2.35	0.47
1:A:147:LEU:HD23	1:A:183:THR:HG22	1.96	0.47
3:M:138:CYS:CB	3:M:198:CYS:HG	2.26	0.47
1:B:331:LEU:O	1:B:335:ILE:HG22	2.15	0.47
3:M:146:LYS:HB3	3:M:177:TYR:CD2	2.50	0.47
2:I:169:HIS:HE1	3:M:142:ASN:OD1	1.97	0.47
3:L:150:VAL:HA	3:L:199:GLU:O	2.15	0.47
1:A:327:ILE:CG2	1:A:331:LEU:HB2	2.43	0.47
3:L:153:LYS:O	3:L:197:THR:HG22	2.15	0.46
3:M:51:SER:HB3	3:M:63:GLY:O	2.16	0.46
1:A:163:GLU:OE1	1:A:163:GLU:N	2.48	0.46
2:H:129:LEU:HB2	2:H:144:GLY:O	2.14	0.46
3:M:122:PHE:HA	3:M:123:PRO:HD3	1.75	0.46
3:L:11:LEU:HD21	3:L:21:ILE:HD11	1.97	0.46
3:M:165:ASN:HD22	3:M:181:SER:HA	1.80	0.46
2:I:119:ALA:HB1	5:I:277:HOH:O	2.15	0.46
2:I:6:GLU:HG3	2:I:111:GLY:HA2	1.98	0.46
1:B:192:GLU:HG3	1:B:221:GLY:CA	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151:ILE:HG22	1:A:153:LEU:HD13	1.98	0.46
1:A:172:LEU:HD11	1:A:331:LEU:HD22	1.98	0.46
1:A:332:GLY:C	1:A:334:ARG:H	2.19	0.46
1:A:172:LEU:HD23	1:A:172:LEU:O	2.16	0.45
3:L:119:VAL:HG12	3:L:140:LEU:HG	1.99	0.45
1:A:254:ILE:HD12	1:A:254:ILE:N	2.31	0.45
2:H:176:GLN:CD	3:L:164:LEU:HD11	2.36	0.45
3:M:72:LEU:C	3:M:72:LEU:HD23	2.36	0.45
1:A:329:LYS:O	1:A:333:GLU:HG2	2.16	0.45
2:I:142:THR:O	3:M:122:PHE:HZ	2.00	0.45
1:A:193:ASN:HD22	1:A:193:ASN:C	2.19	0.45
1:A:201:ASN:HD22	1:A:201:ASN:C	2.19	0.45
3:L:90:TRP:HA	3:L:95:TRP:CD1	2.51	0.45
1:B:313:LYS:HB3	1:B:313:LYS:HZ3	1.80	0.45
3:L:141:ASN:ND2	3:L:178:SER:HB3	2.30	0.45
1:A:178:ILE:HG23	1:A:183:THR:O	2.17	0.45
2:I:33:THR:HB	2:I:52:SER:HA	1.98	0.45
1:B:251:VAL:HG11	1:B:335:ILE:CD1	2.44	0.45
1:B:313:LYS:NZ	1:B:313:LYS:HB3	2.32	0.45
1:B:211:VAL:HG12	1:B:215:LYS:CE	2.47	0.45
3:M:106:LYS:HE3	3:M:106:LYS:HB2	1.83	0.45
3:L:151:LYS:HE3	3:L:158:GLU:OE2	2.16	0.45
1:B:151:ILE:HG22	1:B:153:LEU:CD1	2.47	0.45
3:M:202:HIS:CE1	3:M:204:THR:HG23	2.52	0.45
2:H:50:VAL:CG1	2:H:58:TYR:HB2	2.47	0.45
2:I:104:TYR:CZ	3:M:48:TYR:HB3	2.51	0.45
1:A:307:ALA:HB1	1:A:314:HIS:HB3	1.99	0.45
3:M:165:ASN:ND2	3:M:181:SER:HA	2.31	0.45
3:M:90:TRP:HA	3:M:95:TRP:CD1	2.51	0.45
3:L:155:ASP:OD2	3:L:193:HIS:HB3	2.17	0.44
1:B:234:ARG:NE	1:B:272:ASP:HB3	2.32	0.44
1:B:302:GLU:O	1:B:306:ILE:HG13	2.18	0.44
1:B:283:ILE:HD11	1:B:331:LEU:HD12	2.00	0.44
1:A:184:GLN:HB3	1:A:200:LEU:O	2.18	0.44
2:H:71:ARG:CD	2:H:73:ASN:ND2	2.79	0.44
2:I:66:ARG:HG2	2:I:83:ASN:O	2.18	0.44
2:I:71:ARG:CD	2:I:73:ASN:ND2	2.81	0.44
2:I:193:TRP:CD1	2:I:194:PRO:HA	2.53	0.44
1:B:192:GLU:CG	1:B:222:ARG:H	2.31	0.43
3:M:82:PHE:O	3:M:83:ALA:HB2	2.17	0.43
1:A:249:LYS:HE3	1:A:279:GLN:HG2	1.99	0.43
2:I:6:GLU:HG3	2:I:111:GLY:N	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:235:LYS:HG3	1:B:235:LYS:O	2.19	0.43
1:B:151:ILE:HB	1:B:187:ILE:HD12	2.00	0.43
1:A:295:SER:HB2	1:A:297:GLU:HG3	2.01	0.43
1:B:211:VAL:C	1:B:215:LYS:HE2	2.39	0.43
1:B:151:ILE:HD12	1:B:187:ILE:HD11	2.00	0.43
3:M:206:THR:O	3:M:208:PRO:HD3	2.19	0.43
1:A:213:ALA:C	1:A:215:LYS:H	2.21	0.43
3:M:139:PHE:C	3:M:140:LEU:HD12	2.39	0.43
3:M:154:ILE:HG22	3:M:196:TYR:CD1	2.53	0.43
1:A:289:TYR:HB3	1:A:296:THR:HG22	1.99	0.43
3:M:3:GLN:HE21	3:M:3:GLN:HB2	1.65	0.43
1:B:153:LEU:HD21	1:B:169:LEU:HD11	2.01	0.43
2:I:164:LEU:HA	2:I:164:LEU:HD23	1.82	0.43
1:A:309:GLU:OE2	1:A:310:PRO:HA	2.18	0.43
1:B:223:GLN:HE22	3:M:93:ASN:HD21	1.67	0.42
1:B:289:TYR:HB3	1:B:296:THR:HG22	2.00	0.42
1:B:153:LEU:HD13	1:B:187:ILE:HG23	2.01	0.42
2:H:129:LEU:HB2	2:H:144:GLY:C	2.39	0.42
3:L:51:SER:HB3	3:L:63:GLY:O	2.20	0.42
2:H:122:THR:HG23	2:H:123:PRO:HD2	2.01	0.42
1:B:286:LEU:CD1	1:B:317:ASN:HD21	2.20	0.42
2:H:140:MET:HE2	2:H:187:THR:HG22	2.01	0.42
1:A:331:LEU:C	1:A:331:LEU:HD23	2.39	0.42
2:I:193:TRP:CG	2:I:194:PRO:HA	2.54	0.42
2:I:6:GLU:HG3	2:I:111:GLY:H	1.84	0.42
1:A:151:ILE:HG22	1:A:153:LEU:CD1	2.48	0.42
3:L:1:GLN:H3	3:L:1:GLN:CD	2.22	0.42
1:A:281:PHE:CZ	1:A:335:ILE:HG12	2.54	0.42
1:A:147:LEU:HD23	1:A:147:LEU:N	2.35	0.42
3:M:119:VAL:HG23	3:M:119:VAL:O	2.19	0.42
1:A:206:THR:O	1:A:210:LEU:HG	2.19	0.42
2:H:51:ILE:HA	2:H:56:HIS:O	2.20	0.42
2:H:161:SER:N	2:H:201:ASN:ND2	2.54	0.42
3:M:186:THR:OG1	3:M:189:GLU:HG3	2.19	0.42
2:H:22:CYS:SG	2:H:95:CYS:CB	3.01	0.42
2:H:171:PHE:N	2:H:171:PHE:CD1	2.87	0.42
3:M:117:PRO:HB3	3:M:143:PHE:HB3	2.02	0.42
1:A:215:LYS:HB2	1:A:215:LYS:HE3	1.93	0.42
1:A:192:GLU:CG	1:A:222:ARG:H	2.32	0.42
3:M:80:GLU:O	3:M:80:GLU:HG3	2.20	0.42
2:H:103:GLY:HA3	3:L:90:TRP:HB2	2.01	0.42
3:L:114:ASP:OD2	3:L:203:LYS:HD2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:186:GLY:N	1:B:200:LEU:HD23	2.35	0.42
1:B:227:ALA:HB3	1:B:262:ASP:CG	2.41	0.42
3:M:119:VAL:HG23	3:M:211:LYS:HD3	2.01	0.41
2:H:104:TYR:CZ	3:L:48:TYR:HB3	2.55	0.41
1:B:201:ASN:ND2	1:B:201:ASN:C	2.74	0.41
1:A:192:GLU:HG3	1:A:221:GLY:CA	2.49	0.41
2:I:6:GLU:H	2:I:6:GLU:HG2	1.30	0.41
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.85	0.41
1:A:252:MET:SD	1:A:254:ILE:HD11	2.60	0.41
2:I:124:PRO:HB3	2:I:150:TYR:HB3	2.01	0.41
3:M:79:PRO:O	3:M:105:ILE:HD12	2.20	0.41
2:I:51:ILE:HA	2:I:56:HIS:O	2.21	0.41
1:B:209:VAL:O	1:B:210:LEU:C	2.59	0.41
1:B:150:VAL:O	1:B:252:MET:HA	2.21	0.41
3:L:24:SER:HA	3:L:68:THR:O	2.21	0.41
2:H:178:ASP:O	2:H:179:LEU:HD23	2.20	0.41
1:A:222:ARG:HB3	3:L:95:TRP:CZ2	2.56	0.41
3:L:90:TRP:C	3:L:90:TRP:CD1	2.94	0.41
1:B:172:LEU:C	1:B:174:LYS:H	2.24	0.41
1:B:213:ALA:C	1:B:215:LYS:H	2.25	0.41
1:A:255:VAL:HG22	1:A:283:ILE:HD12	2.02	0.41
3:L:196:TYR:O	3:L:212:SER:HB2	2.21	0.41
3:M:11:LEU:C	3:M:11:LEU:HD12	2.40	0.41
1:A:316:PHE:HB3	1:A:327:ILE:HD13	2.03	0.41
2:H:172:PRO:HG2	3:L:166:SER:OG	2.20	0.41
1:A:245:ARG:HB2	1:A:248:VAL:HG21	2.03	0.40
3:L:15:VAL:HA	3:L:77:LEU:O	2.21	0.40
2:H:182:LEU:O	2:H:182:LEU:HD12	2.21	0.40
3:L:158:GLU:CD	3:L:160:GLN:HE21	2.24	0.40
3:L:72:LEU:C	3:L:72:LEU:HD23	2.41	0.40
2:H:97:ARG:HH21	2:H:106:ASP:CG	2.25	0.40
1:A:248:VAL:HG12	1:A:249:LYS:N	2.36	0.40
3:M:115:ALA:O	3:M:143:PHE:HA	2.21	0.40
1:B:201:ASN:HD22	1:B:201:ASN:C	2.25	0.40
2:H:189:PRO:O	2:H:192:THR:HB	2.22	0.40
2:I:129:LEU:HB2	2:I:144:GLY:O	2.22	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	184/223 (82%)	164 (89%)	18 (10%)	2 (1%)	21	16
1	B	166/223 (74%)	147 (89%)	17 (10%)	2 (1%)	19	14
2	H	206/226 (91%)	201 (98%)	5 (2%)	0	100	100
2	I	206/226 (91%)	202 (98%)	4 (2%)	0	100	100
3	L	208/213 (98%)	198 (95%)	9 (4%)	1 (0%)	38	38
3	M	208/213 (98%)	195 (94%)	12 (6%)	1 (0%)	38	38
All	All	1178/1324 (89%)	1107 (94%)	65 (6%)	6 (0%)	38	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLY
1	B	236	GLU
1	A	333	GLU
3	L	83	ALA
1	B	173	LEU
3	M	160	GLN

### 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	164/194 (84%)	157 (96%)	7 (4%)	40	47
1	B	153/194 (79%)	148 (97%)	5 (3%)	50	60
2	H	177/190 (93%)	170 (96%)	7 (4%)	42	51
2	I	177/190 (93%)	166 (94%)	11 (6%)	26	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	187/190 (98%)	179 (96%)	8 (4%)	40	47
3	M	187/190 (98%)	179 (96%)	8 (4%)	40	47
All	All	1045/1148 (91%)	999 (96%)	46 (4%)	39	45

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	163	GLU
1	A	193	ASN
1	A	201	ASN
1	A	219	ARG
1	A	234	ARG
1	A	268	GLN
2	H	38	ARG
2	H	96	THR
2	H	113	LEU
2	H	152	PRO
2	H	154	PRO
2	H	155	VAL
2	H	199	THR
3	L	4	LEU
3	L	49	LEU
3	L	77	LEU
3	L	90	TRP
3	L	104	GLU
3	L	146	LYS
3	L	159	ARG
3	L	211	LYS
1	B	147	LEU
1	B	171	ASP
1	B	201	ASN
1	B	234	ARG
1	B	238	PHE
2	I	6	GLU
2	I	38	ARG
2	I	43	LYS
2	I	66	ARG
2	I	95	CYS
2	I	113	LEU
2	I	143	LEU

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Mol	Chain	Res	Type
2	I	152	PRO
2	I	154	PRO
2	I	155	VAL
2	I	164	LEU
3	M	4	LEU
3	M	9	SER
3	M	15	VAL
3	M	77	LEU
3	M	90	TRP
3	M	99	GLN
3	M	105	ILE
3	M	194	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	157	ASN
1	A	170	ASN
1	A	193	ASN
1	A	201	ASN
1	A	214	ASN
1	A	218	GLN
1	A	261	HIS
1	A	268	GLN
1	A	271	GLN
1	A	279	GLN
1	A	314	HIS
2	H	3	GLN
2	H	73	ASN
2	H	76	ASN
2	H	169	HIS
2	H	201	ASN
3	L	1	GLN
3	L	3	GLN
3	L	93	ASN
3	L	141	ASN
3	L	160	GLN
3	L	165	ASN
1	B	157	ASN
1	B	201	ASN
1	B	218	GLN

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Mol	Chain	Res	Type
1	B	261	HIS
1	B	268	GLN
1	B	288	HIS
1	B	314	HIS
1	B	317	ASN
2	I	73	ASN
2	I	169	HIS
2	I	201	ASN
3	M	3	GLN
3	M	36	GLN
3	M	93	ASN
3	M	99	GLN
3	M	141	ASN
3	M	160	GLN
3	M	165	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	188/223 (84%)	0.46	9 (4%) 29 29	28, 59, 77, 83	0
1	B	176/223 (78%)	0.78	17 (9%) 8 7	33, 66, 91, 96	0
2	H	210/226 (92%)	0.10	0 100 100	22, 31, 49, 58	0
2	I	210/226 (92%)	0.06	0 100 100	24, 34, 50, 61	0
3	L	210/213 (98%)	0.19	7 (3%) 44 45	22, 42, 74, 86	0
3	M	210/213 (98%)	0.20	9 (4%) 34 34	24, 41, 68, 86	0
All	All	1204/1324 (90%)	0.28	42 (3%) 42 42	22, 42, 78, 96	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	5.0
1	B	147	LEU	4.5
1	B	179	GLY	4.3
1	B	237	ALA	4.2
1	A	146	GLN	4.1
3	L	154	ILE	3.9
3	M	154	ILE	3.8
3	M	214	ASN	3.7
1	B	334	ARG	3.4
3	M	192	ARG	3.2
3	L	209	ILE	3.2
1	A	147	LEU	3.1
1	B	336	PHE	3.1
1	B	313	LYS	3.1
1	B	311	THR	2.9
1	B	148	ASP	2.8
1	B	312	GLU	2.8
1	A	313	LYS	2.7
1	A	331	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	195	SER	2.6
1	B	172	LEU	2.6
1	B	327	ILE	2.6
1	B	245	ARG	2.6
1	B	322	LEU	2.5
1	A	248	VAL	2.5
1	A	178	ILE	2.4
3	L	210	VAL	2.4
1	B	289	TYR	2.4
1	B	182	GLN	2.3
3	L	214	ASN	2.3
3	M	210	VAL	2.2
1	B	240	GLU	2.2
3	L	213	PHE	2.2
1	A	281	PHE	2.2
3	M	119	VAL	2.2
3	M	209	ILE	2.1
1	A	334	ARG	2.1
1	A	238	PHE	2.1
3	M	153	LYS	2.1
3	L	151	LYS	2.1
3	M	199	GLU	2.0
3	L	192	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	401	1/1	0.15	1.33	54,54,54,54	0
4	MG	A	400	1/1	0.12	-0.30	47,47,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.