Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:49 PM UTC

PDB ID	:	4XZU / pdb_00004xzu
Title	:	Crystal Structure of the Human Factor VIII C2 Domain in Complex with Murine 3E6 Inhibitory Antibody
Authors	:	Spiegel, P.C.; Wuerth, M.E.
Deposited on	:	2015-02-05
Resolution	:	2.61 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:

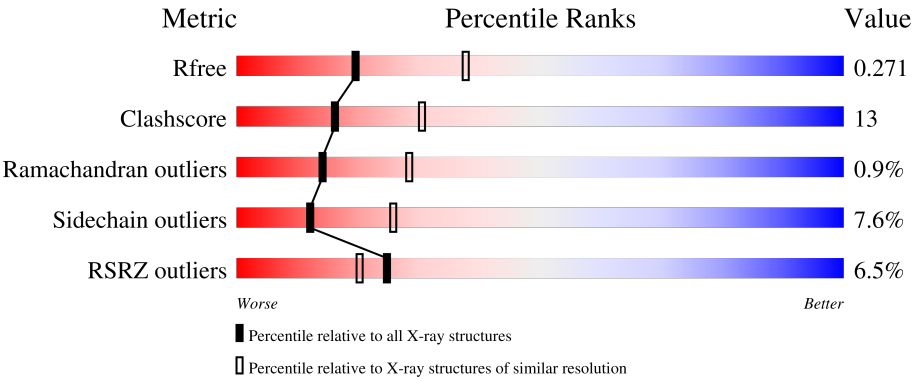
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	219	82% 16% ·
1	E	219	12% 72% 18% · · 5%
2	B	213	% 77% 18% 5%
2	F	213	20% 58% 25% 7% · 8%
3	G	154	% 68% 26% 5% ·

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Mol	Chain	Length	Quality of chain
3	M	154	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9034 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 3E6 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1619	1029	265	319	6			
1	E	208	Total	C	N	O	S	0	0	0
			1581	1007	257	312	5			

- Molecule 2 is a protein called 3E6 antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1633	1016	271	337	9			
2	F	195	Total	C	N	O	S	0	0	0
			1495	937	244	306	8			

- Molecule 3 is a protein called Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	154	Total	C	N	O	S	0	0	0
			1231	785	214	224	8			
3	G	154	Total	C	N	O	S	0	0	0
			1231	785	214	224	8			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

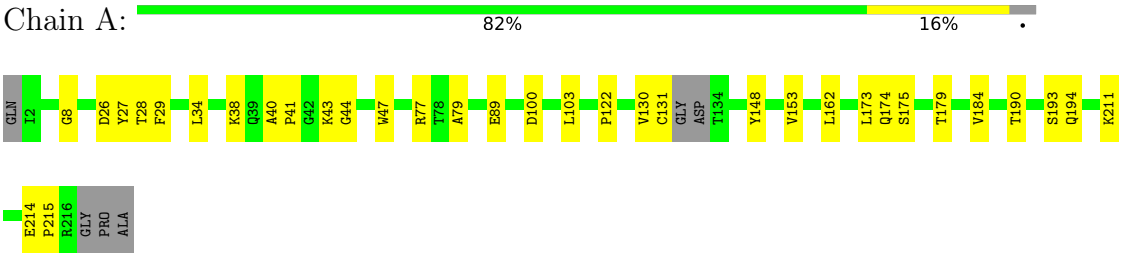
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	73	Total O 73 73	0	0
5	B	49	Total O 49 49	0	0
5	M	30	Total O 30 30	0	0
5	E	41	Total O 41 41	0	0
5	F	27	Total O 27 27	0	0
5	G	21	Total O 21 21	0	0

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.

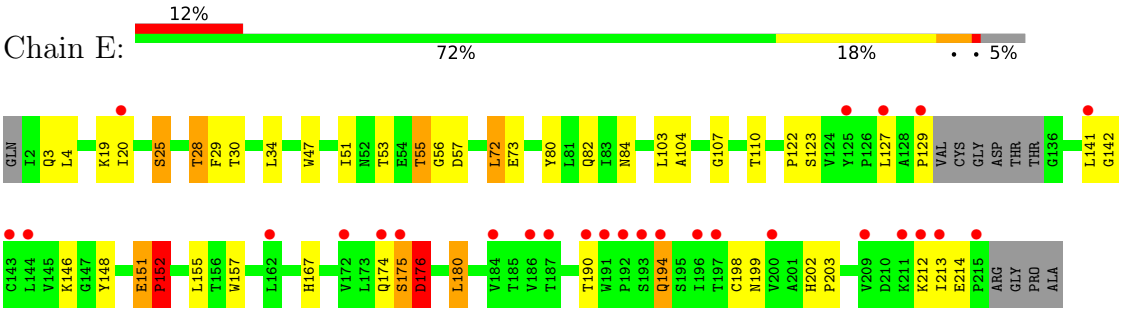
• Molecule 1: 3E6 antibody Fab heavy chain

Chain A:



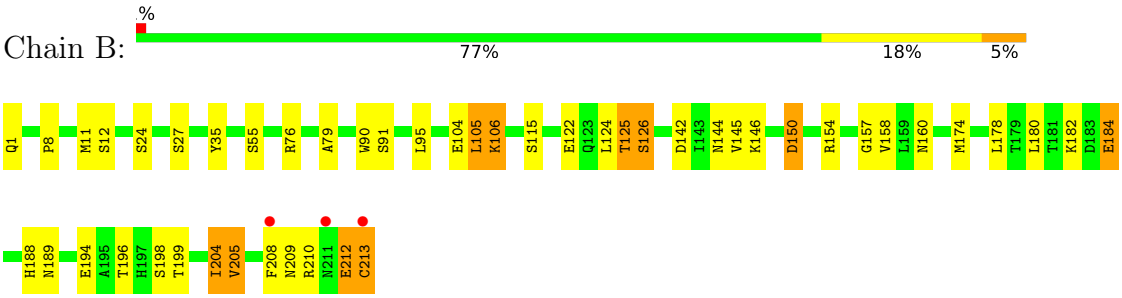
• Molecule 1: 3E6 antibody Fab heavy chain

Chain E:



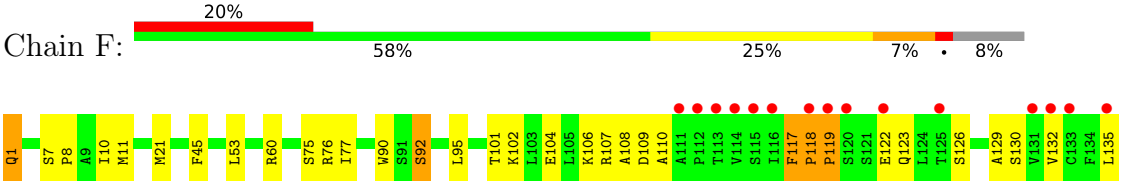
• Molecule 2: 3E6 antibody Fab light chain

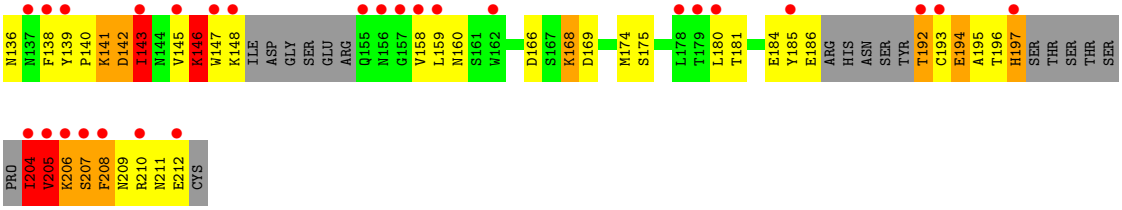
Chain B:



• Molecule 2: 3E6 antibody Fab light chain

Chain F:



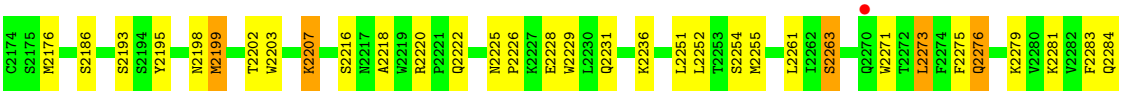


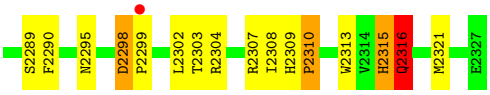
• Molecule 3: Coagulation factor VIII

Chain M:

• Molecule 3: Coagulation factor VIII

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	43.23Å 148.49Å 188.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 2.61 39.78 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.78-2.61) 95.0 (39.78-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.68 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.267 0.206 , 0.271	Depositor DCC
R_{free} test set	1848 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9034	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	0.64	0/1660	0.94	7/2266 (0.3%)
1	E	0.84	2/1622 (0.1%)	1.03	8/2214 (0.4%)
2	B	0.60	0/1672	0.87	1/2274 (0.0%)
2	F	0.82	5/1528 (0.3%)	1.01	6/2074 (0.3%)
3	G	0.53	0/1263	0.91	5/1713 (0.3%)
3	M	0.59	0/1263	0.84	2/1713 (0.1%)
All	All	0.69	7/9008 (0.1%)	0.94	29/12254 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	202	HIS	C-O	-6.70	1.18	1.24
2	F	204	ILE	C-N	6.47	1.42	1.33
2	F	205	VAL	C-N	6.00	1.42	1.33
2	F	119	PRO	N-CD	5.78	1.55	1.47
2	F	117	PHE	C-N	5.75	1.40	1.33
2	F	118	PRO	N-CD	5.26	1.55	1.47
1	E	129	PRO	N-CD	5.08	1.54	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	176	ASP	N-CA-C	-11.75	101.22	114.62
1	E	151	GLU	C-N-CD	8.96	140.31	120.60
1	A	28	THR	N-CA-C	-8.91	91.81	110.80
1	A	8	GLY	CA-C-N	7.55	127.60	119.90
1	A	8	GLY	C-N-CA	7.55	127.60	119.90
1	A	173	LEU	N-CA-C	7.42	120.89	108.20
3	G	2316	GLN	N-CA-C	7.35	122.00	110.32
2	F	117	PHE	CA-C-N	-7.24	112.92	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	117	PHE	C-N-CA	-7.24	112.92	120.38
1	E	29	PHE	N-CA-C	7.10	123.08	111.37
1	E	25	SER	N-CA-C	-6.45	97.06	110.80
1	E	152	PRO	CA-N-CD	-6.31	102.66	111.50
2	B	157	GLY	N-CA-C	-6.27	107.06	115.21
2	F	118	PRO	CA-C-N	-6.23	113.53	119.89
2	F	118	PRO	C-N-CA	-6.23	113.53	119.89
3	G	2321	MET	N-CA-C	6.21	118.22	108.96
3	G	2315	HIS	N-CA-C	-6.16	98.38	108.67
1	A	173	LEU	CB-CA-C	-6.00	101.18	110.78
2	F	146	LYS	N-CA-C	-5.71	99.84	108.46
1	A	40	ALA	CA-C-N	5.57	126.80	119.84
1	A	40	ALA	C-N-CA	5.57	126.80	119.84
2	F	194	GLU	N-CA-C	5.44	118.34	107.62
1	E	146	LYS	N-CA-C	5.11	117.29	109.07
1	E	202	HIS	CA-C-N	-5.08	113.69	119.28
1	E	202	HIS	C-N-CA	-5.08	113.69	119.28
3	M	2321	MET	N-CA-C	5.01	116.43	108.96
3	G	2251	LEU	CB-CA-C	-5.01	110.82	116.63
3	M	2314	VAL	N-CA-C	5.01	114.78	107.37
3	G	2303	THR	N-CA-C	5.00	116.44	108.79

There are no chirality outliers.

There are no planarity outliers.

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	1619	0	1587	23	0
1	E	1581	0	1548	48	0
2	B	1633	0	1554	29	0
2	F	1495	0	1429	103	0
3	G	1231	0	1218	31	0
3	M	1231	0	1218	20	0
4	A	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	1	0	0	0	0
5	A	73	0	0	0	1
5	B	49	0	0	1	0
5	E	41	0	0	6	0
5	F	27	0	0	1	0
5	G	21	0	0	2	0
5	M	30	0	0	3	1
All	All	9034	0	8554	228	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 13.

All (228) 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:F:186:GLU:HA	2:F:210:ARG:NH2	1.21	1.41
2:F:185:TYR:CE2	2:F:210:ARG:HD2	1.65	1.30
2:F:186:GLU:CA	2:F:210:ARG:NH2	1.94	1.30
2:F:185:TYR:CZ	2:F:210:ARG:HD2	1.71	1.24
1:E:167:HIS:HD2	2:F:136:ASN:ND2	1.37	1.19
1:E:212:LYS:HD2	1:E:214:GLU:OE1	1.45	1.16
2:F:204:ILE:O	2:F:205:VAL:HG13	1.44	1.14
2:F:186:GLU:HA	2:F:210:ARG:CZ	1.78	1.13
1:E:167:HIS:CD2	2:F:136:ASN:ND2	2.19	1.11
1:E:30:THR:HG22	1:E:53:THR:O	1.51	1.07
2:F:195:ALA:H	2:F:205:VAL:HG12	1.22	1.01
2:F:186:GLU:C	2:F:210:ARG:HH22	1.68	1.00
2:F:143:ILE:HD11	2:F:197:HIS:CE1	1.98	0.99
2:F:143:ILE:CD1	2:F:197:HIS:ND1	2.26	0.98
1:E:174:GLN:HG3	2:F:159:LEU:CD1	1.96	0.95
1:E:174:GLN:HG3	2:F:159:LEU:HD12	1.48	0.95
2:F:195:ALA:N	2:F:205:VAL:HG12	1.80	0.95
2:F:148:LYS:O	2:F:192:THR:N	2.00	0.94
2:F:185:TYR:CZ	2:F:210:ARG:CD	2.50	0.94
2:F:186:GLU:C	2:F:210:ARG:NH2	2.24	0.92
2:F:204:ILE:O	2:F:205:VAL:CG1	2.16	0.92
2:F:204:ILE:C	2:F:205:VAL:HG13	1.94	0.92
2:F:143:ILE:HD11	2:F:197:HIS:ND1	1.83	0.91
3:G:2263:SER:HG	3:G:2309:HIS:HE2	1.14	0.90
2:F:186:GLU:HA	2:F:210:ARG:HH21	1.34	0.90
1:E:28:THR:HG21	5:E:305:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:THR:CG2	5:E:305:HOH:O	2.20	0.88
2:F:185:TYR:CE2	2:F:210:ARG:CD	2.56	0.87
1:E:167:HIS:HD2	2:F:136:ASN:HD21	1.18	0.87
1:E:212:LYS:CD	1:E:214:GLU:OE1	2.24	0.84
1:A:100:ASP:OD1	3:M:2215:ARG:NH1	2.13	0.82
3:M:2174:CYS:N	5:M:2501:HOH:O	2.13	0.81
1:E:194:GLN:HA	1:E:194:GLN:NE2	1.95	0.79
2:F:123:GLN:OE1	2:F:130:SER:N	2.17	0.78
1:E:167:HIS:CD2	2:F:136:ASN:HD22	2.02	0.76
3:G:2284:GLN:O	5:G:2401:HOH:O	2.05	0.75
2:F:194:GLU:HA	2:F:205:VAL:HG12	1.67	0.74
2:B:180:LEU:HD22	2:B:184:GLU:HG2	1.69	0.73
2:F:185:TYR:O	2:F:210:ARG:NH1	2.21	0.73
2:F:135:LEU:HD13	2:F:174:MET:HG2	1.71	0.72
1:E:176:ASP:OD2	1:E:176:ASP:N	2.21	0.70
1:A:27:TYR:O	1:A:29:PHE:N	2.24	0.70
2:F:123:GLN:O	2:F:126:SER:N	2.23	0.69
2:F:194:GLU:HA	2:F:205:VAL:CG1	2.21	0.69
2:B:79:ALA:HA	2:B:105:LEU:HD22	1.74	0.69
1:E:174:GLN:HG3	2:F:159:LEU:HD11	1.74	0.69
2:F:186:GLU:CA	2:F:210:ARG:HH21	1.95	0.69
2:F:107:ARG:HG3	2:F:108:ALA:N	2.08	0.69
2:F:143:ILE:HD12	2:F:197:HIS:HA	1.75	0.68
2:F:143:ILE:HD12	2:F:197:HIS:ND1	2.09	0.68
1:E:203:PRO:HD2	5:E:313:HOH:O	1.92	0.68
2:F:142:ASP:OD1	2:F:143:ILE:HD13	1.94	0.68
2:F:195:ALA:HB3	2:F:204:ILE:O	1.95	0.66
3:G:2229:TRP:HZ3	3:G:2231:GLN:HB2	1.61	0.66
1:E:34:LEU:HD23	1:E:53:THR:HG21	1.77	0.66
2:F:1:GLN:O	2:F:1:GLN:NE2	2.26	0.65
3:M:2254:SER:HB2	3:M:2289:SER:HB3	1.78	0.65
3:G:2276:GLN:HG2	3:G:2281:LYS:HD2	1.80	0.64
2:F:192:THR:HG22	2:F:193:CYS:H	1.63	0.64
2:F:185:TYR:O	2:F:210:ARG:CZ	2.47	0.63
3:M:2220:ARG:NH2	3:M:2316:GLN:OE1	2.31	0.63
2:F:123:GLN:OE1	2:F:130:SER:HB2	1.99	0.62
3:G:2307:ARG:NH1	5:G:2402:HOH:O	2.29	0.62
2:B:160:ASN:HB3	2:B:174:MET:HE3	1.82	0.62
2:F:138:PHE:CD1	2:F:143:ILE:HG12	2.35	0.62
1:E:55:THR:HG22	1:E:57:ASP:H	1.65	0.61
2:B:125:THR:HG22	2:B:125:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:LEU:CD2	5:E:303:HOH:O	2.48	0.61
2:F:166:ASP:C	2:F:168:LYS:H	2.08	0.61
1:A:43:LYS:HD2	1:A:44:GLY:H	1.63	0.61
1:E:127:LEU:HB2	1:E:142:GLY:C	2.26	0.61
3:G:2298:ASP:HA	3:G:2299:PRO:C	2.26	0.60
2:F:147:TRP:HE3	2:F:192:THR:O	1.84	0.60
2:B:24:SER:HB3	3:G:2222:GLN:HE22	1.66	0.60
1:E:180:LEU:C	1:E:180:LEU:HD23	2.25	0.60
2:F:104:GLU:OE2	2:F:139:TYR:OH	2.15	0.60
3:G:2229:TRP:CZ3	3:G:2231:GLN:HB2	2.36	0.59
3:M:2215:ARG:NH1	5:M:2502:HOH:O	2.26	0.59
2:F:143:ILE:HD13	2:F:143:ILE:N	2.18	0.59
2:F:135:LEU:HD12	2:F:135:LEU:N	2.17	0.59
2:F:209:ASN:C	2:F:211:ASN:H	2.10	0.59
1:A:89:GLU:OE2	1:A:89:GLU:N	2.35	0.59
2:B:24:SER:HB3	3:G:2222:GLN:NE2	2.17	0.58
3:G:2313:TRP:HD1	3:G:2315:HIS:O	1.86	0.58
2:F:92:SER:HB2	3:G:2186:SER:HB3	1.85	0.58
3:M:2304:ARG:HD3	3:M:2305:TYR:CE1	2.38	0.58
1:E:167:HIS:HD2	2:F:136:ASN:HD22	1.34	0.58
2:F:138:PHE:CE1	2:F:143:ILE:HG12	2.39	0.58
2:F:145:VAL:HG12	2:F:146:LYS:N	2.19	0.58
3:G:2236:LYS:H	3:G:2304:ARG:HG3	1.68	0.57
2:F:147:TRP:CD1	2:F:158:VAL:HG22	2.39	0.57
1:E:167:HIS:CD2	2:F:136:ASN:HD21	2.04	0.57
2:F:102:LYS:HE3	5:F:426:HOH:O	2.04	0.57
2:F:147:TRP:HD1	2:F:158:VAL:CG2	2.18	0.57
1:A:100:ASP:CG	3:M:2215:ARG:HH12	2.13	0.56
2:F:166:ASP:OD2	2:F:168:LYS:HB2	2.05	0.56
3:G:2220:ARG:HD2	3:G:2255:MET:HE1	1.87	0.56
2:F:147:TRP:CE3	2:F:192:THR:O	2.60	0.56
2:F:147:TRP:O	2:F:148:LYS:HG3	2.06	0.55
2:F:186:GLU:O	2:F:210:ARG:NH2	2.33	0.55
3:M:2234:PHE:O	3:M:2235:GLN:HB2	2.07	0.55
2:F:195:ALA:N	2:F:205:VAL:CG1	2.63	0.55
3:G:2207:LYS:HG2	3:G:2216:SER:O	2.07	0.54
2:F:180:LEU:HB3	2:F:184:GLU:HG3	1.87	0.54
2:F:205:VAL:HG23	2:F:205:VAL:O	2.07	0.54
2:F:208:PHE:CD1	2:F:208:PHE:C	2.85	0.54
2:F:209:ASN:O	2:F:211:ASN:N	2.35	0.54
1:E:28:THR:HG23	5:E:305:HOH:O	1.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:PRO:O	2:F:142:ASP:OD1	2.25	0.53
2:F:142:ASP:OD1	2:F:142:ASP:N	2.39	0.53
2:B:150:ASP:OD2	2:B:188:HIS:HB3	2.08	0.53
2:F:147:TRP:HD1	2:F:158:VAL:HG22	1.73	0.53
2:F:104:GLU:OE2	2:F:139:TYR:CZ	2.61	0.53
3:G:2255:MET:SD	3:G:2316:GLN:HG3	2.49	0.53
2:B:8:PRO:HG2	2:B:11:MET:HB3	1.91	0.53
3:G:2263:SER:OG	3:G:2309:HIS:NE2	2.19	0.53
1:A:34:LEU:HD23	1:A:79:ALA:HB2	1.89	0.52
2:B:124:LEU:C	2:B:126:SER:H	2.18	0.52
1:A:211:LYS:NZ	2:B:122:GLU:OE1	2.43	0.52
2:F:211:ASN:ND2	2:F:212:GLU:N	2.57	0.52
1:A:47:TRP:CD2	2:B:95:LEU:HB3	2.45	0.52
2:B:158:VAL:HG23	2:B:178:LEU:HD13	1.92	0.52
1:E:56:GLY:HA2	1:E:72:LEU:HD11	1.92	0.51
2:F:145:VAL:CG1	2:F:146:LYS:N	2.73	0.51
3:M:2234:PHE:C	3:M:2236:LYS:H	2.18	0.51
1:A:43:LYS:CD	1:A:44:GLY:H	2.23	0.51
1:A:162:LEU:HD21	1:A:184:VAL:HG21	1.92	0.51
2:B:1:GLN:N	2:B:1:GLN:CD	2.69	0.50
2:F:141:LYS:O	2:F:142:ASP:HB3	2.11	0.50
2:B:154:ARG:HD3	2:B:178:LEU:HD11	1.93	0.50
1:A:130:VAL:HG11	2:B:208:PHE:HB2	1.94	0.50
1:A:38:LYS:NZ	1:A:89:GLU:O	2.45	0.49
3:M:2276:GLN:NE2	3:M:2298:ASP:O	2.45	0.49
1:E:51:ILE:HG12	1:E:72:LEU:HD21	1.93	0.49
2:F:21:MET:HG2	2:F:101:THR:HG21	1.93	0.49
3:G:2195:TYR:HA	3:G:2220:ARG:O	2.13	0.49
2:B:194:GLU:HG2	2:B:205:VAL:HG12	1.93	0.49
3:G:2308:ILE:O	3:G:2310:PRO:HD3	2.12	0.49
1:A:131:CYS:N	2:B:213:CYS:SG	2.86	0.48
3:M:2250:SER:HB3	3:M:2255:MET:HE2	1.95	0.48
2:F:206:LYS:C	2:F:207:SER:OG	2.55	0.48
2:F:143:ILE:HD13	2:F:143:ILE:H	1.76	0.48
3:G:2193:SER:OG	3:G:2228:GLU:OE1	2.27	0.48
1:E:127:LEU:HB2	1:E:142:GLY:CA	2.43	0.48
2:F:211:ASN:CG	2:F:212:GLU:N	2.71	0.48
2:B:12:SER:OG	2:B:106:LYS:HG3	2.13	0.48
2:B:204:ILE:HD11	5:B:348:HOH:O	2.13	0.48
3:G:2236:LYS:N	3:G:2304:ARG:HG3	2.29	0.48
1:E:73:GLU:HB2	1:E:80:TYR:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:GLU:OE2	2:F:139:TYR:CE2	2.66	0.47
1:E:4:LEU:O	1:E:107:GLY:HA2	2.14	0.47
2:F:129:ALA:HB3	2:F:180:LEU:O	2.14	0.47
3:M:2236:LYS:O	3:M:2304:ARG:HG3	2.15	0.47
1:E:190:THR:O	1:E:194:GLN:HB2	2.15	0.47
2:F:209:ASN:C	2:F:211:ASN:N	2.73	0.47
3:G:2254:SER:HB2	3:G:2289:SER:HB3	1.97	0.47
3:G:2313:TRP:CD1	3:G:2315:HIS:O	2.68	0.46
1:A:174:GLN:HA	1:A:175:SER:HA	1.69	0.46
3:M:2234:PHE:HZ	3:M:2323:VAL:HG11	1.80	0.46
3:M:2235:GLN:HA	3:M:2304:ARG:HE	1.79	0.46
2:B:189:ASN:O	2:B:209:ASN:HA	2.16	0.46
3:G:2261:LEU:HB3	3:G:2273:LEU:HD21	1.98	0.46
3:M:2258:LYS:NZ	5:M:2505:HOH:O	2.48	0.46
1:E:175:SER:N	1:E:176:ASP:OD2	2.37	0.46
1:A:27:TYR:O	1:A:27:TYR:CG	2.69	0.45
1:A:130:VAL:HG12	2:B:213:CYS:HB3	1.98	0.45
1:E:47:TRP:CD2	2:F:95:LEU:HB3	2.51	0.45
1:E:47:TRP:CD1	2:F:95:LEU:HD22	2.51	0.45
1:E:127:LEU:HD11	2:F:132:VAL:HG11	1.97	0.45
3:G:2263:SER:HB2	3:G:2271:TRP:HE3	1.81	0.45
1:E:19:LYS:HD2	1:E:82:GLN:HB2	1.99	0.45
2:F:208:PHE:C	2:F:208:PHE:HD1	2.24	0.45
2:F:186:GLU:CB	2:F:210:ARG:HH21	2.29	0.45
2:F:194:GLU:CA	2:F:205:VAL:HG12	2.42	0.45
2:F:135:LEU:HD12	2:F:135:LEU:H	1.80	0.45
1:A:26:ASP:O	1:A:77:ARG:HD2	2.18	0.44
3:G:2225:ASN:HA	3:G:2226:PRO:HD3	1.79	0.44
2:F:148:LYS:HB2	2:F:192:THR:HB	1.98	0.44
2:F:143:ILE:CD1	2:F:197:HIS:CE1	2.80	0.44
1:E:151:GLU:HA	1:E:152:PRO:HA	1.70	0.44
2:F:8:PRO:CD	2:F:11:MET:HE3	2.48	0.44
1:A:122:PRO:HB3	1:A:148:TYR:HB3	2.00	0.43
1:A:190:THR:HG23	1:A:194:GLN:HG3	2.00	0.43
1:E:34:LEU:HD21	5:E:303:HOH:O	2.15	0.43
1:A:214:GLU:HG3	1:A:215:PRO:HD2	1.99	0.43
2:F:160:ASN:HB3	2:F:174:MET:HE3	2.00	0.43
2:F:166:ASP:C	2:F:168:LYS:N	2.72	0.43
1:E:3:GLN:H	1:E:25:SER:HB3	1.83	0.43
1:E:122:PRO:HB3	1:E:148:TYR:HB3	2.01	0.43
3:G:2203:TRP:HE3	3:G:2218:ALA:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:2198:ASN:OD1	3:M:2198:ASN:C	2.61	0.43
1:E:127:LEU:O	2:F:117:PHE:CE2	2.72	0.43
2:B:145:VAL:O	2:B:146:LYS:NZ	2.32	0.43
2:F:211:ASN:ND2	2:F:212:GLU:HB3	2.33	0.43
3:G:2290:PHE:N	3:G:2290:PHE:CD2	2.86	0.43
2:B:76:ARG:NH2	2:F:53:LEU:HD13	2.34	0.43
2:F:60:ARG:HD2	2:F:76:ARG:O	2.19	0.43
2:F:122:GLU:O	2:F:123:GLN:C	2.59	0.43
3:M:2207:LYS:NZ	3:M:2216:SER:HB2	2.34	0.42
1:E:104:ALA:HA	2:F:45:PHE:CD2	2.54	0.42
2:F:181:THR:OG1	2:F:184:GLU:HG2	2.18	0.42
3:G:2283:PHE:HD2	3:G:2295:ASN:CG	2.27	0.42
2:B:12:SER:HA	2:B:104:GLU:O	2.19	0.42
1:E:194:GLN:NE2	1:E:194:GLN:CA	2.72	0.42
1:A:148:TYR:CE2	1:A:153:VAL:HG13	2.54	0.42
2:F:194:GLU:C	2:F:205:VAL:HG12	2.41	0.42
1:A:103:LEU:HB2	2:B:35:TYR:OH	2.19	0.42
2:B:212:GLU:HB3	2:B:213:CYS:H	1.72	0.42
2:B:124:LEU:O	2:B:182:LYS:HD2	2.19	0.41
3:G:2275:PHE:HB2	3:G:2279:LYS:O	2.20	0.41
3:M:2266:GLN:NE2	3:M:2303:THR:HA	2.35	0.41
2:F:110:ALA:O	2:F:197:HIS:NE2	2.42	0.41
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.91	0.41
3:M:2255:MET:HG2	3:M:2316:GLN:HB2	2.02	0.41
1:E:174:GLN:N	1:E:175:SER:HA	2.34	0.41
1:E:194:GLN:HA	1:E:194:GLN:HE21	1.78	0.41
2:F:7:SER:HA	2:F:8:PRO:HA	1.76	0.41
3:M:2234:PHE:CZ	3:M:2323:VAL:HG11	2.55	0.41
1:E:20:ILE:HG12	1:E:110:THR:HG21	2.02	0.41
1:E:155:LEU:HA	1:E:199:ASN:O	2.21	0.41
1:E:56:GLY:HA2	1:E:72:LEU:CD1	2.51	0.41
2:F:174:MET:HG3	2:F:175:SER:N	2.36	0.41
2:B:144:ASN:HD22	2:B:196:THR:HB	1.86	0.40
2:B:124:LEU:C	2:B:126:SER:N	2.79	0.40
3:G:2203:TRP:CH2	3:G:2216:SER:HA	2.55	0.40
1:E:141:LEU:HD22	1:E:213:ILE:HG21	2.03	0.40
1:E:157:TRP:CZ3	1:E:198:CYS:HB3	2.56	0.40
3:G:2198:ASN:HB2	3:G:2199:MET:H	1.79	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:438:HOH:O	5:M:2526:HOH:O[1_455]	2.15	0.05

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	146/219 (67%)	133 (91%)	12 (8%)	1 (1%)	18	35
1	E	204/219 (93%)	188 (92%)	15 (7%)	1 (0%)	24	44
2	B	211/213 (99%)	203 (96%)	6 (3%)	2 (1%)	14	28
2	F	187/213 (88%)	166 (89%)	17 (9%)	4 (2%)	5	10
3	G	152/154 (99%)	128 (84%)	23 (15%)	1 (1%)	18	35
3	M	152/154 (99%)	140 (92%)	12 (8%)	0	100	100
All	All	1052/1172 (90%)	958 (91%)	85 (8%)	9 (1%)	14	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	205	VAL
2	F	142	ASP
2	F	143	ILE
2	B	212	GLU
2	B	125	THR
2	F	109	ASP
3	G	2310	PRO
1	A	41	PRO
1	E	152	PRO

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	79/186 (42%)	77 (98%)	2 (2%)	42 68
1	E	178/186 (96%)	168 (94%)	10 (6%)	19 39
2	B	188/188 (100%)	171 (91%)	17 (9%)	9 18
2	F	171/188 (91%)	150 (88%)	21 (12%)	4 9
3	G	139/139 (100%)	128 (92%)	11 (8%)	11 24
3	M	139/139 (100%)	132 (95%)	7 (5%)	22 44
All	All	894/1026 (87%)	826 (92%)	68 (8%)	12 26

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	THR
1	A	193	SER
2	B	27	SER
2	B	55	SER
2	B	90	TRP
2	B	91	SER
2	B	105	LEU
2	B	106	LYS
2	B	115	SER
2	B	126	SER
2	B	142	ASP
2	B	150	ASP
2	B	184	GLU
2	B	198	SER
2	B	199	THR
2	B	204	ILE
2	B	205	VAL
2	B	210	ARG
2	B	213	CYS
3	M	2213	GLN
3	M	2237	THR
3	M	2252	LEU
3	M	2270	GLN
3	M	2287	GLN
3	M	2302	LEU
3	M	2308	ILE
1	E	28	THR

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Mol	Chain	Res	Type
1	E	55	THR
1	E	72	LEU
1	E	84	ASN
1	E	103	LEU
1	E	123	SER
1	E	175	SER
1	E	176	ASP
1	E	180	LEU
1	E	194	GLN
2	F	1	GLN
2	F	10	ILE
2	F	75	SER
2	F	77	ILE
2	F	90	TRP
2	F	92	SER
2	F	106	LYS
2	F	118	PRO
2	F	119	PRO
2	F	141	LYS
2	F	143	ILE
2	F	146	LYS
2	F	168	LYS
2	F	169	ASP
2	F	192	THR
2	F	196	THR
2	F	197	HIS
2	F	204	ILE
2	F	206	LYS
2	F	207	SER
2	F	208	PHE
3	G	2176	MET
3	G	2199	MET
3	G	2202	THR
3	G	2207	LYS
3	G	2252	LEU
3	G	2263	SER
3	G	2273	LEU
3	G	2276	GLN
3	G	2298	ASP
3	G	2302	LEU
3	G	2316	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
3	M	2276	GLN
1	E	39	GLN
1	E	167	HIS
1	E	194	GLN
2	F	37	GLN
2	F	136	ASN
3	G	2222	GLN
3	G	2269	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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	213/219 (97%)	-0.41	0 100 100	25, 33, 55, 79	0
1	E	208/219 (94%)	0.46	27 (12%) 7 6	31, 47, 96, 114	0
2	B	213/213 (100%)	-0.23	3 (1%) 73 70	25, 37, 71, 97	0
2	F	195/213 (91%)	0.70	42 (21%) 2 2	30, 50, 130, 163	0
3	G	154/154 (100%)	0.16	2 (1%) 75 71	38, 56, 74, 84	0
3	M	154/154 (100%)	-0.33	0 100 100	25, 38, 60, 72	0
All	All	1137/1172 (97%)	0.06	74 (6%) 25 20	25, 42, 99, 163	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	129	PRO	5.4
2	F	204	ILE	5.4
1	E	193	SER	4.9
2	F	133	CYS	4.5
1	E	213	ILE	4.2
2	F	206	LYS	4.1
2	F	135	LEU	4.0
2	F	207	SER	3.8
2	F	148	LYS	3.8
2	F	113	THR	3.6
1	E	143	CYS	3.4
1	E	127	LEU	3.4
2	F	208	PHE	3.4
2	F	112	PRO	3.4
2	F	116	ILE	3.3
2	F	156	ASN	3.3
1	E	144	LEU	3.2
2	F	178	LEU	3.2
2	F	197	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	192	PRO	3.0
2	F	131	VAL	3.0
2	F	114	VAL	2.9
1	E	187	THR	2.8
2	F	139	TYR	2.8
2	F	180	LEU	2.8
1	E	191	TRP	2.7
2	F	137	ASN	2.7
2	F	111	ALA	2.7
1	E	20	ILE	2.7
2	F	155	GLN	2.7
1	E	141	LEU	2.7
2	B	211	ASN	2.7
2	F	192	THR	2.6
1	E	196	ILE	2.6
2	B	208	PHE	2.6
2	F	157	GLY	2.6
1	E	209	VAL	2.6
2	F	118	PRO	2.6
2	F	210	ARG	2.5
1	E	172	VAL	2.5
2	F	147	TRP	2.5
2	F	159	LEU	2.5
2	F	115	SER	2.5
2	F	138	PHE	2.5
1	E	174	GLN	2.5
2	F	132	VAL	2.5
2	F	145	VAL	2.5
2	F	212	GLU	2.4
2	F	205	VAL	2.4
2	F	162	TRP	2.4
1	E	212	LYS	2.4
1	E	200	VAL	2.4
2	F	143	ILE	2.4
2	F	179	THR	2.4
2	F	120	SER	2.4
1	E	211	LYS	2.4
1	E	186	VAL	2.4
1	E	162	LEU	2.3
1	E	175	SER	2.3
1	E	190	THR	2.2
2	F	185	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	125	TYR	2.2
1	E	184	VAL	2.2
2	F	193	CYS	2.2
1	E	215	PRO	2.2
2	F	158	VAL	2.1
1	E	194	GLN	2.1
2	B	213	CYS	2.1
2	F	122	GLU	2.1
2	F	125	THR	2.1
2	F	119	PRO	2.1
1	E	197	THR	2.0
3	G	2270	GLN	2.0
3	G	2299	PRO	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, 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	MG	A	301	1/1	0.64	0.13	75,75,75,75	0
4	MG	F	301	1/1	0.77	0.12	96,96,96,96	0
4	MG	M	2401	1/1	0.94	0.21	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.