Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:06 PM GMT

PDB ID	:	4KK8
Title	:	Structure of the E148Q mutant of CLC-ec1 deltaNC construct in 100mM fluoride
Authors	:	Lim, H.-H.; Miller, C.
Deposited on	:	2013-05-05
Resolution	:	2.86 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

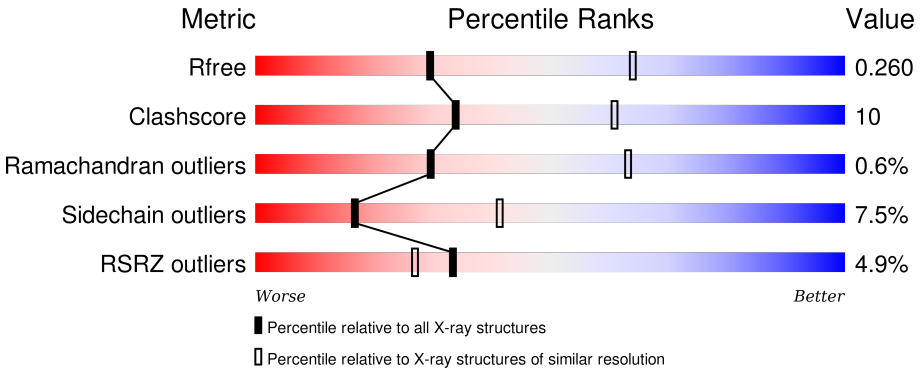
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.86 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 <=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	446	2% 72% 23%
1	B	446	3% 71% 24%
2	C	222	7% 77% 21%
2	E	222	7% 75% 22%
3	D	211	9% 69% 29%

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Mol	Chain	Length	Quality of chain
3	F	211	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13227 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3315	2180	558	557	20			
1	B	443	Total	C	N	O	S	0	0	0
			3324	2185	559	560	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	EXPRESSION TAG	UNP P37019
A	148	GLN	GLU	ENGINEERED MUTATION	UNP P37019
A	461	LYS	-	EXPRESSION TAG	UNP P37019
B	16	MET	-	EXPRESSION TAG	UNP P37019
B	148	GLN	GLU	ENGINEERED MUTATION	UNP P37019
B	461	LYS	-	EXPRESSION TAG	UNP P37019

- Molecule 2 is a protein called Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is FLUORIDE ION (three-letter code: F) (formula: F).

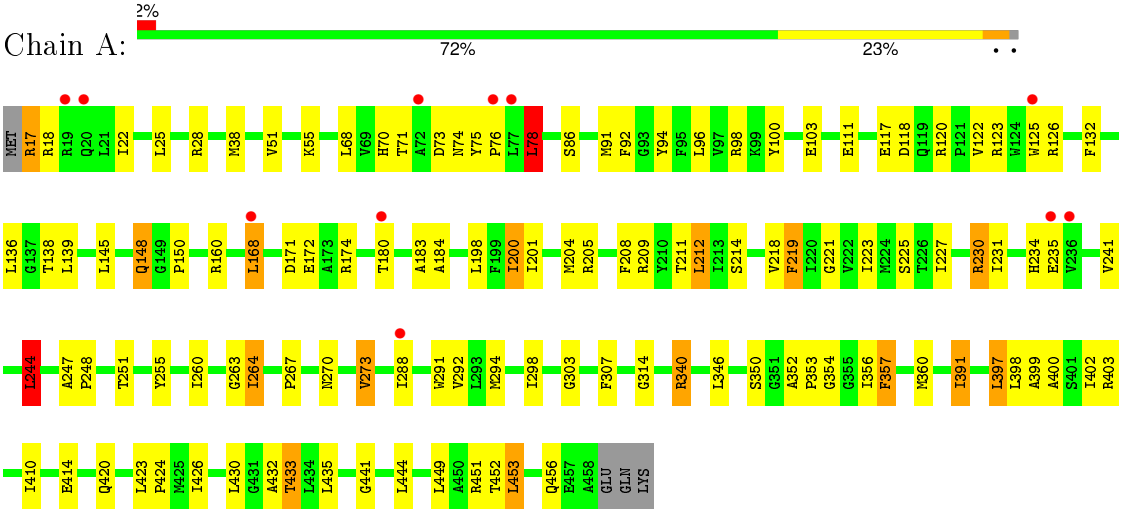
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total F 1 1	0	0
4	A	1	Total F 1 1	0	0

3 Residue-property plots (i)

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.

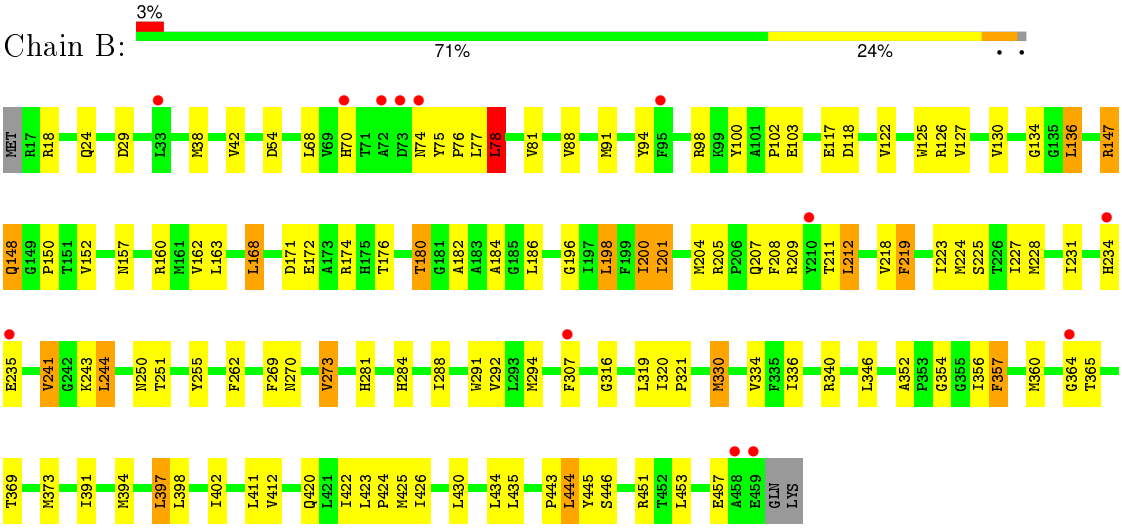
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



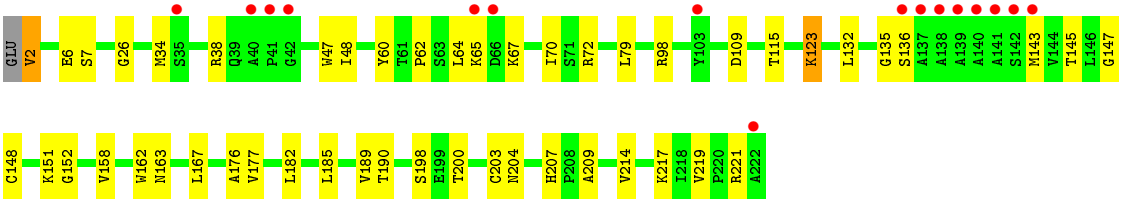
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:

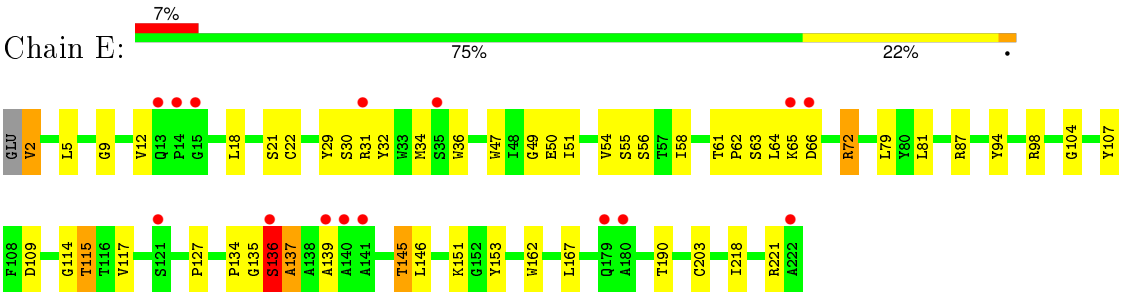


- Molecule 2: Fab, heavy chain

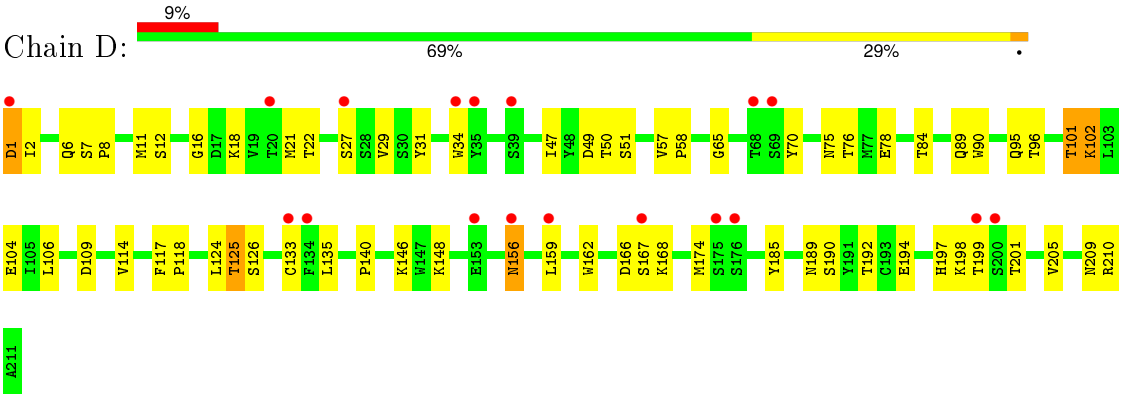
Chain C:



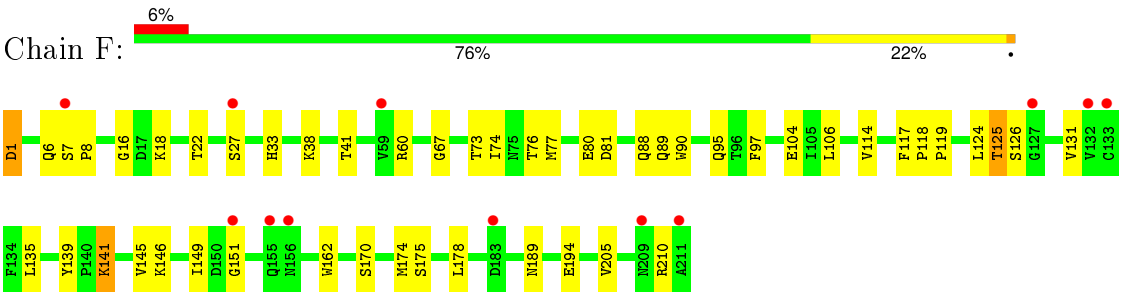
• Molecule 2: Fab, heavy chain



• Molecule 3: Fab, light chain



• Molecule 3: Fab, light chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.23Å 98.90Å 170.02Å 90.00° 131.77° 90.00°	Depositor
Resolution (Å)	24.95 – 2.86 24.95 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.95-2.86) 99.0 (24.95-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.210 , 0.256 0.222 , 0.260	Depositor DCC
R_{free} test set	3326 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.8	EDS
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 65741 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13227	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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, 0.375 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: F

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	0.41	0/3387	0.57	2/4597 (0.0%)
1	B	0.42	0/3396	0.58	1/4609 (0.0%)
2	C	0.49	0/1721	0.63	0/2355
2	E	0.44	0/1721	0.59	0/2355
3	D	0.43	0/1660	0.59	0/2257
3	F	0.43	0/1660	0.60	0/2257
All	All	0.43	0/13545	0.59	3/18430 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	78	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	78	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	244	LEU	CA-CB-CG	5.27	127.42	115.30

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	3315	0	3472	78	0
1	B	3324	0	3478	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1672	0	1654	25	0
2	E	1672	0	1654	31	0
3	D	1621	0	1546	42	0
3	F	1621	0	1546	31	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
All	All	13227	0	13350	267	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 10.

All (267) 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)
3:F:95:GLN:N	3:F:95:GLN:OE1	2.06	0.88
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.60	0.82
3:D:95:GLN:N	3:D:95:GLN:OE1	2.12	0.79
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.48	0.78
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.67	0.77
1:A:183:ALA:HB2	1:A:200:ILE:HG12	1.67	0.76
2:E:136:SER:O	2:E:137:ALA:HB2	1.86	0.75
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.68	0.73
2:C:163:ASN:HD22	2:C:167:LEU:HD13	1.53	0.72
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.04	0.71
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.71	0.71
1:A:360:MET:HG2	1:A:397:LEU:HD13	1.72	0.71
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.72	0.70
2:E:136:SER:O	2:E:137:ALA:CB	2.39	0.70
3:F:1:ASP:OD2	3:F:1:ASP:N	2.25	0.69
3:F:38:LYS:NZ	3:F:80:GLU:O	2.25	0.69
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.29	0.68
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.26	0.68
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.76	0.67
1:B:98:ARG:HH21	1:B:102:PRO:HB3	1.58	0.67
3:D:1:ASP:N	3:D:1:ASP:OD2	2.18	0.67
3:F:38:LYS:O	3:F:41:THR:HG22	1.95	0.66
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.77	0.65
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.78	0.65
1:A:100:TYR:O	1:A:126:ARG:NH1	2.28	0.65
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.80	0.64
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.29	0.62
2:E:9:GLY:H	2:E:115:THR:HG21	1.65	0.62
1:B:198:LEU:HD13	1:B:201:ILE:HD11	1.82	0.61
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.82	0.60
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.34	0.60
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.36	0.60
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.36	0.60
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.17	0.59
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.83	0.59
2:E:61:THR:O	2:E:63:SER:N	2.35	0.59
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.38	0.59
3:D:89:GLN:O	3:D:95:GLN:HB2	2.03	0.59
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.85	0.59
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.85	0.58
3:D:12:SER:HA	3:D:104:GLU:O	2.02	0.58
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.86	0.58
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.86	0.58
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.84	0.58
1:B:422:ILE:HA	1:B:425:MET:HE3	1.85	0.58
2:E:145:THR:OG1	2:E:190:THR:OG1	2.20	0.57
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.86	0.57
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.86	0.57
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.39	0.57
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.40	0.56
1:B:320:ILE:HG23	1:B:365:THR:HG21	1.87	0.56
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.20	0.56
1:B:88:VAL:HA	1:B:91:MET:HE2	1.85	0.56
1:A:214:SER:O	1:A:218:VAL:HG23	2.05	0.56
1:B:176:THR:O	1:B:180:THR:HG23	2.05	0.56
1:B:212:LEU:H	1:B:212:LEU:HD12	1.71	0.56
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.70	0.56
1:B:180:THR:HA	1:B:218:VAL:HG13	1.89	0.55
3:D:21:MET:SD	3:D:101:THR:HG21	2.47	0.55
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.89	0.55
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.89	0.55
3:D:124:LEU:C	3:D:126:SER:H	2.11	0.54
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.43	0.54
1:B:360:MET:HG2	1:B:397:LEU:HD13	1.90	0.54
1:B:241:VAL:HG13	1:B:244:LEU:HD21	1.90	0.54
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.89	0.53
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.41	0.53
1:A:200:ILE:HA	1:A:204:MET:HB2	1.90	0.53
3:D:29:VAL:O	3:D:70:TYR:OH	2.20	0.53
3:D:185:TYR:CZ	3:D:210:ARG:HD3	2.44	0.53
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.90	0.53
1:A:212:LEU:HD12	1:A:212:LEU:H	1.73	0.53
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.90	0.53
2:E:135:GLY:O	2:E:137:ALA:N	2.42	0.53
1:B:148:GLN:CD	1:B:357:PHE:HB2	2.29	0.52
2:C:152:GLY:HA2	2:C:182:LEU:HB3	1.92	0.52
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.44	0.52
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.92	0.52
1:B:38:MET:O	1:B:42:VAL:HG23	2.10	0.52
1:A:172:GLU:HA	1:A:212:LEU:HD13	1.92	0.52
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.45	0.52
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.92	0.51
1:A:28:ARG:NE	1:B:207:GLN:HG3	2.24	0.51
1:A:227:ILE:O	1:A:231:ILE:HG12	2.11	0.51
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.93	0.51
1:B:118:ASP:OD1	1:B:174:ARG:NH2	2.35	0.51
3:D:49:ASP:O	3:D:51:SER:N	2.38	0.51
2:E:32:TYR:O	2:E:72:ARG:NH2	2.38	0.51
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.92	0.51
1:A:410:ILE:O	1:A:414:GLU:HG3	2.11	0.50
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.93	0.50
1:B:172:GLU:HG3	1:B:212:LEU:O	2.11	0.50
1:B:171:ASP:OD2	1:B:174:ARG:NH1	2.36	0.50
1:A:148:GLN:CD	1:A:357:PHE:HB2	2.32	0.50
1:B:130:VAL:O	1:B:134:GLY:N	2.34	0.50
3:D:101:THR:O	3:D:102:LYS:O	2.30	0.50
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.93	0.50
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.92	0.50
3:D:125:THR:HG22	3:D:125:THR:O	2.11	0.50
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.92	0.50
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.46	0.49
1:A:294:MET:O	1:A:298:ILE:HG13	2.12	0.49
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.92	0.49
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.81	0.49
1:B:68:LEU:HD22	1:B:78:LEU:HD22	1.94	0.49
3:D:109:ASP:HB3	3:D:199:THR:HG22	1.95	0.49
1:A:234:HIS:CD2	1:A:235:GLU:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.47	0.49
1:A:403:ARG:HE	1:A:433:THR:HG22	1.78	0.49
2:C:135:GLY:HA2	2:C:221:ARG:HD3	1.94	0.49
2:E:145:THR:HG22	3:F:117:PHE:HZ	1.77	0.48
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.95	0.48
3:F:145:VAL:HA	3:F:194:GLU:O	2.13	0.48
1:A:403:ARG:NH2	1:B:29:ASP:OD1	2.46	0.48
1:A:18:ARG:O	1:A:22:ILE:HG13	2.13	0.48
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.13	0.48
3:D:124:LEU:O	3:D:126:SER:N	2.47	0.48
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.96	0.48
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.47	0.48
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.39	0.48
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.82	0.48
1:B:269:PHE:O	1:B:273:VAL:HG12	2.14	0.48
3:D:6:GLN:HA	3:D:22:THR:O	2.13	0.48
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.49	0.47
1:A:68:LEU:HD13	1:A:307:PHE:CD1	2.49	0.47
1:B:91:MET:HG2	1:B:292:VAL:O	2.14	0.47
1:B:224:MET:O	1:B:228:MET:HG2	2.14	0.47
2:C:145:THR:HG22	3:D:117:PHE:HZ	1.79	0.47
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.50	0.47
3:F:88:GLN:HG3	3:F:97:PHE:CE1	2.49	0.47
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.49	0.47
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.95	0.47
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.95	0.47
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.49	0.47
1:B:234:HIS:HD1	1:B:234:HIS:H	1.62	0.47
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.96	0.47
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.96	0.47
2:E:47:TRP:HZ2	2:E:50:GLU:HG2	1.79	0.47
3:F:124:LEU:C	3:F:126:SER:H	2.18	0.47
1:B:54:ASP:OD1	1:B:147:ARG:NH2	2.44	0.47
1:A:139:LEU:CD2	1:A:145:LEU:HB2	2.45	0.47
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.50	0.46
1:B:227:ILE:O	1:B:231:ILE:HG12	2.15	0.46
3:D:166:ASP:OD1	3:D:167:SER:N	2.49	0.46
1:A:71:THR:O	1:A:78:LEU:HB2	2.16	0.46
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.75	0.46
2:C:143:MET:HB3	2:C:190:THR:CG2	2.45	0.46
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HD22	1:A:402:ILE:HD12	1.97	0.46
3:F:149:ILE:HD11	3:F:178:LEU:HD21	1.97	0.46
2:C:167:LEU:HD23	2:C:189:VAL:HG21	1.97	0.46
1:A:314:GLY:O	1:A:340:ARG:NH2	2.48	0.46
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.81	0.46
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.80	0.46
2:E:94:TYR:O	2:E:114:GLY:HA2	2.15	0.46
2:C:123:LYS:HB3	2:C:123:LYS:HE2	1.75	0.46
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.81	0.46
1:A:241:VAL:HG13	1:A:244:LEU:HD21	1.97	0.46
2:E:146:LEU:HD22	2:E:218:ILE:HG21	1.97	0.46
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.51	0.46
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.51	0.46
2:C:158:VAL:HG12	2:C:207:HIS:HB2	1.97	0.46
2:C:217:LYS:HE2	2:C:219:VAL:HG12	1.98	0.46
1:A:91:MET:HG2	1:A:292:VAL:O	2.17	0.45
1:A:132:PHE:O	1:A:136:LEU:HB2	2.16	0.45
1:B:316:GLY:O	1:B:319:LEU:HG	2.16	0.45
1:A:98:ARG:HB3	1:A:288:ILE:HG13	1.98	0.45
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.98	0.45
3:D:2:ILE:O	3:D:96:THR:HG21	2.16	0.45
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.98	0.45
1:A:74:ASN:OD1	1:A:76:PRO:HD2	2.16	0.45
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.20	0.45
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.98	0.44
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.98	0.44
1:A:356:ILE:O	1:A:360:MET:HE2	2.17	0.44
1:B:369:THR:O	1:B:373:MET:HG3	2.17	0.44
1:A:399:ALA:O	1:A:403:ARG:HA	2.17	0.44
3:F:6:GLN:HA	3:F:22:THR:O	2.17	0.44
3:D:167:SER:OG	3:D:168:LYS:HG3	2.17	0.44
2:C:6:GLU:OE1	2:C:6:GLU:N	2.50	0.44
1:B:98:ARG:HB3	1:B:288:ILE:HG13	1.99	0.44
2:E:134:PRO:HD3	2:E:146:LEU:HD23	2.00	0.44
2:E:2:VAL:HG11	2:E:98:ARG:HH22	1.83	0.44
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.47	0.44
1:A:92:PHE:O	1:A:96:LEU:HD23	2.17	0.44
1:B:402:ILE:HD13	1:B:445:TYR:CE1	2.52	0.44
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.99	0.44
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.17	0.44
1:B:394:MET:HE2	1:B:412:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.98	0.44
1:A:51:VAL:O	1:A:55:LYS:HG2	2.18	0.43
1:B:330:MET:O	1:B:334:VAL:HG23	2.17	0.43
1:B:100:TYR:O	1:B:126:ARG:NH1	2.45	0.43
2:E:22:CYS:HB3	2:E:79:LEU:HB3	2.00	0.43
3:F:106:LEU:HD23	3:F:139:TYR:OH	2.19	0.43
1:B:356:ILE:HG22	4:B:501:F:F	2.07	0.43
1:A:346:LEU:O	1:A:350:SER:HB3	2.17	0.43
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.00	0.43
3:D:18:LYS:HG3	3:D:75:ASN:HA	1.99	0.43
1:A:17:ARG:NH2	1:B:117:GLU:O	2.46	0.43
3:D:174:MET:HE2	3:D:174:MET:HB3	1.86	0.43
1:A:260:ILE:O	1:A:264:ILE:HG23	2.19	0.43
3:D:8:PRO:HB2	3:D:11:MET:HB3	2.01	0.43
1:B:234:HIS:CD2	1:B:235:GLU:HG2	2.54	0.42
1:A:73:ASP:OD1	1:A:73:ASP:N	2.37	0.42
2:C:7:SER:HA	2:C:115:THR:HG21	2.01	0.42
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.54	0.42
3:F:119:PRO:HD3	3:F:131:VAL:HG22	2.02	0.42
1:A:25:LEU:HD23	1:B:208:PHE:HE1	1.84	0.42
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.54	0.42
1:B:262:PHE:HZ	1:B:364:GLY:HA2	1.84	0.42
2:C:177:VAL:HG21	3:D:159:LEU:HD13	2.02	0.42
3:D:146:LYS:HB3	3:D:194:GLU:HB2	2.01	0.42
3:F:7:SER:HB3	3:F:22:THR:HB	2.02	0.42
3:D:156:ASN:N	3:D:156:ASN:OD1	2.52	0.42
2:C:38:ARG:HD3	2:C:48:ILE:HD11	2.01	0.42
1:A:357:PHE:O	1:A:360:MET:HB2	2.19	0.42
2:C:60:TYR:CE2	2:C:70:ILE:HG13	2.52	0.42
1:B:270:ASN:OD1	1:B:444:LEU:HG	2.19	0.42
3:F:162:TRP:NE1	3:F:174:MET:HG3	2.34	0.42
3:F:106:LEU:HA	3:F:139:TYR:OH	2.20	0.42
3:D:140:PRO:HD2	3:D:197:HIS:HE2	1.85	0.42
2:E:2:VAL:HG11	2:E:98:ARG:NH2	2.34	0.42
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.76	0.42
2:E:34:MET:HB3	2:E:79:LEU:HD22	2.01	0.42
1:A:270:ASN:O	1:A:273:VAL:HG13	2.20	0.42
2:C:176:ALA:HB2	2:C:185:LEU:HD23	2.01	0.41
3:F:141:LYS:HB2	3:F:141:LYS:HE2	1.88	0.41
3:D:57:VAL:HA	3:D:58:PRO:HD2	1.87	0.41
2:E:32:TYR:CE2	2:E:98:ARG:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:O	1:B:163:LEU:HB3	2.19	0.41
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.55	0.41
1:A:136:LEU:HA	1:A:136:LEU:HD12	1.86	0.41
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.55	0.41
1:B:152:VAL:HG13	1:B:182:ALA:HB1	2.02	0.41
1:B:294:MET:HE2	1:B:294:MET:HB3	1.80	0.41
1:A:180:THR:CG2	1:A:221:GLY:HA3	2.49	0.41
3:D:124:LEU:C	3:D:126:SER:N	2.73	0.41
3:F:189:ASN:HA	3:F:210:ARG:HG3	2.03	0.41
2:E:29:TYR:CE1	2:E:34:MET:HG3	2.55	0.41
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.56	0.41
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.56	0.41
1:A:267:PRO:HG3	1:A:441:GLY:HA3	2.03	0.41
1:A:139:LEU:HD21	1:A:145:LEU:HB2	2.02	0.41
2:C:132:LEU:HB2	2:C:147:GLY:HA3	2.03	0.41
2:E:51:ILE:HG13	2:E:58:ILE:HG12	2.02	0.41
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.21	0.41
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.86	0.41
1:A:449:LEU:HG	1:A:453:LEU:HD22	2.03	0.41
1:A:86:SER:OG	1:A:303:GLY:HA3	2.21	0.41
1:B:336:ILE:O	1:B:340:ARG:HG3	2.20	0.41
3:D:31:TYR:HA	3:D:50:THR:OG1	2.21	0.41
1:B:75:TYR:HB3	1:B:76:PRO:HD3	2.02	0.41
1:A:247:ALA:HA	1:A:248:PRO:HD3	1.96	0.41
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.55	0.40
1:B:422:ILE:HD12	1:B:425:MET:HE3	2.03	0.40
3:D:162:TRP:CG	3:D:174:MET:HG3	2.55	0.40
2:C:2:VAL:HA	2:C:26:GLY:HA3	2.02	0.40
3:D:189:ASN:O	3:D:209:ASN:HA	2.22	0.40
1:B:136:LEU:HA	1:B:136:LEU:HD12	1.73	0.40
3:F:95:GLN:CD	3:F:95:GLN:H	2.11	0.40
3:F:89:GLN:O	3:F:95:GLN:HB2	2.22	0.40
1:B:435:LEU:HD13	1:B:435:LEU:HA	1.80	0.40
3:D:84:THR:HA	3:D:102:LYS:HA	2.03	0.40
1:B:243:LYS:HB3	2:E:31:ARG:HH21	1.86	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	440/446 (99%)	415 (94%)	25 (6%)	0	100	100
1	B	441/446 (99%)	414 (94%)	27 (6%)	0	100	100
2	C	219/222 (99%)	202 (92%)	16 (7%)	1 (0%)	34	67
2	E	219/222 (99%)	201 (92%)	14 (6%)	4 (2%)	11	33
3	D	209/211 (99%)	190 (91%)	17 (8%)	2 (1%)	19	49
3	F	209/211 (99%)	192 (92%)	14 (7%)	3 (1%)	14	40
All	All	1737/1758 (99%)	1614 (93%)	113 (6%)	10 (1%)	30	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102	LYS
2	E	136	SER
2	E	137	ALA
3	D	125	THR
2	E	62	PRO
2	E	139	ALA
2	C	62	PRO
3	F	125	THR
3	F	67	GLY
3	F	151	GLY

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	333/337 (99%)	304 (91%)	29 (9%)	13	33
1	B	334/337 (99%)	305 (91%)	29 (9%)	13	33
2	C	181/182 (100%)	170 (94%)	11 (6%)	23	52
2	E	181/182 (100%)	165 (91%)	16 (9%)	12	33
3	D	185/185 (100%)	176 (95%)	9 (5%)	31	63
3	F	185/185 (100%)	174 (94%)	11 (6%)	24	54
All	All	1399/1408 (99%)	1294 (92%)	105 (8%)	17	41

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	70	HIS
1	A	78	LEU
1	A	103	GLU
1	A	148	GLN
1	A	168	LEU
1	A	171	ASP
1	A	200	ILE
1	A	201	ILE
1	A	205	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	230	ARG
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	273	VAL
1	A	340	ARG
1	A	357	PHE
1	A	391	ILE
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU
1	A	433	THR
1	A	444	LEU
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	70	HIS

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Mol	Chain	Res	Type
1	B	78	LEU
1	B	81	VAL
1	B	103	GLU
1	B	136	LEU
1	B	147	ARG
1	B	148	GLN
1	B	162	VAL
1	B	168	LEU
1	B	180	THR
1	B	198	LEU
1	B	200	ILE
1	B	201	ILE
1	B	205	ARG
1	B	211	THR
1	B	212	LEU
1	B	219	PHE
1	B	241	VAL
1	B	244	LEU
1	B	251	THR
1	B	273	VAL
1	B	330	MET
1	B	346	LEU
1	B	357	PHE
1	B	397	LEU
1	B	420	GLN
1	B	444	LEU
1	B	451	ARG
1	B	453	LEU
2	C	2	VAL
2	C	65	LYS
2	C	72	ARG
2	C	123	LYS
2	C	136	SER
2	C	148	CYS
2	C	151	LYS
2	C	198	SER
2	C	200	THR
2	C	204	ASN
2	C	214	VAL
3	D	1	ASP
3	D	27	SER
3	D	78	GLU

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Mol	Chain	Res	Type
3	D	101	THR
3	D	106	LEU
3	D	133	CYS
3	D	156	ASN
3	D	190	SER
3	D	201	THR
2	E	2	VAL
2	E	5	LEU
2	E	12	VAL
2	E	21	SER
2	E	30	SER
2	E	55	SER
2	E	64	LEU
2	E	65	LYS
2	E	66	ASP
2	E	72	ARG
2	E	87	ARG
2	E	115	THR
2	E	136	SER
2	E	145	THR
2	E	151	LYS
2	E	167	LEU
3	F	1	ASP
3	F	18	LYS
3	F	27	SER
3	F	73	THR
3	F	74	ILE
3	F	77	MET
3	F	104	GLU
3	F	125	THR
3	F	141	LYS
3	F	170	SER
3	F	175	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	B	157	ASN
2	C	163	ASN
3	D	36	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 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.

No monomer is involved in short contacts.

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^{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	442/446 (99%)	0.01	11 (2%)	61	56	44, 62, 90, 113	0
1	B	443/446 (99%)	0.01	13 (2%)	55	49	42, 63, 98, 130	0
2	C	221/222 (99%)	-0.06	16 (7%)	18	12	33, 58, 92, 117	0
2	E	221/222 (99%)	0.02	15 (6%)	20	14	37, 59, 88, 126	0
3	D	211/211 (100%)	0.23	18 (8%)	13	8	44, 68, 88, 93	0
3	F	211/211 (100%)	0.10	12 (5%)	27	21	38, 54, 99, 116	0
All	All	1749/1758 (99%)	0.04	85 (4%)	33	27	33, 61, 92, 130	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	GLU	5.3
2	C	65	LYS	4.9
2	E	136	SER	4.7
1	B	72	ALA	4.7
2	E	222	ALA	4.6
2	E	141	ALA	4.3
1	B	235	GLU	4.3
1	A	72	ALA	4.3
1	A	168	LEU	3.9
3	D	39	SER	3.8
1	B	73	ASP	3.7
2	E	139	ALA	3.7
1	B	459	GLU	3.7
2	E	140	ALA	3.5
3	D	27	SER	3.5
2	E	13	GLN	3.4
2	C	141	ALA	3.3
2	C	136	SER	3.3
3	F	183	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	15	GLY	3.3
3	F	156	ASN	3.3
3	F	127	GLY	3.3
2	C	140	ALA	3.2
2	E	65	LYS	3.2
2	C	42	GLY	3.1
1	A	77	LEU	3.1
3	D	35	TYR	3.0
2	C	41	PRO	3.0
3	F	133	CYS	3.0
2	E	66	ASP	3.0
3	F	211	ALA	3.0
2	E	179	GLN	3.0
3	F	155	GLN	2.9
1	A	76	PRO	2.9
2	C	103	TYR	2.8
3	D	167	SER	2.8
3	D	133	CYS	2.8
2	E	121	SER	2.8
3	D	68	THR	2.8
1	B	234	HIS	2.7
2	E	14	PRO	2.7
2	C	137	ALA	2.7
2	E	31	ARG	2.7
1	B	70	HIS	2.7
2	C	138	ALA	2.6
1	A	180	THR	2.5
3	F	59	VAL	2.5
3	F	132	VAL	2.5
3	F	151	GLY	2.5
1	B	33	LEU	2.4
1	A	236	VAL	2.4
2	C	143	MET	2.4
1	A	288	ILE	2.4
3	D	153	GLU	2.4
3	D	69	SER	2.4
2	E	180	ALA	2.3
3	D	34	TRP	2.3
3	D	156	ASN	2.3
2	C	139	ALA	2.3
3	D	159	LEU	2.3
2	E	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	1	ASP	2.3
3	D	199	THR	2.3
1	B	74	ASN	2.3
1	A	125	TRP	2.3
3	F	209	ASN	2.2
2	C	222	ALA	2.2
2	C	142	SER	2.2
3	D	200	SER	2.2
3	D	175	SER	2.2
1	A	19	ARG	2.2
3	F	7	SER	2.1
2	C	35	SER	2.1
3	F	27	SER	2.1
2	C	40	ALA	2.1
3	D	176	SER	2.1
1	B	364	GLY	2.0
3	D	134	PHE	2.0
2	C	66	ASP	2.0
3	D	20	THR	2.0
1	B	458	ALA	2.0
1	B	307	PHE	2.0
1	A	20	GLN	2.0
1	B	210	TYR	2.0
1	B	95	PHE	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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	F	A	501	1/1	0.91	0.16	-0.71	60,60,60,60	0
4	F	B	501	1/1	0.94	0.14	-0.79	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.