Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 07:40 PM EDT

PDB ID	:	5HD8
Title	:	Crystal structure of disulfide cross-linked D417C ClC-ec1
Authors	:	Mathews, I.I.; Khantwal, C.M.; Maduke, M.
Deposited on	:	2016-01-05
Resolution	:	3.15 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:

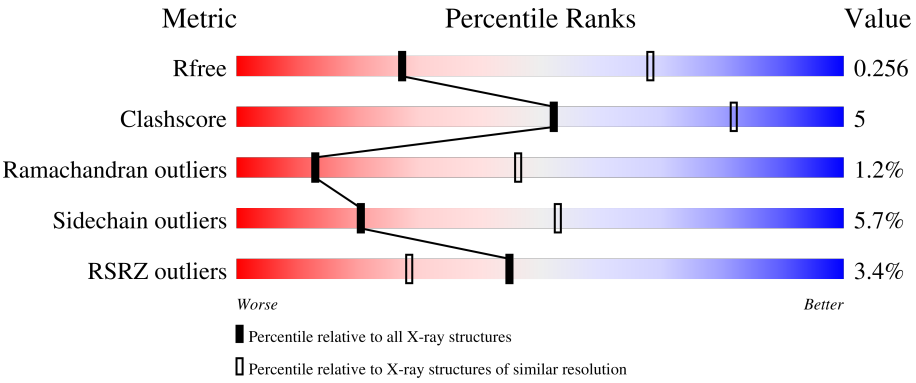
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	450	2% 79% 15%
1	B	450	4% 81% 14%
2	C	222	4% 81% 17%
2	E	222	84% 12%
3	D	211	6% 87% 11%

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Mol	Chain	Length	Quality of chain
3	F	211	4% 81% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	502	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13068 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	433	Total	C	N	O	S	0	0	0
			3248	2137	547	543	21			
1	B	432	Total	C	N	O	S	0	0	0
			3236	2131	542	542	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	initiating methionine	UNP P37019
A	417	CYS	ASP	engineered mutation	UNP P37019
B	16	MET	-	initiating methionine	UNP P37019
B	417	CYS	ASP	engineered mutation	UNP P37019

- Molecule 2 is a protein called FAB FRAGMENT (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	220	Total	C	N	O	S	0	0	0
			1666	1074	273	313	6			

- Molecule 3 is a protein called FAB FRAGMENT (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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

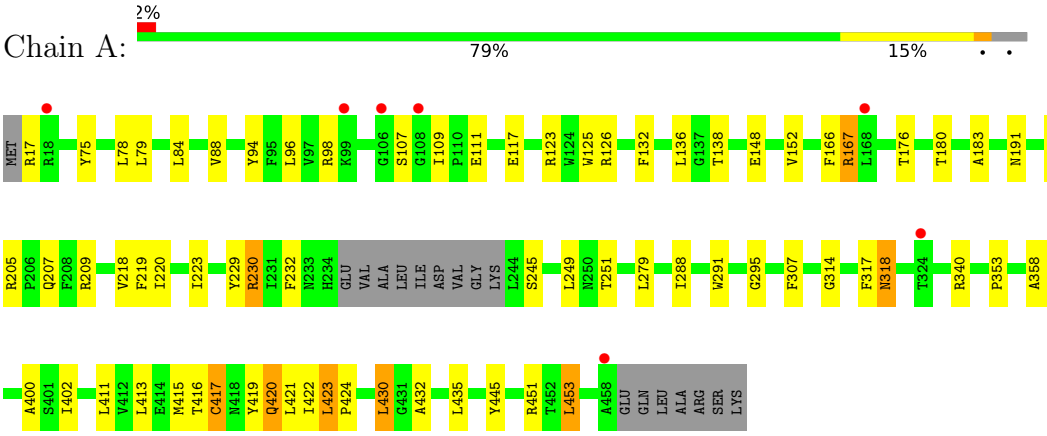
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	2	Total Cl 2 2	0	0

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.

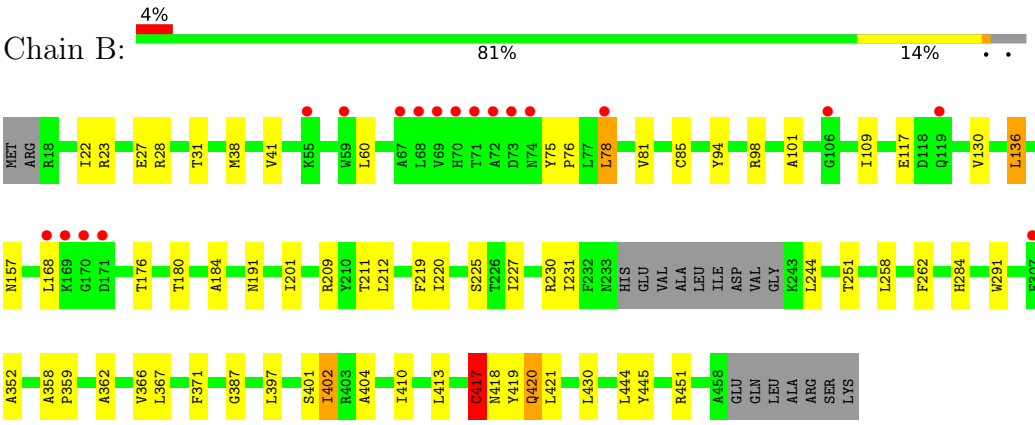
• Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



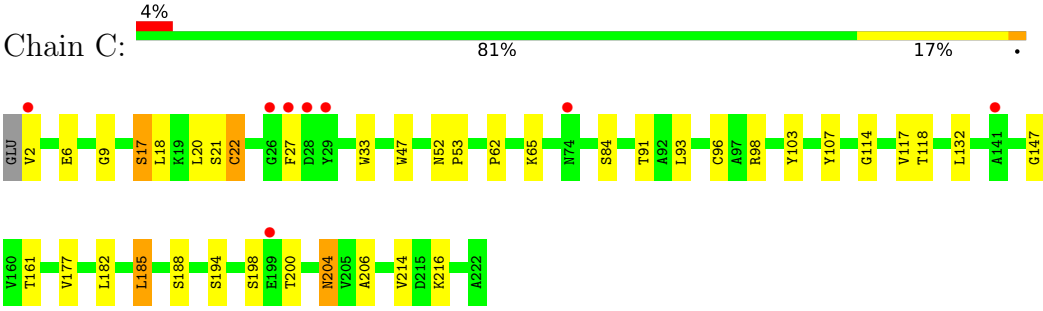
• Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:



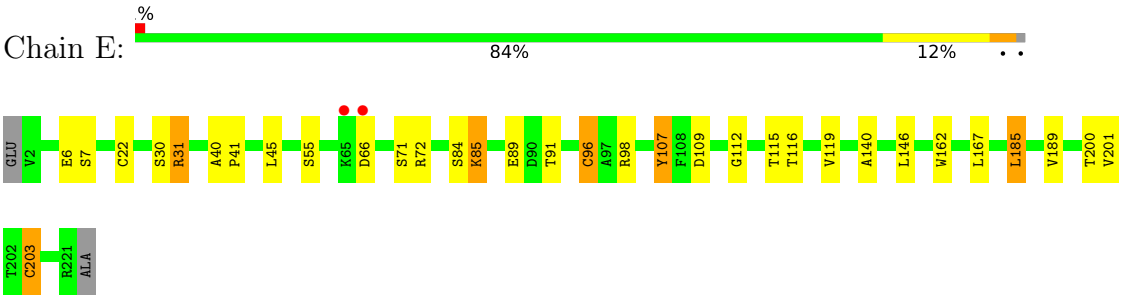
• Molecule 2: FAB FRAGMENT (HEAVY CHAIN)

Chain C:



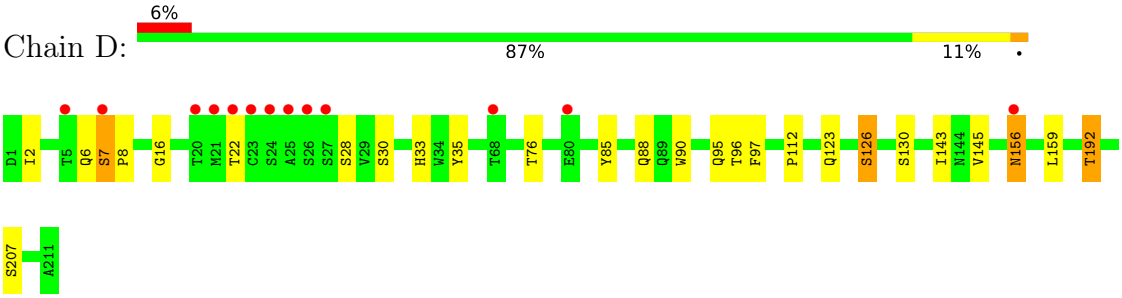
• Molecule 2: FAB FRAGMENT (HEAVY CHAIN)

Chain E:



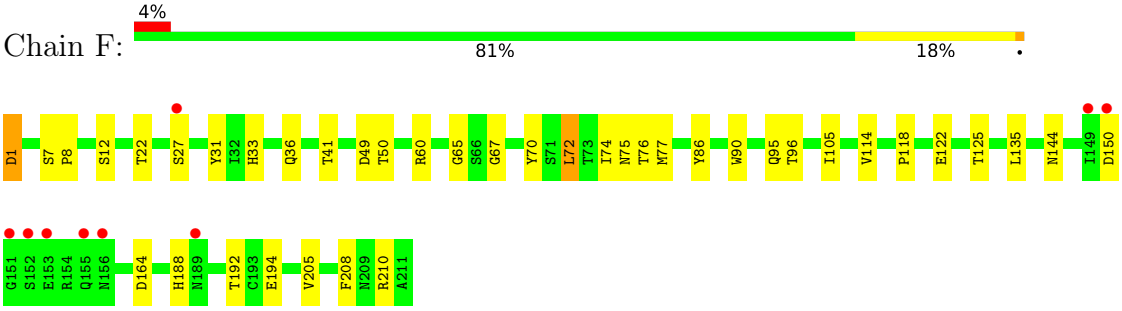
• Molecule 3: FAB FRAGMENT (LIGHT CHAIN)

Chain D:



• Molecule 3: FAB FRAGMENT (LIGHT CHAIN)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.74Å 96.06Å 169.95Å 90.00° 131.58° 90.00°	Depositor
Resolution (Å)	39.20 – 3.15 39.21 – 3.15	Depositor EDS
% Data completeness (in resolution range)	90.7 (39.20-3.15) 90.7 (39.21-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.205 , 0.257 0.203 , 0.256	Depositor DCC
R_{free} test set	2202 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	95.9	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13068	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: 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	0.37	0/3319	0.56	0/4503
1	B	0.37	0/3306	0.53	0/4485
2	C	0.38	0/1721	0.61	0/2355
2	E	0.41	0/1715	0.61	0/2348
3	D	0.35	0/1660	0.54	0/2257
3	F	0.42	0/1660	0.62	0/2257
All	All	0.38	0/13381	0.57	0/18205

There are no bond length outliers.

There are no bond angle outliers.

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	3248	0	3398	52	0
1	B	3236	0	3391	43	0
2	C	1672	0	1654	21	0
2	E	1666	0	1649	15	0
3	D	1621	0	1546	16	0
3	F	1621	0	1546	16	0
4	A	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	1	0
All	All	13068	0	13184	143	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 (143) 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	2.09	0.86
3:D:95:GLN:OE1	3:D:95:GLN:N	2.20	0.73
1:A:413:LEU:HD22	1:A:422:ILE:HD11	1.72	0.71
2:C:17:SER:HB3	2:C:84:SER:HA	1.73	0.69
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.29	0.65
3:F:31:TYR:HA	3:F:50:THR:OG1	1.97	0.65
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.33	0.64
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.80	0.62
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.81	0.61
1:A:249:LEU:HD13	1:B:231:ILE:HD13	1.83	0.60
2:C:93:LEU:HD11	2:C:114:GLY:HA3	1.83	0.60
2:C:177:VAL:HG21	3:D:159:LEU:HD13	1.84	0.59
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.86	0.57
1:B:262:PHE:CE1	1:B:367:LEU:HD23	2.39	0.57
1:A:416:THR:O	1:A:417:CYS:C	2.43	0.57
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.86	0.56
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.40	0.56
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.87	0.56
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.87	0.56
1:A:419:TYR:HB2	1:B:417:CYS:HB2	1.88	0.56
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.36	0.56
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.41	0.56
1:A:183:ALA:HB2	1:A:200:ILE:HD13	1.88	0.55
3:F:1:ASP:OD1	3:F:1:ASP:N	2.35	0.55
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.41	0.55
1:A:148:GLU:H	1:A:148:GLU:CD	2.09	0.54
1:A:180:THR:HG22	1:A:218:VAL:HA	1.90	0.54
1:A:430:LEU:HD11	1:B:220:ILE:HG13	1.90	0.53
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.90	0.53
1:B:362:ALA:O	1:B:366:VAL:HG23	2.09	0.53
2:E:30:SER:O	2:E:31:ARG:HB2	2.09	0.52
1:B:176:THR:O	1:B:180:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:189:VAL:O	2:E:189:VAL:HG13	2.10	0.52
1:B:148:GLU:H	1:B:148:GLU:CD	2.13	0.51
3:D:88:GLN:HB2	3:D:97:PHE:CD2	2.46	0.51
1:B:60:LEU:HD12	1:B:136:LEU:HD12	1.93	0.51
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.93	0.51
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.46	0.50
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.44	0.50
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.94	0.50
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.93	0.50
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.94	0.50
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.94	0.50
1:B:23:ARG:O	1:B:27:GLU:HG2	2.11	0.49
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.27	0.49
1:A:430:LEU:HD11	1:B:220:ILE:CG1	2.42	0.49
3:D:192:THR:HB	3:D:207:SER:HB3	1.95	0.49
1:A:419:TYR:HB2	1:B:417:CYS:CB	2.43	0.48
2:C:194:SER:O	2:C:198:SER:OG	2.30	0.48
1:A:249:LEU:HD21	1:B:230:ARG:HB3	1.95	0.48
3:F:72:LEU:C	3:F:72:LEU:HD23	2.33	0.48
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.96	0.48
2:C:2:VAL:HG12	2:C:27:PHE:CD1	2.49	0.47
2:E:30:SER:O	2:E:31:ARG:CB	2.62	0.47
1:B:284:HIS:CE1	1:B:291:TRP:CE3	3.02	0.47
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.94	0.47
1:A:107:SER:N	4:A:502:CL:CL	2.82	0.47
1:A:423:LEU:HB3	1:A:424:PRO:CD	2.45	0.47
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.96	0.47
3:F:188:HIS:O	3:F:210:ARG:NE	2.47	0.47
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.82	0.46
1:A:109:ILE:HG12	1:A:152:VAL:HG11	1.98	0.46
1:A:402:ILE:HD12	1:A:445:TYR:CE2	2.50	0.46
1:A:411:LEU:HG	1:A:415:MET:HE2	1.97	0.46
1:B:109:ILE:HG12	1:B:152:VAL:HG11	1.96	0.46
2:E:6:GLU:HA	2:E:22:CYS:HA	1.96	0.46
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.97	0.46
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.47	0.46
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.96	0.46
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.97	0.46
1:A:148:GLU:OE2	1:A:358:ALA:HB2	2.15	0.46
1:A:94:TYR:CE1	1:A:295:GLY:HA3	2.51	0.46
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD13	1:B:219:PHE:HB3	1.98	0.45
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.51	0.45
1:A:176:THR:O	1:A:180:THR:HG23	2.16	0.45
1:A:183:ALA:HB2	1:A:200:ILE:CD1	2.45	0.45
1:A:249:LEU:HD12	2:C:103:TYR:CD1	2.51	0.45
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.51	0.45
1:A:84:LEU:O	1:A:88:VAL:HG23	2.17	0.45
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.82	0.45
1:A:200:ILE:HG22	1:A:201:ILE:HG23	1.98	0.45
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.99	0.45
2:E:185:LEU:C	2:E:185:LEU:HD12	2.37	0.45
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.51	0.44
1:A:132:PHE:O	1:A:136:LEU:HB2	2.17	0.44
3:F:118:PRO:HB3	3:F:208:PHE:CE2	2.52	0.44
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.99	0.44
1:B:402:ILE:HD11	1:B:404:ALA:HB3	1.98	0.44
1:A:166:PHE:O	1:A:167:ARG:C	2.56	0.44
1:A:314:GLY:O	1:A:340:ARG:NH2	2.50	0.44
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.53	0.44
1:B:358:ALA:HB3	1:B:359:PRO:CD	2.48	0.44
1:B:445:TYR:OH	4:B:501:CL:CL	2.66	0.44
2:C:152:GLY:O	2:C:182:LEU:HD22	2.17	0.44
1:A:249:LEU:HD12	2:C:103:TYR:HD1	1.83	0.44
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.53	0.44
2:E:45:LEU:HD11	3:F:86:TYR:CD2	2.53	0.43
1:A:360:MET:HG2	1:A:397:LEU:HD13	2.00	0.43
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.86	0.43
1:A:232:PHE:CD1	1:A:232:PHE:N	2.87	0.43
3:D:6:GLN:HA	3:D:22:THR:O	2.18	0.43
2:C:6:GLU:HA	2:C:22:CYS:HA	1.99	0.43
2:E:40:ALA:HB1	2:E:41:PRO:HD2	2.01	0.42
1:A:453:LEU:HB3	1:B:22:ILE:HD11	2.00	0.42
1:B:413:LEU:O	1:B:417:CYS:HA	2.19	0.42
2:E:91:THR:HG1	2:E:119:VAL:H	1.65	0.42
1:A:419:TYR:O	1:A:421:LEU:N	2.52	0.42
1:A:279:LEU:HD23	1:A:279:LEU:O	2.19	0.42
2:C:161:THR:OG1	2:C:204:ASN:OD1	2.37	0.42
2:C:185:LEU:C	2:C:185:LEU:HD12	2.39	0.42
3:D:2:ILE:O	3:D:96:THR:HG21	2.20	0.42
2:E:6:GLU:OE1	2:E:96:CYS:N	2.48	0.42
3:F:60:ARG:HG3	3:F:74:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:MET:HE1	1:A:402:ILE:HD11	2.01	0.41
2:C:6:GLU:HA	2:C:21:SER:O	2.19	0.41
1:A:78:LEU:HD21	1:A:307:PHE:CE2	2.56	0.41
2:E:6:GLU:OE2	2:E:112:GLY:HA3	2.19	0.41
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.55	0.41
3:D:35:TYR:O	3:D:85:TYR:HA	2.19	0.41
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.55	0.41
1:B:157:ASN:HD22	1:B:157:ASN:N	2.19	0.41
2:C:159:THR:OG1	2:C:206:ALA:HB3	2.21	0.41
1:B:244:LEU:HD11	1:B:387:GLY:HA3	2.02	0.41
1:B:212:LEU:HD12	1:B:212:LEU:N	2.36	0.41
1:B:419:TYR:O	1:B:421:LEU:N	2.53	0.41
2:C:132:LEU:N	2:C:147:GLY:O	2.48	0.41
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.86	0.41
1:B:227:ILE:O	1:B:231:ILE:HG12	2.20	0.41
2:C:2:VAL:HG12	2:C:27:PHE:HD1	1.85	0.41
2:C:91:THR:HG23	2:C:118:THR:HA	2.02	0.41
3:D:156:ASN:OD1	3:D:156:ASN:N	2.54	0.41
1:A:107:SER:HB3	4:A:502:CL:CL	2.58	0.41
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.21	0.41
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.56	0.41
2:C:20:LEU:HD21	2:C:117:VAL:CG2	2.51	0.40
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.56	0.40
3:D:112:PRO:HG3	3:D:143:ILE:HD11	2.03	0.40
3:D:123:GLN:O	3:D:126:SER:HB2	2.21	0.40
3:F:77:MET:HE1	3:F:105:ILE:HD12	2.03	0.40
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.57	0.40
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.52	0.40
2:E:84:SER:O	2:E:85:LYS:C	2.60	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	429/450 (95%)	405 (94%)	18 (4%)	6 (1%)	11	43
1	B	428/450 (95%)	402 (94%)	24 (6%)	2 (0%)	29	65
2	C	219/222 (99%)	201 (92%)	15 (7%)	3 (1%)	11	43
2	E	218/222 (98%)	194 (89%)	21 (10%)	3 (1%)	11	43
3	D	209/211 (99%)	189 (90%)	18 (9%)	2 (1%)	15	51
3	F	209/211 (99%)	188 (90%)	17 (8%)	4 (2%)	8	36
All	All	1712/1766 (97%)	1579 (92%)	113 (7%)	20 (1%)	13	46

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
1	A	420	GLN
1	B	417	CYS
2	C	65	LYS
2	E	140	ALA
1	B	420	GLN
2	C	9	GLY
3	D	126	SER
2	E	31	ARG
1	A	318	ASN
1	A	417	CYS
2	C	62	PRO
1	A	202	GLU
3	F	49	ASP
3	F	76	THR
1	A	245	SER
2	E	85	LYS
3	F	150	ASP
3	D	7	SER
3	F	67	GLY

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	326/340 (96%)	310 (95%)	16 (5%)	25 59
1	B	325/340 (96%)	307 (94%)	18 (6%)	21 54
2	C	181/182 (100%)	170 (94%)	11 (6%)	18 50
2	E	181/182 (100%)	167 (92%)	14 (8%)	13 41
3	D	185/185 (100%)	179 (97%)	6 (3%)	39 70
3	F	185/185 (100%)	171 (92%)	14 (8%)	13 41
All	All	1383/1414 (98%)	1304 (94%)	79 (6%)	20 53

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	96	LEU
1	A	111	GLU
1	A	205	ARG
1	A	230	ARG
1	A	251	THR
1	A	288	ILE
1	A	317	PHE
1	A	318	ASN
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU
1	A	430	LEU
1	A	435	LEU
1	A	451	ARG
1	A	453	LEU
1	B	31	THR
1	B	41	VAL
1	B	78	LEU
1	B	85	CYS
1	B	136	LEU
1	B	201	ILE
1	B	211	THR
1	B	251	THR
1	B	319	LEU
1	B	397	LEU
1	B	401	SER
1	B	402	ILE
1	B	410	ILE
1	B	417	CYS

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Mol	Chain	Res	Type
1	B	418	ASN
1	B	420	GLN
1	B	444	LEU
1	B	451	ARG
2	C	17	SER
2	C	18	LEU
2	C	22	CYS
2	C	96	CYS
2	C	98	ARG
2	C	185	LEU
2	C	188	SER
2	C	200	THR
2	C	204	ASN
2	C	214	VAL
2	C	216	LYS
3	D	28	SER
3	D	30	SER
3	D	130	SER
3	D	145	VAL
3	D	156	ASN
3	D	192	THR
2	E	7	SER
2	E	55	SER
2	E	66	ASP
2	E	71	SER
2	E	72	ARG
2	E	89	GLU
2	E	96	CYS
2	E	107	TYR
2	E	115	THR
2	E	116	THR
2	E	167	LEU
2	E	185	LEU
2	E	200	THR
2	E	203	CYS
3	F	1	ASP
3	F	12	SER
3	F	22	THR
3	F	27	SER
3	F	36	GLN
3	F	41	THR
3	F	72	LEU

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Mol	Chain	Res	Type
3	F	75	ASN
3	F	96	THR
3	F	122	GLU
3	F	125	THR
3	F	144	ASN
3	F	164	ASP
3	F	192	THR

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

Mol	Chain	Res	Type
1	A	418	ASN
1	A	420	GLN
3	F	75	ASN
3	F	144	ASN

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 4 ligands modelled in this entry, 4 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	433/450 (96%)	-0.16	7 (1%) 72 59	77, 101, 140, 186	0
1	B	432/450 (96%)	-0.08	19 (4%) 34 20	81, 112, 155, 216	0
2	C	221/222 (99%)	-0.26	8 (3%) 42 26	64, 100, 145, 171	0
2	E	220/222 (99%)	-0.48	2 (0%) 84 75	67, 95, 139, 184	0
3	D	211/211 (100%)	-0.11	13 (6%) 20 11	79, 116, 148, 159	0
3	F	211/211 (100%)	-0.18	9 (4%) 35 21	59, 89, 141, 162	0
All	All	1728/1766 (97%)	-0.19	58 (3%) 45 28	59, 104, 147, 216	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	7	SER	4.5
3	F	153	GLU	4.5
1	B	70	HIS	4.5
3	F	155	GLN	4.1
1	B	73	ASP	3.8
1	B	71	THR	3.8
3	F	156	ASN	3.6
3	D	27	SER	3.4
1	B	67	ALA	3.2
1	B	170	GLY	3.1
1	B	69	VAL	3.1
1	B	171	ASP	3.1
3	D	23	CYS	3.1
3	D	26	SER	3.0
1	B	55	LYS	3.0
3	D	5	THR	2.9
3	D	20	THR	2.9
3	D	24	SER	2.9
3	D	21	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	2.8
3	F	152	SER	2.8
3	D	156	ASN	2.8
2	C	2	VAL	2.8
2	E	65	LYS	2.8
1	B	168	LEU	2.7
2	C	141	ALA	2.7
1	B	78	LEU	2.7
1	B	169	LYS	2.6
2	C	28	ASP	2.6
3	F	151	GLY	2.6
2	C	29	TYR	2.5
1	A	324	THR	2.5
1	A	99	LYS	2.5
2	C	27	PHE	2.5
1	B	307	PHE	2.4
3	D	22	THR	2.4
3	F	189	ASN	2.4
1	A	458	ALA	2.4
1	A	18	ARG	2.3
3	D	68	THR	2.3
2	C	199	GLU	2.3
1	B	74	ASN	2.3
2	E	66	ASP	2.2
2	C	26	GLY	2.2
3	F	27	SER	2.2
1	B	106	GLY	2.2
1	B	59	TRP	2.2
3	F	149	ILE	2.1
1	A	168	LEU	2.1
3	D	80	GLU	2.1
2	C	74	ASN	2.1
3	D	25	ALA	2.1
1	B	119	GLN	2.1
1	A	106	GLY	2.0
1	B	308	VAL	2.0
3	F	150	ASP	2.0
1	A	108	GLY	2.0
1	B	68	LEU	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	B	502	1/1	0.75	0.38	113,113,113,113	0
4	CL	A	502	1/1	0.87	0.67	140,140,140,140	0
4	CL	A	501	1/1	0.90	0.47	115,115,115,115	0
4	CL	B	501	1/1	0.94	0.21	104,104,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.