



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:32 AM UTC

PDB ID : 4LOU / pdb_00004lou
Title : Structure of the E148Q mutant of CLC-ec1 deltaNC construct in the absence of halide
Authors : Lim, H.-H.; Miller, C.
Deposited on : 2013-07-13
Resolution : 2.98 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

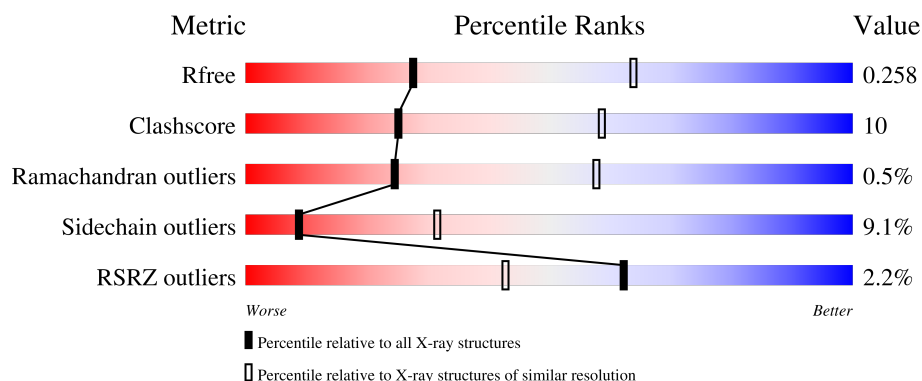
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 $\leq 5\%$. 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	3% 73% 23% .
1	B	446	% 66% 29% ..
2	C	222	3% 79% 19% .
2	E	222	4% 73% 23% .
3	D	211	2% 76% 21% ..

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Mol	Chain	Length	Quality of chain
3	F	211	2% 78% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13243 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	444	Total	C	N	O	S	0	0	0
			3333	2190	561	562	20			
1	B	442	Total	C	N	O	S	0	0	0
			3315	2180	558	557	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	initiating methionine	UNP P37019
A	148	GLN	GLU	engineered mutation	UNP P37019
A	461	LYS	-	expression tag	UNP P37019
B	16	MET	-	initiating methionine	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	222	Total	C	N	O	S	0	0	0
			1681	1082	275	318	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

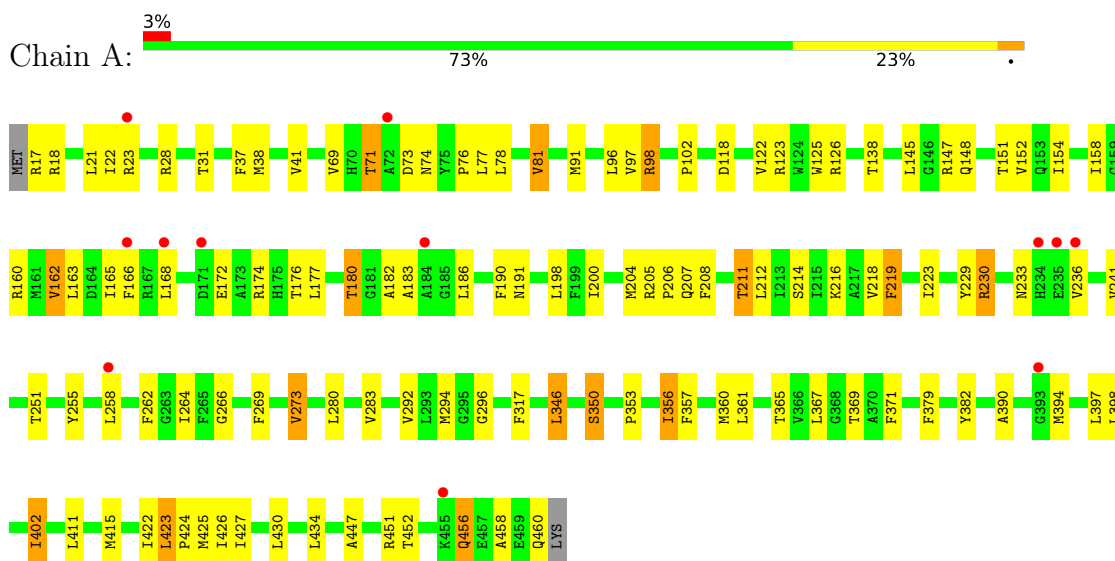
- Molecule 3 is a protein called Fab light chain.

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			

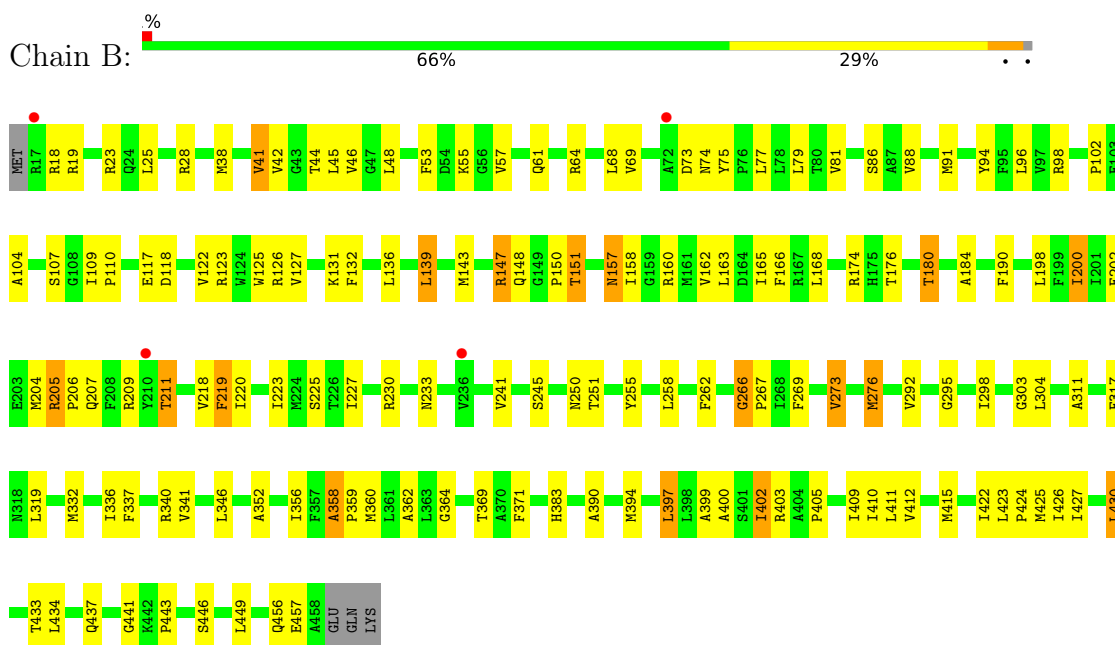
3 Residue-property plots

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.

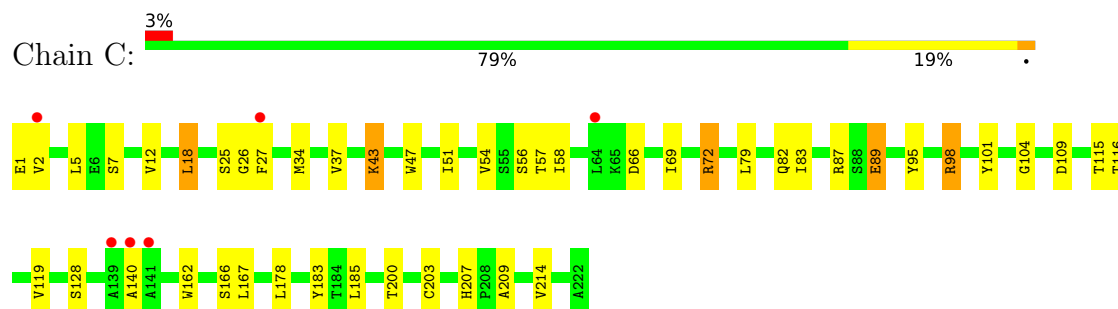
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



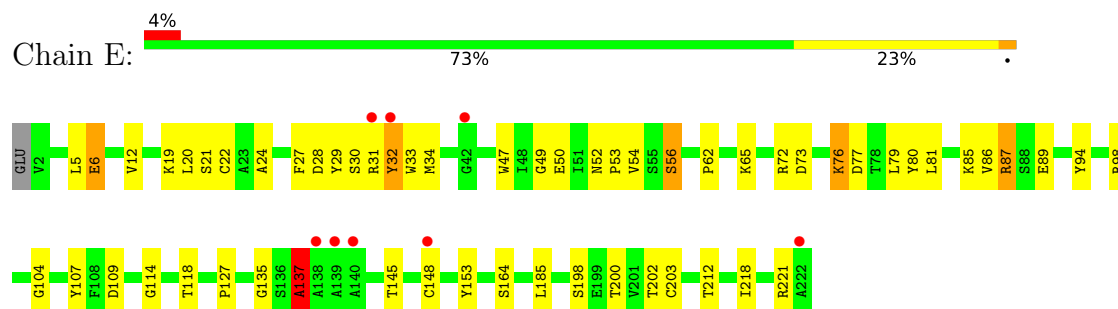
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA



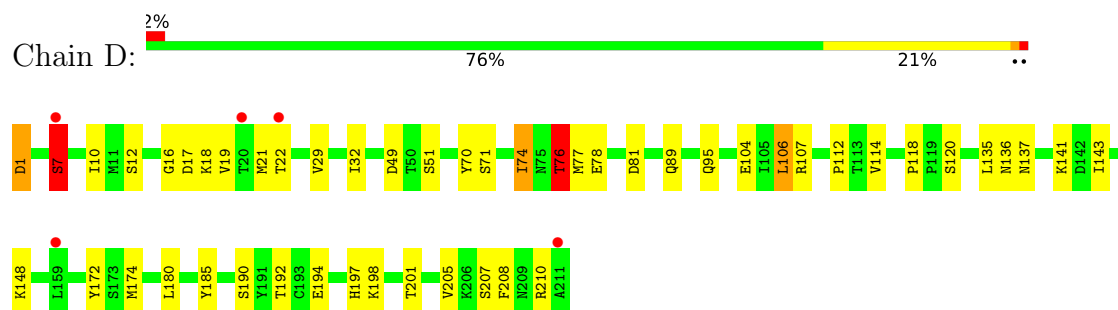
- Molecule 2: Fab heavy chain



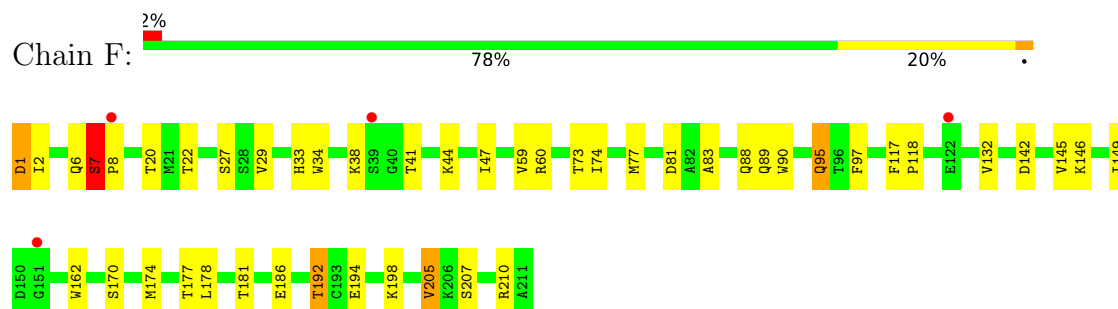
- Molecule 2: Fab heavy chain



- Molecule 3: Fab light chain



- Molecule 3: Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.62Å 100.32Å 170.96Å 90.00° 131.71° 90.00°	Depositor
Resolution (Å)	39.72 – 2.98 39.72 – 2.98	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.72-2.98) 98.2 (39.72-2.98)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.210 , 0.253 0.214 , 0.258	Depositor DCC
R_{free} test set	2981 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13243	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/3405	0.92	2/4621 (0.0%)
1	B	0.55	0/3387	0.95	4/4597 (0.1%)
2	C	0.61	0/1730	0.92	1/2367 (0.0%)
2	E	0.58	0/1721	0.92	2/2355 (0.1%)
3	D	0.58	0/1660	0.97	6/2257 (0.3%)
3	F	0.58	0/1660	0.87	1/2257 (0.0%)
All	All	0.57	0/13563	0.93	16/18454 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	GLN	CB-CA-C	10.87	132.90	110.40
1	B	266	GLY	CA-C-N	7.64	127.53	119.05
1	B	266	GLY	C-N-CA	7.64	127.53	119.05
3	D	7	SER	CA-C-N	-7.26	110.77	119.84
3	D	7	SER	C-N-CA	-7.26	110.77	119.84
2	E	32	TYR	N-CA-C	-6.81	97.15	108.32
3	D	136	ASN	N-CA-C	6.32	119.99	109.95
1	B	358	ALA	CA-C-N	-6.07	113.43	119.56
1	B	358	ALA	C-N-CA	-6.07	113.43	119.56
2	E	137	ALA	N-CA-C	-6.05	97.90	110.80
1	A	266	GLY	CA-C-N	6.01	126.44	119.47
1	A	266	GLY	C-N-CA	6.01	126.44	119.47
3	D	114	VAL	N-CA-C	5.39	116.00	108.89
3	D	74	ILE	N-CA-C	5.23	113.91	106.53
2	C	119	VAL	N-CA-C	5.11	114.84	106.72
3	D	137	ASN	N-CA-C	5.02	116.78	110.91

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	3333	0	3486	81	0
1	B	3315	0	3472	99	0
2	C	1681	0	1663	18	0
2	E	1672	0	1656	34	0
3	D	1621	0	1546	26	0
3	F	1621	0	1546	28	0
All	All	13243	0	13369	257	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 (257) 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:7:SER:HB2	3:F:8:PRO:CD	1.55	1.27
2:E:148:CYS:SG	2:E:218:ILE:HD11	1.86	1.15
3:F:7:SER:HB2	3:F:8:PRO:HD2	1.14	1.10
2:E:30:SER:O	2:E:31:ARG:HB2	1.72	0.89
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.56	0.88
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.58	0.86
3:F:7:SER:CB	3:F:8:PRO:CD	2.43	0.86
2:E:148:CYS:SG	2:E:218:ILE:CD1	2.64	0.85
3:D:95:GLN:OE1	3:D:95:GLN:N	2.08	0.85
1:A:180:THR:HB	1:A:218:VAL:HA	1.59	0.82
3:F:7:SER:HB2	3:F:8:PRO:HD3	1.60	0.80
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.64	0.79
3:D:1:ASP:OD2	3:D:1:ASP:N	2.19	0.76
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.20	0.75
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.69	0.74
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.68	0.74
3:F:192:THR:HB	3:F:207:SER:HB3	1.70	0.73
3:F:186:GLU:O	3:F:210:ARG:NH2	2.21	0.73
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.71	0.72
1:B:394:MET:HE2	1:B:412:VAL:HG22	1.71	0.72
3:F:95:GLN:H	3:F:95:GLN:CD	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:TYR:H	2:E:53:PRO:HG3	1.55	0.71
3:D:29:VAL:O	3:D:70:TYR:OH	2.06	0.70
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.25	0.69
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.28	0.69
1:A:28:ARG:HH11	1:B:207:GLN:HG2	1.56	0.69
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.25	0.69
3:F:1:ASP:OD1	3:F:1:ASP:N	2.26	0.68
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.75	0.68
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.75	0.67
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.76	0.66
1:B:422:ILE:HA	1:B:425:MET:HE3	1.78	0.65
1:A:411:LEU:HG	1:A:415:MET:HE2	1.78	0.65
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.79	0.64
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.80	0.63
3:F:95:GLN:CD	3:F:95:GLN:N	2.56	0.63
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.80	0.62
1:B:147:ARG:O	1:B:151:THR:OG1	2.16	0.62
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.32	0.62
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.35	0.61
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.66	0.60
1:A:205:ARG:HH12	1:B:205:ARG:HH12	1.47	0.60
3:D:29:VAL:HG12	3:D:32:ILE:HD11	1.83	0.60
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.83	0.60
1:B:38:MET:O	1:B:42:VAL:HG23	2.01	0.60
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.66	0.60
1:B:200:ILE:HA	1:B:204:MET:HB2	1.84	0.60
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.83	0.60
1:A:17:ARG:HH22	1:A:21:LEU:HD13	1.67	0.59
3:F:145:VAL:HG11	3:F:174:MET:HE1	1.84	0.59
3:D:192:THR:HG22	3:D:207:SER:HB3	1.84	0.58
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.68	0.58
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.86	0.58
1:B:157:ASN:N	1:B:157:ASN:HD22	2.02	0.58
1:A:183:ALA:HB2	1:A:200:ILE:HG12	1.87	0.56
1:B:44:THR:O	1:B:48:LEU:HG	2.06	0.56
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.87	0.56
3:F:149:ILE:HD11	3:F:178:LEU:HD21	1.88	0.56
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.87	0.55
1:A:77:LEU:O	1:A:81:VAL:HG13	2.07	0.55
2:E:30:SER:O	2:E:31:ARG:CB	2.44	0.54
3:D:197:HIS:CG	3:D:198:LYS:H	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.90	0.54
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.90	0.53
1:B:269:PHE:O	1:B:273:VAL:HG12	2.09	0.53
2:C:87:ARG:HH21	2:C:89:GLU:CD	2.15	0.53
1:B:176:THR:O	1:B:180:THR:HG23	2.09	0.53
3:D:17:ASP:OD1	3:D:18:LYS:N	2.37	0.53
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.09	0.53
3:F:38:LYS:HG2	3:F:83:ALA:HB2	1.90	0.53
1:A:38:MET:HB3	1:A:177:LEU:HD11	1.91	0.53
1:B:319:LEU:HD11	1:B:362:ALA:HB1	1.90	0.53
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.90	0.52
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.42	0.52
3:D:192:THR:HG22	3:D:207:SER:CB	2.39	0.52
3:D:29:VAL:CG1	3:D:32:ILE:HD11	2.38	0.52
1:B:360:MET:HG2	1:B:397:LEU:HD13	1.91	0.52
3:F:7:SER:CB	3:F:8:PRO:HD3	2.29	0.52
1:B:255:TYR:CD1	1:B:424:PRO:HB3	2.44	0.52
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.90	0.51
1:A:28:ARG:HH21	1:B:443:PRO:HB3	1.75	0.51
1:A:422:ILE:HA	1:A:425:MET:HE3	1.92	0.51
1:A:172:GLU:HG3	1:A:212:LEU:HB3	1.92	0.51
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.46	0.51
3:D:16:GLY:HA2	3:D:76:THR:OG1	2.11	0.51
1:B:332:MET:O	1:B:336:ILE:HG13	2.10	0.51
1:A:200:ILE:HD13	1:A:204:MET:HG3	1.93	0.51
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.93	0.51
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.46	0.50
1:B:262:PHE:HZ	1:B:364:GLY:HA2	1.76	0.50
1:B:88:VAL:HA	1:B:91:MET:HE2	1.92	0.50
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.93	0.50
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.12	0.50
1:B:383:HIS:NE2	2:E:50:GLU:OE1	2.45	0.50
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.48	0.49
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.77	0.49
1:A:200:ILE:HA	1:A:204:MET:HB2	1.94	0.49
1:A:361:LEU:HD13	1:A:415:MET:HE1	1.94	0.49
1:B:64:ARG:O	1:B:68:LEU:HG	2.13	0.49
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.47	0.49
1:B:41:VAL:O	1:B:45:LEU:HG	2.13	0.48
3:D:89:GLN:O	3:D:95:GLN:HB2	2.13	0.48
1:A:207:GLN:HG2	1:B:28:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MET:HE3	1:B:298:ILE:HG22	1.94	0.48
2:E:31:ARG:H	2:E:53:PRO:HB3	1.78	0.48
1:A:430:LEU:HD11	1:B:219:PHE:CG	2.48	0.48
1:B:19:ARG:NH1	1:B:19:ARG:HA	2.28	0.48
1:A:430:LEU:HD23	1:B:220:ILE:HG12	1.94	0.48
2:C:7:SER:HA	2:C:115:THR:HG21	1.94	0.48
1:A:91:MET:HG2	1:A:292:VAL:O	2.14	0.48
2:E:33:TRP:CZ2	2:E:52:ASN:HB3	2.48	0.48
2:E:31:ARG:HG3	2:E:31:ARG:HH11	1.78	0.48
3:F:194:GLU:HG2	3:F:205:VAL:HB	1.94	0.47
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.29	0.47
1:A:183:ALA:HB2	1:A:200:ILE:CG1	2.44	0.47
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.96	0.47
1:A:458:ALA:C	1:A:460:GLN:H	2.22	0.47
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.61	0.47
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.96	0.47
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.97	0.47
1:B:157:ASN:HD22	1:B:157:ASN:H	1.61	0.47
2:C:101:TYR:HB2	2:C:104:GLY:HA2	1.96	0.47
1:B:276:MET:HE3	1:B:276:MET:HB2	1.69	0.47
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.23	0.47
1:B:267:PRO:HG3	1:B:441:GLY:HA3	1.96	0.47
1:B:409:ILE:HD13	1:B:426:ILE:HG12	1.96	0.47
3:D:77:MET:HE3	3:D:78:GLU:O	2.15	0.47
1:B:165:ILE:HG22	1:B:166:PHE:CD2	2.50	0.47
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.74	0.47
1:A:346:LEU:O	1:A:350:SER:HB3	2.16	0.46
1:A:365:THR:HG23	1:A:390:ALA:HB1	1.97	0.46
3:F:186:GLU:HG2	3:F:210:ARG:NH1	2.30	0.46
1:B:337:PHE:O	1:B:341:VAL:HG23	2.14	0.46
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.50	0.46
1:B:118:ASP:OD1	1:B:174:ARG:NH2	2.28	0.46
1:A:229:TYR:O	1:A:233:ASN:HB2	2.15	0.46
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.50	0.46
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.97	0.46
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.45	0.46
1:B:180:THR:HB	1:B:218:VAL:HA	1.97	0.46
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.97	0.46
3:D:106:LEU:HD23	3:D:107:ARG:N	2.31	0.46
3:F:34:TRP:HB2	3:F:47:ILE:HB	1.97	0.46
1:B:42:VAL:O	1:B:46:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:TYR:N	2:E:53:PRO:HG3	2.28	0.46
1:A:262:PHE:CE2	1:A:367:LEU:HD23	2.51	0.46
3:D:112:PRO:HG3	3:D:143:ILE:HD11	1.97	0.46
1:B:411:LEU:O	1:B:415:MET:HG3	2.16	0.45
2:E:6:GLU:CD	2:E:114:GLY:H	2.25	0.45
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.52	0.45
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.52	0.45
2:E:53:PRO:HA	2:E:72:ARG:CZ	2.47	0.45
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.98	0.45
3:D:12:SER:HA	3:D:104:GLU:O	2.16	0.45
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.81	0.45
1:A:165:ILE:HG22	1:A:166:PHE:CD2	2.52	0.45
1:B:202:GLU:OE2	1:B:405:PRO:HD2	2.16	0.45
1:A:31:THR:O	1:B:437:GLN:NE2	2.48	0.45
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.97	0.45
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.98	0.45
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.50	0.45
1:B:75:TYR:CZ	1:B:79:LEU:HD21	2.52	0.45
1:A:205:ARG:HH12	1:B:205:ARG:NH1	2.10	0.45
1:A:360:MET:HE1	1:A:402:ILE:CG2	2.47	0.45
1:A:427:ILE:HD11	1:B:227:ILE:HD11	1.99	0.45
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.85	0.45
1:B:369:THR:OG1	1:B:390:ALA:HB2	2.17	0.44
1:A:255:TYR:CD1	1:A:424:PRO:HB3	2.52	0.44
1:B:250:ASN:OD1	2:E:104:GLY:HA3	2.17	0.44
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.98	0.44
1:A:152:VAL:HG13	1:A:182:ALA:HB1	2.00	0.44
1:A:369:THR:OG1	1:A:390:ALA:HB2	2.18	0.44
3:D:49:ASP:O	3:D:51:SER:N	2.44	0.44
2:E:24:ALA:HB1	2:E:27:PHE:CZ	2.52	0.44
1:A:190:PHE:HE2	1:A:317:PHE:HZ	1.65	0.44
1:B:311:ALA:O	1:B:340:ARG:HD2	2.18	0.44
1:B:430:LEU:HA	1:B:433:THR:HG22	1.99	0.44
1:B:53:PHE:O	1:B:57:VAL:HG23	2.18	0.44
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.99	0.44
3:F:20:THR:HG23	3:F:73:THR:OG1	2.18	0.44
1:B:91:MET:HG2	1:B:292:VAL:O	2.17	0.43
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.52	0.43
1:B:399:ALA:O	1:B:403:ARG:HA	2.18	0.43
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.34	0.43
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:HA	1:B:160:ARG:HD2	1.79	0.43
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.75	0.43
1:B:86:SER:OG	1:B:303:GLY:HA3	2.18	0.43
1:B:131:LYS:HE2	1:B:150:PRO:HA	1.99	0.43
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.53	0.43
2:E:87:ARG:NE	2:E:89:GLU:OE1	2.51	0.43
1:A:176:THR:O	1:A:180:THR:HG22	2.18	0.43
1:B:46:VAL:HG22	1:B:158:ILE:HD12	2.00	0.43
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.53	0.43
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.54	0.43
2:E:19:LYS:HE2	2:E:80:TYR:CD2	2.54	0.43
1:A:269:PHE:O	1:A:273:VAL:HG12	2.18	0.43
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.85	0.43
2:E:148:CYS:SG	2:E:203:CYS:CB	3.07	0.43
2:E:185:LEU:C	2:E:185:LEU:HD12	2.43	0.43
2:E:135:GLY:O	2:E:137:ALA:N	2.51	0.43
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.83	0.42
1:A:214:SER:O	1:A:218:VAL:HG23	2.18	0.42
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.18	0.42
2:E:85:LYS:HD3	2:E:85:LYS:HA	1.67	0.42
1:A:208:PHE:HE1	1:B:25:LEU:HD23	1.84	0.42
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.34	0.42
1:B:132:PHE:O	1:B:136:LEU:HG	2.19	0.42
1:A:294:MET:HB3	1:A:294:MET:HE2	1.80	0.42
1:B:360:MET:HE1	1:B:402:ILE:HG21	2.01	0.42
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.55	0.42
3:D:7:SER:HB3	3:D:22:THR:HB	2.01	0.42
1:B:198:LEU:HD13	1:B:198:LEU:HA	1.85	0.42
2:C:1:GLU:O	2:C:26:GLY:HA3	2.20	0.42
3:F:77:MET:HB3	3:F:77:MET:HE2	1.76	0.42
1:B:55:LYS:HA	1:B:55:LYS:HD3	1.82	0.42
1:B:204:MET:HE3	1:B:204:MET:HB3	1.95	0.42
3:D:21:MET:H	3:D:21:MET:HG2	1.67	0.42
2:E:29:TYR:HE1	2:E:34:MET:HE2	1.85	0.42
1:A:394:MET:HE2	1:A:415:MET:HE3	2.02	0.42
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.35	0.42
1:A:74:ASN:OD1	1:A:76:PRO:HD2	2.19	0.41
1:B:358:ALA:HB3	1:B:359:PRO:HD3	2.02	0.41
1:A:71:THR:O	1:A:78:LEU:HD23	2.19	0.41
2:E:94:TYR:O	2:E:114:GLY:HA2	2.21	0.41
3:F:7:SER:CB	3:F:8:PRO:HD2	2.10	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:VAL:HG13	2:C:27:PHE:CD1	2.55	0.41
3:D:106:LEU:HD23	3:D:107:ARG:H	1.85	0.41
2:C:12:VAL:HG21	2:C:18:LEU:HD23	2.03	0.41
2:C:69:ILE:HB	2:C:82:GLN:HB2	2.01	0.41
1:A:160:ARG:HA	1:A:160:ARG:HD2	1.84	0.41
2:C:54:VAL:HG23	2:C:56:SER:HB3	2.02	0.41
1:A:447:ALA:O	1:A:451:ARG:HG3	2.21	0.41
1:B:110:PRO:O	1:B:449:LEU:HD13	2.20	0.41
1:B:163:LEU:HD12	1:B:168:LEU:HB2	2.02	0.41
1:B:139:LEU:HD12	1:B:147:ARG:HG3	2.02	0.41
1:B:266:GLY:HA3	1:B:400:ALA:HB1	2.02	0.41
1:A:18:ARG:O	1:A:22:ILE:HG13	2.20	0.41
1:A:280:LEU:HD22	1:A:294:MET:SD	2.60	0.41
1:B:102:PRO:C	1:B:104:ALA:H	2.29	0.41
2:E:31:ARG:HG3	2:E:31:ARG:NH1	2.36	0.41
1:A:280:LEU:HA	1:A:280:LEU:HD23	1.81	0.41
1:A:158:ILE:O	1:A:162:VAL:HG13	2.22	0.40
1:B:94:TYR:CD1	1:B:295:GLY:HA3	2.56	0.40
3:F:162:TRP:CE2	3:F:174:MET:HG3	2.56	0.40
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.27	0.40
1:A:160:ARG:NE	1:A:163:LEU:HD23	2.37	0.40
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.57	0.40
3:F:89:GLN:O	3:F:95:GLN:HB2	2.21	0.40
2:C:37:VAL:O	2:C:95:TYR:HB2	2.21	0.40
2:E:73:ASP:OD1	2:E:76:LYS:HB2	2.22	0.40
1:A:154:ILE:O	1:A:158:ILE:HG13	2.21	0.40
2:C:43:LYS:HE2	2:C:43:LYS:HB3	1.74	0.40
3:D:185:TYR:CZ	3:D:210:ARG:HD3	2.55	0.40
2:E:28:ASP:O	2:E:30:SER:O	2.38	0.40
1:A:206:PRO:HG2	1:A:211:THR:HG21	2.03	0.40
1:B:184:ALA:HB1	1:B:225:SER:HB2	2.03	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	442/446 (99%)	410 (93%)	32 (7%)	0	100	100
1	B	440/446 (99%)	408 (93%)	31 (7%)	1 (0%)	43	73
2	C	220/222 (99%)	200 (91%)	18 (8%)	2 (1%)	14	45
2	E	219/222 (99%)	193 (88%)	23 (10%)	3 (1%)	9	34
3	D	209/211 (99%)	184 (88%)	23 (11%)	2 (1%)	12	42
3	F	209/211 (99%)	196 (94%)	12 (6%)	1 (0%)	24	58
All	All	1739/1758 (99%)	1591 (92%)	139 (8%)	9 (0%)	24	58

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	65	LYS
2	E	137	ALA
3	F	7	SER
2	C	140	ALA
1	B	233	ASN
3	D	7	SER
3	D	76	THR
2	E	62	PRO
2	C	25	SER

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	335/337 (99%)	302 (90%)	33 (10%)	7	28
1	B	333/337 (99%)	300 (90%)	33 (10%)	7	28
2	C	182/182 (100%)	166 (91%)	16 (9%)	9	33
2	E	181/182 (100%)	166 (92%)	15 (8%)	10	35
3	D	185/185 (100%)	173 (94%)	12 (6%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	185/185 (100%)	167 (90%)	18 (10%)	8	29
All	All	1401/1408 (100%)	1274 (91%)	127 (9%)	9	31

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	41	VAL
1	A	69	VAL
1	A	71	THR
1	A	73	ASP
1	A	81	VAL
1	A	96	LEU
1	A	97	VAL
1	A	98	ARG
1	A	145	LEU
1	A	148	GLN
1	A	151	THR
1	A	162	VAL
1	A	168	LEU
1	A	180	THR
1	A	211	THR
1	A	219	PHE
1	A	230	ARG
1	A	236	VAL
1	A	241	VAL
1	A	251	THR
1	A	264	ILE
1	A	273	VAL
1	A	283	VAL
1	A	346	LEU
1	A	350	SER
1	A	356	ILE
1	A	357	PHE
1	A	397	LEU
1	A	402	ILE
1	A	423	LEU
1	A	452	THR
1	A	456	GLN
1	B	23	ARG
1	B	41	VAL
1	B	69	VAL

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Mol	Chain	Res	Type
1	B	73	ASP
1	B	81	VAL
1	B	96	LEU
1	B	107	SER
1	B	109	ILE
1	B	139	LEU
1	B	147	ARG
1	B	148	GLN
1	B	151	THR
1	B	157	ASN
1	B	162	VAL
1	B	180	THR
1	B	200	ILE
1	B	205	ARG
1	B	211	THR
1	B	219	PHE
1	B	241	VAL
1	B	245	SER
1	B	251	THR
1	B	273	VAL
1	B	276	MET
1	B	304	LEU
1	B	346	LEU
1	B	356	ILE
1	B	397	LEU
1	B	402	ILE
1	B	423	LEU
1	B	427	ILE
1	B	430	LEU
1	B	456	GLN
2	C	5	LEU
2	C	18	LEU
2	C	43	LYS
2	C	57	THR
2	C	66	ASP
2	C	72	ARG
2	C	83	ILE
2	C	89	GLU
2	C	98	ARG
2	C	116	THR
2	C	128	SER
2	C	166	SER

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Mol	Chain	Res	Type
2	C	167	LEU
2	C	185	LEU
2	C	200	THR
2	C	214	VAL
3	D	1	ASP
3	D	10	ILE
3	D	19	VAL
3	D	71	SER
3	D	76	THR
3	D	106	LEU
3	D	120	SER
3	D	135	LEU
3	D	174	MET
3	D	180	LEU
3	D	190	SER
3	D	201	THR
2	E	5	LEU
2	E	6	GLU
2	E	12	VAL
2	E	21	SER
2	E	56	SER
2	E	76	LYS
2	E	86	VAL
2	E	87	ARG
2	E	118	THR
2	E	145	THR
2	E	164	SER
2	E	198	SER
2	E	200	THR
2	E	202	THR
2	E	212	THR
3	F	1	ASP
3	F	2	ILE
3	F	7	SER
3	F	22	THR
3	F	27	SER
3	F	29	VAL
3	F	41	THR
3	F	44	LYS
3	F	59	VAL
3	F	74	ILE
3	F	95	GLN

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Mol	Chain	Res	Type
3	F	142	ASP
3	F	146	LYS
3	F	170	SER
3	F	181	THR
3	F	192	THR
3	F	198	LYS
3	F	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	207	GLN
1	A	281	HIS
1	B	63	GLN
1	B	119	GLN
1	B	157	ASN
1	B	175	HIS
1	B	207	GLN
3	D	197	HIS
3	F	95	GLN
3	F	123	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th 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	444/446 (99%)	0.02	12 (2%) 56 37	25, 44, 69, 114	0
1	B	442/446 (99%)	-0.07	4 (0%) 81 65	26, 45, 83, 115	0
2	C	222/222 (100%)	-0.09	6 (2%) 56 37	11, 36, 71, 102	0
2	E	221/222 (99%)	0.00	8 (3%) 46 29	16, 38, 70, 111	0
3	D	211/211 (100%)	0.04	5 (2%) 59 40	23, 43, 62, 77	0
3	F	211/211 (100%)	-0.22	4 (1%) 66 47	17, 31, 76, 90	0
All	All	1751/1758 (99%)	-0.05	39 (2%) 62 43	11, 41, 73, 115	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	GLU	7.5
2	E	138	ALA	4.6
1	A	168	LEU	4.5
1	B	210	TYR	4.1
3	D	20	THR	4.0
2	E	222	ALA	3.5
1	A	234	HIS	3.5
2	E	148	CYS	3.4
3	D	7	SER	3.1
1	A	166	PHE	3.0
2	C	64	LEU	3.0
1	A	236	VAL	3.0
3	F	122	GLU	2.9
1	A	171	ASP	2.8
2	C	140	ALA	2.7
3	D	211	ALA	2.7
1	B	236	VAL	2.6
2	C	2	VAL	2.6
1	A	72	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	2.6
3	D	159	LEU	2.6
2	C	139	ALA	2.6
3	F	39	SER	2.5
1	A	393	GLY	2.4
1	A	258	LEU	2.4
3	D	22	THR	2.4
1	A	455	LYS	2.3
2	E	32	TYR	2.3
2	E	140	ALA	2.2
1	B	17	ARG	2.2
1	A	23	ARG	2.2
3	F	8	PRO	2.2
2	E	42	GLY	2.2
2	E	139	ALA	2.2
2	C	141	ALA	2.1
2	C	27	PHE	2.1
3	F	151	GLY	2.1
1	A	184	ALA	2.0
2	E	31	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.