



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 AM UTC

PDB ID : 2HTK / pdb_00002htk
Title : Structure of the Escherichia coli ClC chloride channel Y445A mutant and Fab complex
Authors : Accardi, A.; Lobet, S.; Williams, C.; Miller, C.; Dutzler, R.
Deposited on : 2006-07-26
Resolution : 3.41 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

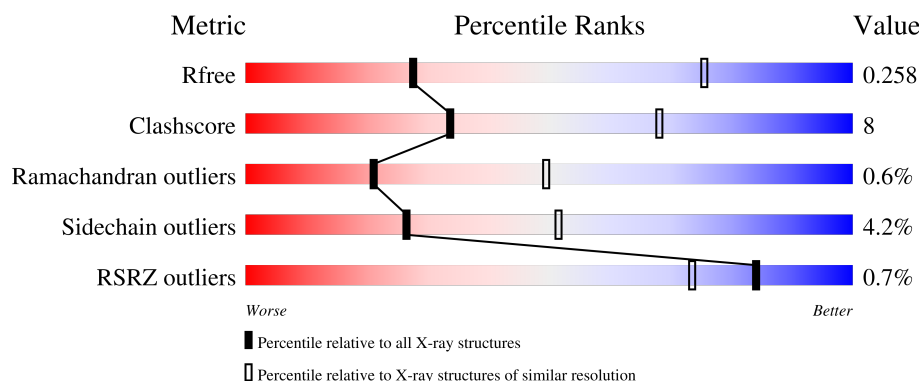
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	473	 2% 74% 18% • 6%
1	B	473	 % 72% 20% • 7%
2	C	221	 88% 11%
2	E	221	 81% 17% •
3	D	211	 86% 14%

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Mol	Chain	Length	Quality of chain
3	F	211	

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	BR	A	474	-	-	X	-
4	BR	B	474	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13211 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
			3326	2184	560	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3297	2168	553	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	ALA	TYR	engineered mutation	UNP P37019
B	445	ALA	TYR	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	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	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 BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Br	0	0
			1	1		



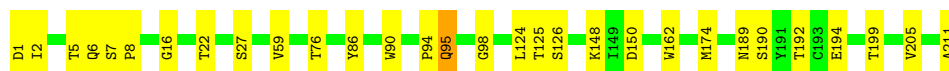
- Molecule 2: Fab fragment, Heavy chain

Chain E: 81% 17% .



- Molecule 3: Fab fragment, Light chain

Chain D: 86% 14%



- Molecule 3: Fab fragment, Light chain

Chain F: 74% 24% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.07Å 98.14Å 171.07Å 90.00° 131.56° 90.00°	Depositor
Resolution (Å)	40.00 – 3.41 40.00 – 3.41	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.00-3.41) 96.1 (40.00-3.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.266 , 0.276 0.246 , 0.258	Depositor DCC
R_{free} test set	1939 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	113.4	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13211	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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](#)

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

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	0.46	0/3397	0.86	0/4610
1	B	0.45	0/3368	0.86	0/4572
2	C	0.47	0/1721	0.75	0/2355
2	E	0.45	0/1721	0.72	0/2355
3	D	0.44	0/1660	0.73	0/2257
3	F	0.43	0/1660	0.75	0/2257
All	All	0.45	0/13527	0.80	0/18406

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 [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	3326	0	3480	64	0
1	B	3297	0	3453	65	0
2	C	1672	0	1654	11	0
2	E	1672	0	1654	21	0
3	D	1621	0	1546	18	0
3	F	1621	0	1546	37	0
4	A	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	2	0
All	All	13211	0	13333	203	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 8.

All (203) 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:HB3	3:F:8:PRO:HD3	1.42	0.98
1:A:381:GLN:H	1:A:381:GLN:HE21	0.95	0.91
1:B:381:GLN:H	1:B:381:GLN:HE21	1.15	0.90
1:B:148:GLU:CD	1:B:148:GLU:H	1.85	0.84
1:A:148:GLU:HG2	1:A:357:PHE:HB3	1.63	0.80
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.64	0.79
1:A:381:GLN:HE21	1:A:381:GLN:N	1.79	0.76
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.69	0.74
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.87	0.74
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.70	0.72
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.71	0.71
3:F:7:SER:HB2	3:F:22:THR:HB	1.73	0.70
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.73	0.69
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.73	0.68
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.59	0.67
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.58	0.67
1:A:200:ILE:HA	1:A:204:MET:HB2	1.76	0.67
1:A:148:GLU:CD	1:A:148:GLU:H	2.02	0.67
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.76	0.67
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.76	0.67
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.76	0.67
1:B:38:MET:O	1:B:42:VAL:HG23	1.95	0.67
1:A:74:ASN:HD22	1:A:76:PRO:HD2	1.60	0.66
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.76	0.66
1:B:381:GLN:HE21	1:B:381:GLN:N	1.91	0.66
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.61	0.66
1:A:176:THR:O	1:A:180:THR:HG23	1.95	0.66
3:D:95:GLN:CD	3:D:95:GLN:H	2.04	0.66
1:A:381:GLN:H	1:A:381:GLN:NE2	1.80	0.65
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.79	0.64
1:B:200:ILE:HA	1:B:204:MET:HB2	1.79	0.63
3:F:7:SER:HB3	3:F:8:PRO:CD	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HG21	1:A:343:THR:HB	1.80	0.62
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.63	0.62
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.81	0.62
1:B:176:THR:O	1:B:180:THR:HG23	2.00	0.62
3:D:95:GLN:CD	3:D:95:GLN:N	2.58	0.61
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.83	0.60
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.84	0.59
3:F:95:GLN:H	3:F:95:GLN:CD	2.10	0.59
2:E:143:MET:HE3	2:E:190:THR:HG22	1.83	0.59
2:E:91:THR:HG23	2:E:118:THR:HA	1.86	0.58
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.84	0.58
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.86	0.57
1:B:180:THR:HG22	1:B:218:VAL:HA	1.87	0.57
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.86	0.57
1:B:143:MET:HE2	1:B:347:CYS:SG	2.45	0.56
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.41	0.56
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.87	0.56
1:A:148:GLU:HG2	1:A:357:PHE:CB	2.35	0.56
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.21	0.55
1:A:360:MET:HG2	1:A:397:LEU:HD12	1.87	0.55
3:F:189:ASN:HD21	3:F:211:ALA:H	1.54	0.55
2:E:6:GLU:HA	2:E:22:CYS:HA	1.89	0.55
2:E:130:TYR:HB3	3:F:120:SER:OG	2.06	0.55
1:A:112:ILE:HD11	1:A:153:GLN:HG3	1.90	0.54
1:A:227:ILE:O	1:A:231:ILE:HG12	2.07	0.54
3:F:77:MET:HE2	3:F:103:LEU:HD11	1.89	0.54
3:D:1:ASP:HB3	3:D:94:PRO:HD2	1.88	0.54
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.42	0.54
3:F:7:SER:CB	3:F:8:PRO:HD3	2.27	0.53
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.41	0.53
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.91	0.53
3:D:124:LEU:C	3:D:126:SER:H	2.17	0.52
3:F:95:GLN:CD	3:F:95:GLN:N	2.67	0.52
2:E:132:LEU:HD11	2:E:149:LEU:HB2	1.92	0.52
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.93	0.52
1:A:110:PRO:HG2	4:A:474:BR:BR	2.65	0.51
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.91	0.51
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.45	0.51
1:A:356:ILE:HG23	1:A:360:MET:CE	2.40	0.51
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.93	0.51
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.41	0.51
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.44	0.51
1:A:398:LEU:HD22	1:A:402:ILE:HD12	1.93	0.51
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.93	0.51
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.76	0.50
1:A:305:LEU:C	1:A:307:PHE:H	2.20	0.50
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.94	0.50
1:A:148:GLU:CG	1:A:357:PHE:HB3	2.39	0.50
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.94	0.50
3:F:189:ASN:HD22	3:F:210:ARG:HB2	1.77	0.50
2:E:30:SER:C	2:E:32:TYR:H	2.20	0.50
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.47	0.49
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.92	0.49
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.77	0.49
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.94	0.49
2:C:91:THR:HG23	2:C:118:THR:HA	1.94	0.49
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.47	0.49
3:D:189:ASN:HD21	3:D:211:ALA:H	1.61	0.49
1:A:160:ARG:HH12	1:A:174:ARG:HD2	1.78	0.48
2:C:30:SER:C	2:C:32:TYR:H	2.20	0.48
3:F:95:GLN:N	3:F:95:GLN:OE1	2.47	0.48
1:A:172:GLU:HG3	1:A:212:LEU:O	2.13	0.48
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.29	0.48
2:E:35:SER:HB2	2:E:99:LEU:HD11	1.95	0.48
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.81	0.48
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.95	0.48
1:A:336:ILE:O	1:A:340:ARG:HG3	2.14	0.47
1:B:148:GLU:O	1:B:149:GLY:C	2.56	0.47
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.79	0.47
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.50	0.47
1:A:376:VAL:HG22	1:A:384:LEU:HB2	1.96	0.47
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.97	0.47
1:A:330:MET:HE1	1:A:370:ALA:HB1	1.97	0.47
3:F:34:TRP:HB2	3:F:47:ILE:HB	1.96	0.47
3:F:150:ASP:HA	3:F:190:SER:HB3	1.97	0.47
3:D:7:SER:CB	3:D:8:PRO:HD3	2.45	0.46
3:F:141:LYS:HB3	3:F:172:TYR:CD1	2.50	0.46
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.50	0.46
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.97	0.46
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.51	0.46
1:B:234:HIS:CD2	1:B:234:HIS:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:TYR:CE2	2:E:98:ARG:HD3	2.50	0.46
1:A:348:PHE:CD1	1:A:356:ILE:HB	2.50	0.45
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.15	0.45
1:B:305:LEU:C	1:B:307:PHE:H	2.24	0.45
3:F:149:ILE:HD11	3:F:178:LEU:HD21	1.97	0.45
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.52	0.45
3:F:7:SER:CB	3:F:22:THR:HB	2.42	0.45
1:B:110:PRO:HG2	4:B:474:BR:BR	2.72	0.45
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.52	0.45
1:A:328:PHE:O	1:A:373:MET:HE1	2.17	0.45
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.65	0.45
1:B:448:ILE:HG21	4:B:474:BR:BR	2.72	0.45
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.97	0.45
1:B:422:ILE:HA	1:B:425:MET:HE3	1.99	0.45
2:C:134:PRO:HD2	2:C:196:TRP:CH2	2.52	0.45
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.98	0.44
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.98	0.44
1:A:451:ARG:HH11	1:A:451:ARG:HB3	1.83	0.44
1:A:42:VAL:HG22	1:A:162:VAL:HG21	1.99	0.44
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.97	0.44
1:B:88:VAL:HA	1:B:91:MET:HE3	1.99	0.44
2:C:52:ASN:HB2	2:C:53:PRO:HD2	2.00	0.44
2:E:6:GLU:HB3	2:E:22:CYS:HB2	2.00	0.44
1:A:28:ARG:HD3	1:B:443:PRO:HG2	2.00	0.44
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.52	0.44
1:A:180:THR:HG22	1:A:218:VAL:HA	1.98	0.44
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.53	0.44
1:B:148:GLU:CD	1:B:148:GLU:N	2.63	0.44
3:D:148:LYS:HB2	3:D:192:THR:HG1	1.81	0.44
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.48	0.44
2:C:195:SER:O	2:C:199:GLU:HB3	2.17	0.44
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.48	0.44
2:C:29:TYR:OH	2:C:79:LEU:HB2	2.18	0.44
1:A:219:PHE:HB3	1:B:430:LEU:CD1	2.48	0.43
2:E:221:ARG:HH22	3:F:120:SER:HA	1.83	0.43
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.86	0.43
1:B:59:TRP:O	1:B:63:GLN:HG2	2.17	0.43
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.83	0.43
2:E:9:GLY:H	2:E:115:THR:HG21	1.84	0.43
1:A:112:ILE:HG13	1:A:153:GLN:HA	2.01	0.43
1:A:413:LEU:HD11	1:A:419:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:150:ASP:HA	3:D:190:SER:HB3	1.99	0.43
1:B:239:ILE:HD13	1:B:394:MET:HE1	1.99	0.43
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.53	0.43
1:B:358:ALA:HB3	1:B:359:PRO:HD3	2.00	0.43
1:A:109:ILE:N	1:A:110:PRO:CD	2.82	0.43
3:F:2:ILE:HD12	3:F:27:SER:HB2	2.00	0.43
3:F:31:TYR:HA	3:F:50:THR:OG1	2.19	0.43
1:A:434:LEU:HD23	1:B:216:LYS:HD3	2.00	0.43
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.54	0.43
1:A:198:LEU:HD11	1:B:198:LEU:HD21	2.01	0.43
1:A:449:LEU:O	1:A:453:LEU:HB2	2.19	0.43
1:B:184:ALA:HB1	1:B:225:SER:HB3	2.00	0.42
2:E:20:LEU:HD12	2:E:81:LEU:HD23	2.01	0.42
3:F:38:LYS:O	3:F:41:THR:HG22	2.19	0.42
1:B:163:LEU:HD12	1:B:168:LEU:HB2	2.01	0.42
1:A:223:ILE:HD12	1:B:430:LEU:HD22	2.01	0.42
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.34	0.42
1:A:38:MET:O	1:A:42:VAL:HG23	2.19	0.42
1:A:119:GLN:HB3	1:A:453:LEU:HD11	2.01	0.42
1:A:372:GLY:O	1:A:376:VAL:HG23	2.18	0.42
1:B:38:MET:HG3	1:B:168:LEU:HD11	2.01	0.42
1:B:381:GLN:H	1:B:381:GLN:NE2	1.98	0.42
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.50	0.42
1:B:360:MET:HE1	1:B:402:ILE:CG2	2.50	0.42
1:B:358:ALA:HA	1:B:361:LEU:HD12	2.01	0.42
1:B:422:ILE:HD12	1:B:425:MET:HE3	2.00	0.42
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.55	0.42
1:A:87:ALA:O	1:A:91:MET:HG3	2.20	0.41
1:A:226:THR:HG21	1:B:423:LEU:HD11	2.02	0.41
3:F:136:ASN:HD22	3:F:173:SER:HB3	1.85	0.41
2:E:16:GLY:O	2:E:86:VAL:HG23	2.20	0.41
2:E:125:THR:HA	2:E:126:PRO:HD2	1.90	0.41
1:B:109:ILE:N	1:B:110:PRO:CD	2.83	0.41
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.85	0.41
1:B:183:ALA:HB2	1:B:200:ILE:HD13	2.03	0.41
3:F:189:ASN:ND2	3:F:210:ARG:HB2	2.34	0.41
1:A:108:GLY:O	1:A:112:ILE:HG12	2.20	0.41
2:E:207:HIS:HA	2:E:208:PRO:HD2	1.93	0.41
2:C:16:GLY:O	2:C:86:VAL:HG23	2.20	0.41
1:A:448:ILE:HG21	4:A:474:BR:BR	2.76	0.41
1:B:397:LEU:HD22	1:B:397:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:O	1:B:231:ILE:CG2	2.69	0.40
3:D:95:GLN:N	3:D:95:GLN:OE1	2.54	0.40
1:B:249:LEU:C	1:B:251:THR:H	2.29	0.40
1:A:163:LEU:HD12	1:A:168:LEU:HB2	2.03	0.40
1:B:174:ARG:O	1:B:178:LEU:HB2	2.21	0.40
1:B:345:LEU:O	1:B:346:LEU:C	2.64	0.40
1:B:370:ALA:O	1:B:374:VAL:HG23	2.21	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	442/473 (93%)	415 (94%)	26 (6%)	1 (0%)	43 71
1	B	439/473 (93%)	408 (93%)	30 (7%)	1 (0%)	43 71
2	C	219/221 (99%)	202 (92%)	16 (7%)	1 (0%)	24 54
2	E	219/221 (99%)	197 (90%)	18 (8%)	4 (2%)	6 26
3	D	209/211 (99%)	187 (90%)	21 (10%)	1 (0%)	24 54
3	F	209/211 (99%)	191 (91%)	16 (8%)	2 (1%)	12 39
All	All	1737/1810 (96%)	1600 (92%)	127 (7%)	10 (1%)	21 49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	65	LYS
2	E	62	PRO
2	E	140	ALA
2	C	62	PRO
3	F	7	SER

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Mol	Chain	Res	Type
3	F	76	THR
1	B	149	GLY
3	D	125	THR
2	E	164	SER
1	A	201	ILE

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	334/357 (94%)	320 (96%)	14 (4%)	26	51
1	B	331/357 (93%)	313 (95%)	18 (5%)	20	46
2	C	181/181 (100%)	174 (96%)	7 (4%)	28	53
2	E	181/181 (100%)	176 (97%)	5 (3%)	38	59
3	D	185/185 (100%)	180 (97%)	5 (3%)	39	60
3	F	185/185 (100%)	176 (95%)	9 (5%)	22	48
All	All	1397/1446 (97%)	1339 (96%)	58 (4%)	26	51

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	148	GLU
1	A	180	THR
1	A	211	THR
1	A	244	LEU
1	A	264	ILE
1	A	340	ARG
1	A	346	LEU
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	430	LEU
1	A	433	THR

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Mol	Chain	Res	Type
1	A	451	ARG
1	B	122	VAL
1	B	136	LEU
1	B	139	LEU
1	B	148	GLU
1	B	200	ILE
1	B	211	THR
1	B	219	PHE
1	B	244	LEU
1	B	324	THR
1	B	357	PHE
1	B	377	GLU
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
1	B	444	LEU
1	B	457	GLU
2	C	98	ARG
2	C	115	THR
2	C	118	THR
2	C	151	LYS
2	C	188	SER
2	C	203	CYS
2	C	218	ILE
3	D	5	THR
3	D	22	THR
3	D	59	VAL
3	D	95	GLN
3	D	199	THR
2	E	5	LEU
2	E	30	SER
2	E	115	THR
2	E	125	THR
2	E	151	LYS
3	F	1	ASP
3	F	32	ILE
3	F	68	THR
3	F	77	MET
3	F	84	THR
3	F	95	GLN

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Mol	Chain	Res	Type
3	F	96	THR
3	F	125	THR
3	F	177	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	74	ASN
1	A	119	GLN
1	A	157	ASN
1	A	175	HIS
1	A	207	GLN
1	A	270	ASN
1	A	281	HIS
1	A	327	ASN
1	A	381	GLN
1	A	420	GLN
1	A	437	GLN
1	B	62	ASN
1	B	74	ASN
1	B	157	ASN
1	B	207	GLN
1	B	234	HIS
1	B	270	ASN
1	B	277	GLN
1	B	327	ASN
1	B	381	GLN
1	B	420	GLN
1	B	437	GLN
3	D	6	GLN
3	D	75	ASN
3	D	137	ASN
3	D	189	ASN
2	E	172	HIS
3	F	6	GLN
3	F	75	ASN
3	F	88	GLN
3	F	136	ASN
3	F	189	ASN

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](#)

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	444/473 (93%)	-0.20	8 (1%) 67 53	40, 96, 146, 200	0
1	B	441/473 (93%)	-0.18	3 (0%) 84 73	44, 97, 154, 200	0
2	C	221/221 (100%)	-0.25	0 100 100	53, 90, 146, 197	0
2	E	221/221 (100%)	-0.24	1 (0%) 87 78	48, 99, 157, 200	0
3	D	211/211 (100%)	-0.19	0 100 100	48, 109, 157, 179	0
3	F	211/211 (100%)	-0.18	0 100 100	40, 89, 147, 181	0
All	All	1749/1810 (96%)	-0.20	12 (0%) 84 73	40, 97, 154, 200	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	ASP	4.1
1	B	73	ASP	3.8
1	A	447	ALA	2.9
1	B	72	ALA	2.7
1	B	143	MET	2.6
1	A	141	GLY	2.6
2	E	105	TYR	2.5
1	A	94	TYR	2.3
1	A	135	GLY	2.3
1	A	139	LEU	2.2
1	A	91	MET	2.2
1	A	308	VAL	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, 95th 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($\text{\AA}^2$)	Q<0.9
4	BR	A	474	1/1	0.81	0.44	56,56,56,56	0
4	BR	B	474	1/1	0.87	0.38	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.