



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:27 AM UTC

PDB ID : 1OTS / pdb_00001ots
Title : Structure of the Escherichia coli ClC Chloride channel and Fab Complex
Authors : Dutzler, R.; Campbell, E.B.; MacKinnon, R.
Deposited on : 2003-03-22
Resolution : 2.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

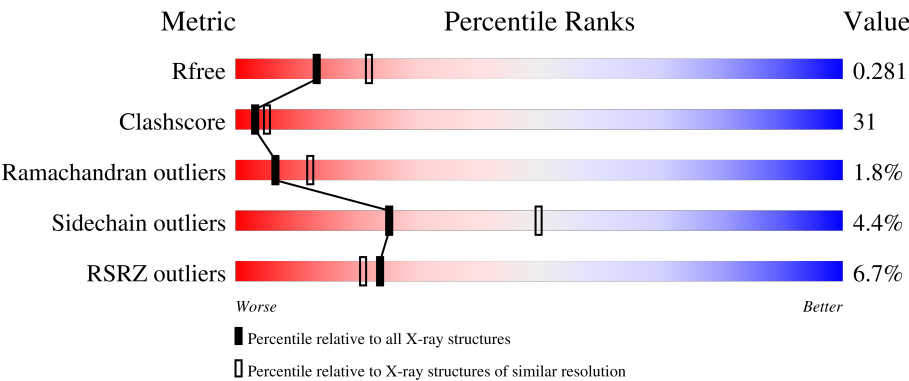
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	465	6% 48% 44% 5%
1	B	465	5% 46% 43% 6% 5%
2	C	222	9% 58% 39%
2	E	222	8% 53% 42% 5%
3	D	211	11% 55% 41%

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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	CL	B	467	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13654 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 Voltage-gated ClC-type chloride channel eriC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

- 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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

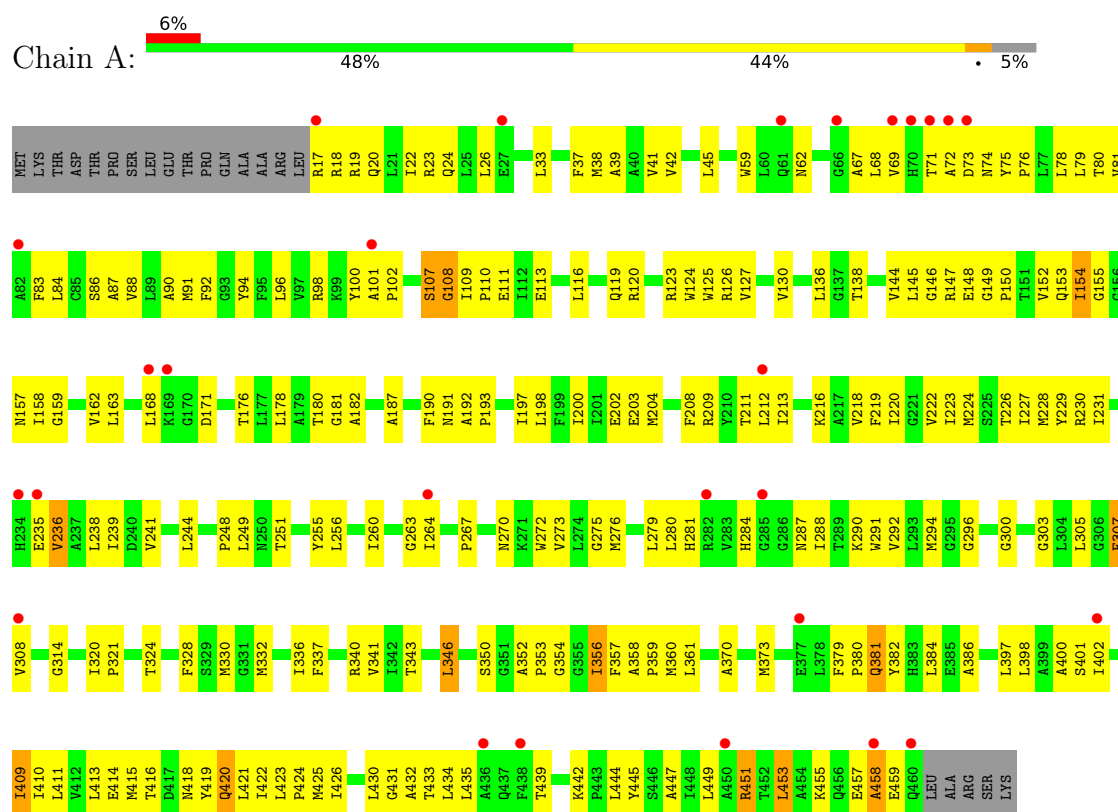
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total 76	O 76	0	0
5	B	91	Total 91	O 91	0	0
5	C	85	Total 85	O 85	0	0
5	D	36	Total 36	O 36	0	0
5	E	69	Total 69	O 69	0	0
5	F	70	Total 70	O 70	0	0

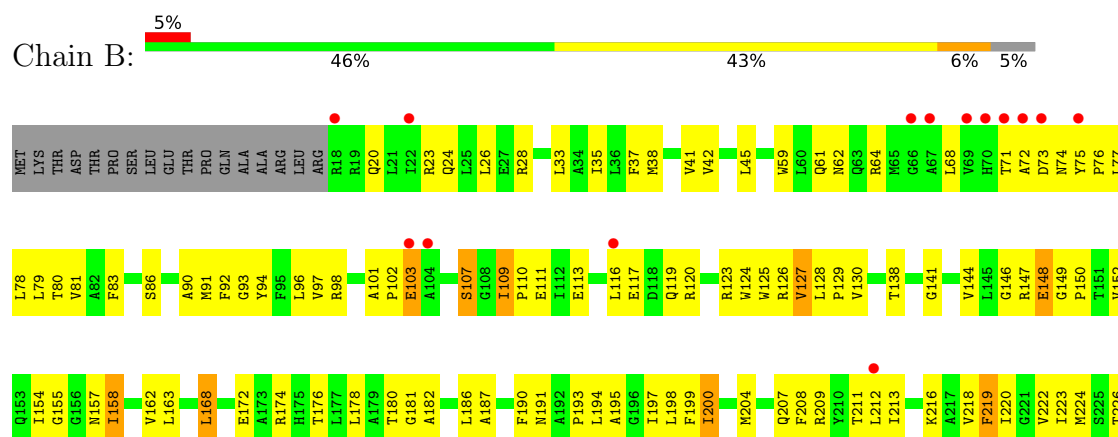
3 Residue-property plots

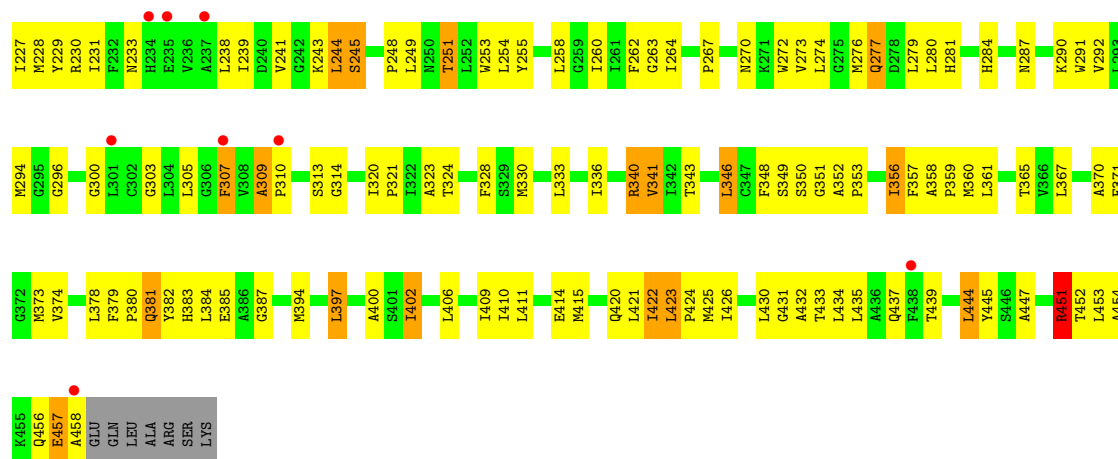
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Voltage-gated ClC-type chloride channel eriC

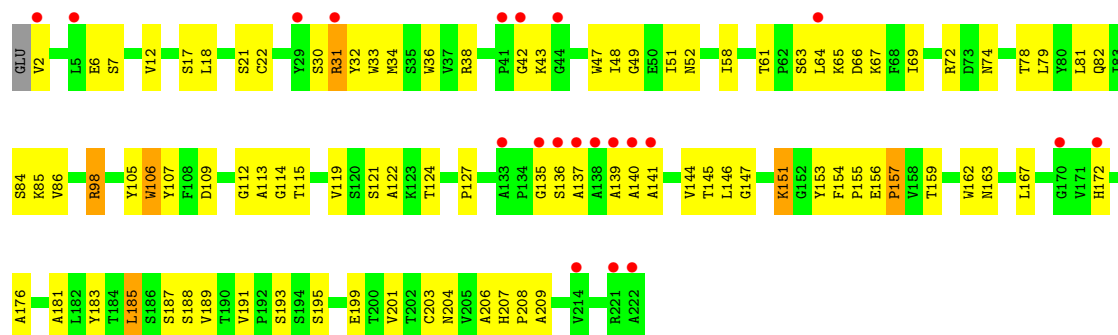


- Molecule 1: Voltage-gated ClC-type chloride channel eriC

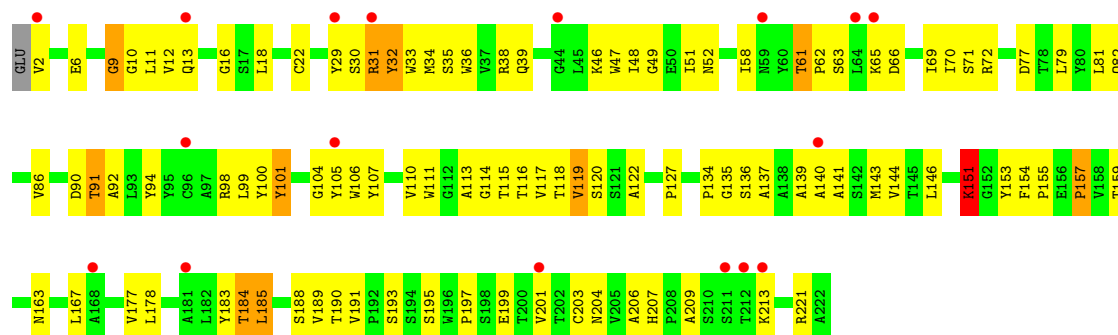




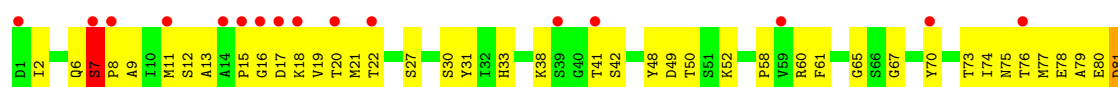
• Molecule 2: Fab fragment (heavy chain)

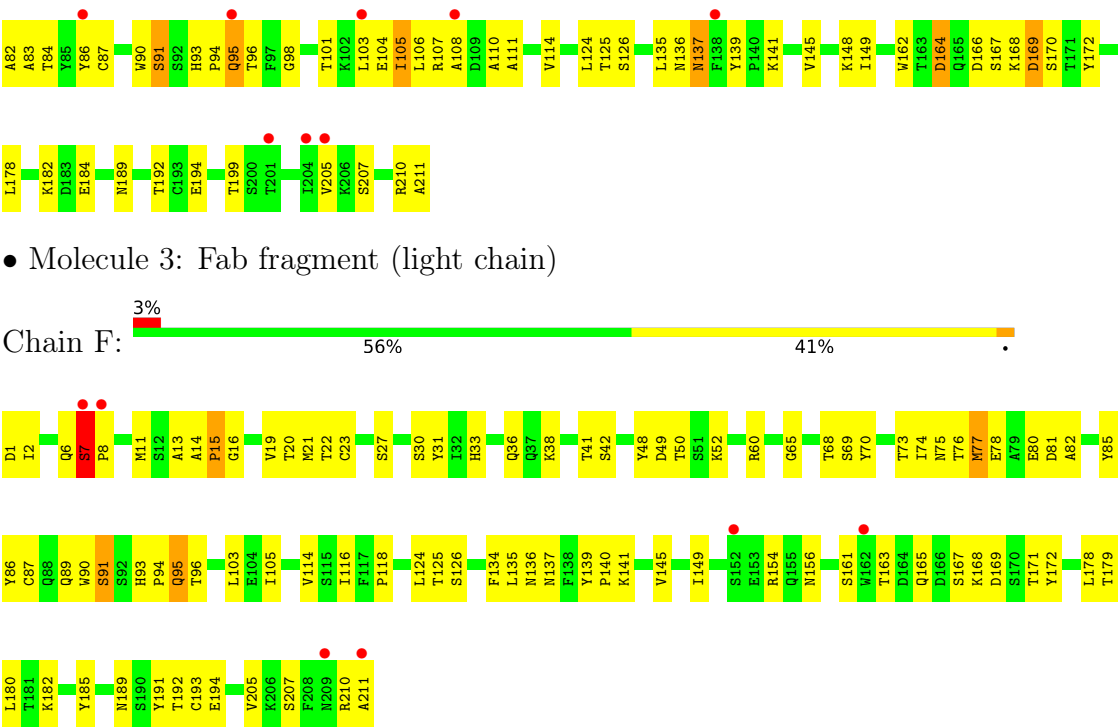


• Molecule 2: Fab fragment (heavy chain)



• Molecule 3: Fab fragment (light chain)





● Molecule 3: Fab fragment (light chain)

Chain F: 3% 56% 41% .

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.94Å 93.87Å 168.54Å 90.00° 131.72° 90.00°	Depositor
Resolution (Å)	24.58 – 2.51 24.58 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.58-2.51) 95.9 (24.58-2.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.264 , 0.299 0.252 , 0.281	Depositor DCC
R_{free} test set	4446 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13654	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

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	0.50	0/3405	0.96	7/4621 (0.2%)
1	B	0.53	1/3376 (0.0%)	0.98	8/4583 (0.2%)
2	C	0.52	0/1721	0.93	3/2355 (0.1%)
2	E	0.52	0/1721	0.95	4/2355 (0.2%)
3	D	0.45	0/1660	0.96	7/2257 (0.3%)
3	F	0.60	0/1660	1.00	6/2257 (0.3%)
All	All	0.52	1/13543 (0.0%)	0.96	35/18428 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	ILE	CA-CB	5.01	1.57	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ILE	N-CA-C	-10.55	102.87	113.10
1	B	356	ILE	N-CA-C	-9.37	103.90	112.90
3	F	7	SER	CA-C-N	-8.02	110.36	120.23
3	F	7	SER	C-N-CA	-8.02	110.36	120.23
2	C	106	TRP	N-CA-C	7.52	120.02	110.24
2	E	66	ASP	N-CA-C	-7.42	100.68	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	7	SER	CA-C-N	-7.39	111.40	119.98
3	D	7	SER	C-N-CA	-7.39	111.40	119.98
3	D	91	SER	N-CA-C	-7.14	103.83	112.54
3	F	137	ASN	N-CA-C	7.08	120.84	111.28
1	A	108	GLY	N-CA-C	-7.05	106.08	114.48
3	F	91	SER	N-CA-C	-6.88	104.88	113.20
3	F	136	ASN	N-CA-C	6.75	121.30	109.96
1	B	361	LEU	N-CA-C	-6.34	104.29	111.14
3	D	164	ASP	N-CA-C	-6.18	102.56	110.53
3	D	137	ASN	N-CA-C	6.12	119.54	111.28
2	E	32	TYR	N-CA-C	5.77	118.36	109.07
2	C	121	SER	N-CA-C	-5.71	106.36	113.38
1	A	256	LEU	N-CA-C	-5.68	105.01	111.14
3	D	136	ASN	N-CA-C	5.63	119.00	109.76
1	B	451	ARG	N-CA-C	-5.57	104.85	111.03
2	E	61	THR	N-CA-C	-5.56	102.05	110.39
1	A	39	ALA	N-CA-C	-5.53	105.41	111.82
2	E	151	LYS	N-CA-C	5.49	117.53	109.24
2	C	151	LYS	N-CA-C	5.46	118.48	109.85
1	A	431	GLY	N-CA-C	-5.46	106.18	112.73
1	B	127	VAL	N-CA-C	5.44	116.07	110.36
1	A	154	ILE	N-CA-C	-5.34	105.17	110.62
1	B	431	GLY	N-CA-C	-5.32	106.35	112.73
1	B	341	VAL	N-CA-C	-5.26	105.25	110.62
3	D	9	ALA	N-CA-C	-5.21	105.68	111.36
1	B	158	ILE	N-CA-C	-5.16	105.36	110.62
1	B	422	ILE	N-CA-C	5.08	115.69	110.36
3	F	163	THR	N-CA-C	-5.06	103.26	110.59
1	A	361	LEU	N-CA-C	-5.05	105.69	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	101	TYR	Sidechain

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	3484	251	0
1	B	3304	0	3457	253	0
2	C	1672	0	1654	83	0
2	E	1672	0	1654	103	0
3	D	1621	0	1546	92	0
3	F	1621	0	1546	99	0
4	A	2	0	0	1	0
4	B	2	0	0	2	0
5	A	76	0	0	4	0
5	B	91	0	0	11	0
5	C	85	0	0	10	0
5	D	36	0	0	7	0
5	E	69	0	0	10	0
5	F	70	0	0	10	0
All	All	13654	0	13341	818	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 31.

All (818) 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)
1:A:119:GLN:HE21	1:A:119:GLN:HA	1.07	1.15
2:E:9:GLY:H	2:E:115:THR:HG21	1.11	1.15
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.38	1.06
3:F:95:GLN:H	3:F:95:GLN:CD	1.66	1.03
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.41	1.03
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.40	1.03
1:A:381:GLN:HE21	1:A:381:GLN:N	1.58	1.00
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.40	1.00
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.44	0.99
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.43	0.99
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.43	0.98
1:B:251:THR:HG21	5:B:529:HOH:O	1.64	0.98
1:B:381:GLN:HE21	1:B:381:GLN:N	1.61	0.98
1:A:180:THR:HG22	1:A:218:VAL:HA	1.46	0.98
3:D:95:GLN:CD	3:D:95:GLN:H	1.69	0.97
1:A:381:GLN:H	1:A:381:GLN:NE2	1.62	0.97
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.48	0.95
1:A:235:GLU:O	1:A:236:VAL:HG23	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.03	0.93
3:D:41:THR:HG23	5:D:222:HOH:O	1.67	0.93
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.47	0.93
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.35	0.91
1:B:381:GLN:H	1:B:381:GLN:NE2	1.66	0.91
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.54	0.89
2:E:9:GLY:N	2:E:115:THR:HG21	1.86	0.88
2:C:113:ALA:HA	3:D:42:SER:OG	1.73	0.88
1:A:119:GLN:HA	1:A:119:GLN:NE2	1.88	0.87
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.56	0.87
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.57	0.87
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.56	0.86
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.56	0.85
1:A:381:GLN:HE21	1:A:381:GLN:H	0.86	0.85
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.59	0.85
3:F:19:VAL:HG21	3:F:77:MET:HE3	1.58	0.85
3:F:95:GLN:CD	3:F:95:GLN:N	2.30	0.85
3:D:95:GLN:CD	3:D:95:GLN:N	2.29	0.84
2:E:46:LYS:HG3	5:E:273:HOH:O	1.75	0.84
1:A:72:ALA:HA	1:A:78:LEU:HD12	1.59	0.84
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.43	0.84
2:E:9:GLY:HA3	2:E:115:THR:HG22	1.58	0.84
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.60	0.84
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.60	0.83
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.41	0.83
2:E:13:GLN:HG2	5:E:264:HOH:O	1.77	0.83
1:B:78:LEU:HD12	1:B:79:LEU:N	1.95	0.82
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.43	0.82
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.60	0.81
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.59	0.81
2:E:221:ARG:HH12	3:F:118:PRO:HB2	1.43	0.81
3:D:17:ASP:H	3:D:76:THR:HA	1.46	0.81
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.61	0.81
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.46	0.81
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.44	0.80
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.63	0.80
1:B:180:THR:HG22	1:B:218:VAL:HA	1.62	0.79
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.65	0.79
1:A:144:VAL:HG21	1:A:343:THR:HB	1.65	0.78
1:B:409:ILE:HD13	1:B:426:ILE:HA	1.66	0.78
3:F:141:LYS:HG2	5:F:254:HOH:O	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.66	0.76
1:B:33:LEU:HD23	1:B:33:LEU:O	1.86	0.75
1:B:148:GLU:OE1	1:B:357:PHE:HB3	1.87	0.75
2:E:134:PRO:O	2:E:221:ARG:HG3	1.86	0.75
3:F:189:ASN:HD21	3:F:211:ALA:H	1.34	0.75
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.21	0.74
1:B:144:VAL:HG21	1:B:343:THR:HB	1.69	0.74
3:D:106:LEU:HD23	3:D:107:ARG:N	2.03	0.74
3:D:189:ASN:HD21	3:D:211:ALA:H	1.37	0.73
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.23	0.73
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.18	0.73
1:B:328:PHE:O	1:B:373:MET:HE1	1.89	0.73
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.70	0.73
1:B:381:GLN:HE21	1:B:381:GLN:H	0.82	0.73
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.71	0.72
1:B:411:LEU:HG	1:B:415:MET:HE2	1.71	0.72
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.70	0.72
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.70	0.72
1:B:176:THR:O	1:B:180:THR:HG23	1.90	0.72
1:A:19:ARG:HB2	1:A:19:ARG:NH1	2.05	0.71
1:A:150:PRO:O	1:A:154:ILE:HG13	1.90	0.71
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.04	0.71
3:F:27:SER:O	3:F:68:THR:HG22	1.90	0.71
1:A:216:LYS:HE2	1:B:433:THR:HG22	1.72	0.71
1:A:411:LEU:HG	1:A:415:MET:HE2	1.73	0.71
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.73	0.71
2:C:7:SER:HA	2:C:115:THR:HG21	1.73	0.71
3:F:38:LYS:O	3:F:41:THR:HG22	1.91	0.71
1:B:346:LEU:O	1:B:350:SER:HB3	1.92	0.70
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.07	0.70
2:E:30:SER:C	2:E:32:TYR:H	1.98	0.70
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.56	0.69
2:E:9:GLY:HA3	2:E:115:THR:CG2	2.23	0.69
2:C:195:SER:O	2:C:199:GLU:HB3	1.93	0.69
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.74	0.69
1:A:433:THR:HG22	1:B:216:LYS:HZ3	1.57	0.69
1:A:148:GLU:OE1	1:A:357:PHE:HB3	1.93	0.69
3:F:95:GLN:H	3:F:95:GLN:NE2	1.90	0.68
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.73	0.68
1:B:92:PHE:O	1:B:96:LEU:HD23	1.93	0.68
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.75	0.68
2:E:221:ARG:NH1	3:F:118:PRO:HB2	2.09	0.68
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.74	0.68
1:A:33:LEU:O	1:A:33:LEU:HD23	1.94	0.68
3:F:38:LYS:NZ	3:F:80:GLU:O	2.27	0.68
1:A:223:ILE:CD1	1:B:426:ILE:HG22	2.21	0.68
1:B:154:ILE:O	1:B:158:ILE:HG12	1.93	0.68
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.09	0.68
2:C:6:GLU:O	2:C:115:THR:HG23	1.93	0.67
3:D:7:SER:HB2	3:D:22:THR:HB	1.76	0.67
2:E:2:VAL:N	5:E:271:HOH:O	2.27	0.67
1:A:180:THR:HG22	1:A:218:VAL:CA	2.24	0.67
2:C:185:LEU:C	2:C:185:LEU:HD12	2.20	0.67
1:B:270:ASN:O	1:B:273:VAL:HG12	1.94	0.67
1:B:75:TYR:CE2	1:B:79:LEU:HD11	2.30	0.66
1:B:211:THR:HG22	1:B:213:ILE:HG13	1.78	0.66
1:B:356:ILE:HG23	1:B:360:MET:CE	2.26	0.66
3:D:137:ASN:ND2	5:D:243:HOH:O	2.29	0.66
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.78	0.66
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.31	0.66
1:A:398:LEU:HD22	1:A:402:ILE:HD12	1.77	0.66
3:D:95:GLN:N	3:D:95:GLN:OE1	2.27	0.65
1:A:220:ILE:CG1	1:B:430:LEU:HD21	2.24	0.65
2:E:195:SER:O	2:E:199:GLU:HB3	1.96	0.65
1:A:226:THR:O	1:A:230:ARG:HG2	1.95	0.65
3:D:192:THR:HG22	3:D:207:SER:CB	2.26	0.65
1:A:38:MET:HG3	1:A:168:LEU:CD1	2.24	0.65
1:A:74:ASN:HD22	1:A:76:PRO:HD2	1.59	0.65
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.26	0.65
1:A:176:THR:O	1:A:180:THR:HG23	1.97	0.65
3:D:192:THR:HG23	5:D:212:HOH:O	1.96	0.65
1:B:109:ILE:O	1:B:113:GLU:HG3	1.96	0.65
1:A:241:VAL:CG1	1:A:244:LEU:HD21	2.27	0.65
1:B:211:THR:CG2	1:B:213:ILE:HG13	2.27	0.65
1:A:86:SER:OG	1:A:303:GLY:HA3	1.97	0.64
3:D:30:SER:HA	3:D:70:TYR:OH	1.98	0.64
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.78	0.64
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.32	0.64
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.61	0.64
2:C:145:THR:HB	5:C:249:HOH:O	1.96	0.64
3:F:141:LYS:HB3	3:F:172:TYR:CD1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:O	1:B:424:PRO:HD2	1.97	0.64
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.63	0.64
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.08	0.64
1:A:382:TYR:HB3	1:A:384:LEU:HD21	1.80	0.64
1:A:433:THR:HG22	1:B:216:LYS:HE2	1.78	0.64
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.33	0.64
3:F:20:THR:HG23	3:F:73:THR:OG1	1.97	0.64
3:F:77:MET:HE2	3:F:103:LEU:HD21	1.80	0.63
1:A:92:PHE:O	1:A:96:LEU:HD23	1.98	0.63
3:D:125:THR:HG22	3:D:125:THR:O	1.98	0.63
1:B:340:ARG:NH1	5:B:474:HOH:O	2.30	0.63
3:D:6:GLN:NE2	3:D:87:CYS:H	1.95	0.63
3:D:79:ALA:C	3:D:81:ASP:H	2.06	0.63
2:C:30:SER:C	2:C:32:TYR:H	2.04	0.63
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.34	0.62
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.81	0.62
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.29	0.62
1:B:91:MET:HG2	1:B:292:VAL:O	1.99	0.62
1:B:148:GLU:CD	1:B:148:GLU:H	2.05	0.62
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.34	0.62
3:D:7:SER:CB	3:D:22:THR:HB	2.30	0.62
3:F:30:SER:HA	3:F:70:TYR:OH	2.00	0.62
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.81	0.62
1:A:346:LEU:O	1:A:350:SER:HB3	1.99	0.62
1:B:241:VAL:CG1	1:B:244:LEU:HD21	2.30	0.62
1:B:409:ILE:CD1	1:B:426:ILE:HA	2.29	0.62
3:D:11:MET:HE2	3:D:19:VAL:HG13	1.82	0.62
1:B:422:ILE:HA	1:B:425:MET:HE3	1.82	0.62
2:E:163:ASN:ND2	2:E:167:LEU:HD22	2.14	0.62
1:A:84:LEU:O	1:A:88:VAL:HG23	2.00	0.61
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.82	0.61
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.82	0.61
1:A:235:GLU:OE2	2:E:101:TYR:O	2.18	0.61
1:A:330:MET:HE1	1:A:370:ALA:HB1	1.82	0.61
3:D:189:ASN:HD22	3:D:210:ARG:HB2	1.66	0.61
1:A:148:GLU:CD	1:A:148:GLU:H	2.07	0.61
3:F:31:TYR:HA	3:F:50:THR:OG1	2.01	0.61
2:C:208:PRO:HG2	5:C:251:HOH:O	2.01	0.61
1:A:212:LEU:N	1:A:212:LEU:HD12	2.16	0.61
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.83	0.61
1:B:402:ILE:HD12	1:B:445:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:LEU:HD12	2:C:67:LYS:HD3	1.83	0.60
1:A:148:GLU:HG2	1:A:357:PHE:HB3	1.82	0.60
3:D:110:ALA:C	3:D:199:THR:HG21	2.26	0.60
3:F:80:GLU:HA	3:F:167:SER:O	2.01	0.60
1:A:37:PHE:CD2	1:A:38:MET:HE2	2.37	0.60
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.15	0.60
3:F:7:SER:HB3	3:F:8:PRO:CD	2.31	0.60
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.01	0.60
1:B:150:PRO:O	1:B:154:ILE:HG13	2.01	0.60
1:A:19:ARG:HB2	1:A:19:ARG:HH11	1.66	0.60
1:B:445:TYR:HB2	5:B:489:HOH:O	2.02	0.60
3:F:6:GLN:NE2	3:F:87:CYS:H	1.99	0.60
3:F:22:THR:HG22	5:F:232:HOH:O	2.02	0.60
1:B:37:PHE:HD2	1:B:38:MET:HE2	1.65	0.60
1:A:356:ILE:HG23	1:A:360:MET:CE	2.31	0.60
1:B:267:PRO:HG2	1:B:439:THR:OG1	2.02	0.60
1:A:422:ILE:HD11	1:B:194:LEU:HD11	1.84	0.60
1:B:38:MET:HA	1:B:41:VAL:HG12	1.83	0.60
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.82	0.60
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.66	0.59
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.24	0.59
1:A:379:PHE:HA	1:A:381:GLN:HE22	1.65	0.59
1:B:37:PHE:CD2	1:B:38:MET:HE2	2.36	0.59
2:C:34:MET:HG2	5:C:239:HOH:O	2.02	0.59
1:B:243:LYS:HB3	2:E:31:ARG:HH21	1.67	0.59
2:E:104:GLY:O	2:E:106:TRP:CD1	2.56	0.59
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.37	0.59
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.37	0.59
1:A:426:ILE:HG22	1:B:223:ILE:CD1	2.27	0.59
3:F:82:ALA:HB2	3:F:105:ILE:HG12	1.85	0.59
3:F:125:THR:O	3:F:125:THR:HG22	2.02	0.59
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.37	0.59
1:A:328:PHE:O	1:A:373:MET:HE1	2.03	0.59
2:C:63:SER:HB3	5:C:284:HOH:O	2.02	0.59
3:D:31:TYR:HA	3:D:50:THR:OG1	2.03	0.59
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.84	0.59
2:E:91:THR:OG1	2:E:119:VAL:HG23	2.03	0.59
1:A:148:GLU:HG3	1:A:190:PHE:CZ	2.38	0.59
1:A:279:LEU:HD23	1:A:279:LEU:O	2.03	0.59
2:C:7:SER:HA	2:C:115:THR:CG2	2.32	0.59
2:C:163:ASN:HD22	2:C:167:LEU:HD22	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.28	0.59
1:B:86:SER:OG	1:B:303:GLY:HA3	2.03	0.59
5:C:232:HOH:O	3:D:52:LYS:HE2	2.03	0.59
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.85	0.59
1:A:235:GLU:HG3	5:A:485:HOH:O	2.03	0.58
3:F:7:SER:CB	3:F:8:PRO:HD3	2.31	0.58
1:A:42:VAL:CG2	1:A:162:VAL:HG21	2.33	0.58
1:A:270:ASN:O	1:A:273:VAL:HG12	2.03	0.58
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.84	0.58
2:C:135:GLY:C	2:C:137:ALA:H	2.11	0.58
1:A:18:ARG:HB2	1:B:119:GLN:OE1	2.02	0.58
1:A:216:LYS:HZ3	1:B:433:THR:HG22	1.68	0.58
3:D:95:GLN:H	3:D:95:GLN:NE2	2.00	0.58
2:E:11:LEU:HD11	2:E:120:SER:HB3	1.86	0.58
3:D:8:PRO:O	3:D:101:THR:HG23	2.03	0.58
1:B:330:MET:HE1	1:B:370:ALA:HB1	1.85	0.58
3:D:7:SER:CB	3:D:8:PRO:HD3	2.33	0.58
2:E:163:ASN:HD22	2:E:167:LEU:HD22	1.67	0.58
1:A:111:GLU:OE2	1:A:120:ARG:NE	2.32	0.58
1:B:279:LEU:O	1:B:279:LEU:HD23	2.03	0.58
2:E:51:ILE:CD1	2:E:72:ARG:HG2	2.33	0.58
1:B:241:VAL:HG12	1:B:244:LEU:CD2	2.33	0.58
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.85	0.58
3:F:189:ASN:HD21	3:F:211:ALA:N	2.00	0.58
3:D:106:LEU:HD23	3:D:107:ARG:H	1.67	0.57
3:F:6:GLN:HA	5:F:223:HOH:O	2.04	0.57
1:B:224:MET:O	1:B:228:MET:HG2	2.04	0.57
3:D:106:LEU:HA	3:D:139:TYR:OH	2.04	0.57
3:D:7:SER:HB3	3:D:8:PRO:CD	2.29	0.57
3:F:169:ASP:OD1	3:F:171:THR:HG23	2.04	0.57
1:A:248:PRO:O	1:A:251:THR:HB	2.05	0.57
2:C:106:TRP:H	2:C:106:TRP:CD1	2.23	0.57
3:D:189:ASN:HD21	3:D:211:ALA:N	2.00	0.57
3:F:13:ALA:HB3	3:F:77:MET:CE	2.34	0.57
1:B:42:VAL:CG2	1:B:162:VAL:HG21	2.35	0.57
1:B:212:LEU:HD12	1:B:212:LEU:N	2.19	0.57
1:B:245:SER:HB3	1:B:385:GLU:OE2	2.05	0.57
3:F:2:ILE:HD12	3:F:27:SER:HB2	1.85	0.57
1:A:267:PRO:HG2	1:A:439:THR:OG1	2.05	0.56
1:B:421:LEU:C	1:B:424:PRO:HD2	2.30	0.56
2:C:112:GLY:O	3:D:42:SER:OG	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:60:ARG:HD2	3:D:76:THR:O	2.05	0.56
1:A:216:LYS:CE	1:B:433:THR:HG22	2.35	0.56
1:A:451:ARG:HH11	1:A:451:ARG:HB3	1.69	0.56
3:D:17:ASP:N	3:D:76:THR:HA	2.17	0.56
1:A:241:VAL:HG12	1:A:244:LEU:CD2	2.35	0.56
1:A:430:LEU:HD21	1:B:220:ILE:CG1	2.34	0.56
1:A:433:THR:HG22	1:B:216:LYS:CE	2.35	0.56
1:B:113:GLU:HB3	5:B:513:HOH:O	2.05	0.56
2:E:6:GLU:CD	2:E:114:GLY:H	2.14	0.56
1:A:422:ILE:HA	1:A:425:MET:HE3	1.88	0.56
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.88	0.56
2:E:69:ILE:HB	2:E:82:GLN:HB2	1.88	0.56
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.14	0.56
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.41	0.56
3:F:95:GLN:N	3:F:95:GLN:OE1	2.39	0.56
1:A:68:LEU:CD2	1:A:81:VAL:HG23	2.36	0.55
1:A:211:THR:CG2	1:A:213:ILE:HG13	2.36	0.55
2:C:72:ARG:NH1	5:C:239:HOH:O	2.39	0.55
3:F:192:THR:HG22	3:F:207:SER:CB	2.37	0.55
1:A:273:VAL:HG11	1:A:444:LEU:HD21	1.88	0.55
1:B:78:LEU:HA	1:B:81:VAL:CG2	2.33	0.55
1:B:200:ILE:HA	1:B:204:MET:HB2	1.87	0.55
1:B:287:ASN:HD22	1:B:290:LYS:CG	2.17	0.55
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.41	0.55
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.89	0.55
1:B:227:ILE:O	1:B:231:ILE:HG13	2.04	0.55
3:F:69:SER:HB2	5:F:268:HOH:O	2.06	0.55
1:A:337:PHE:O	1:A:341:VAL:HG23	2.07	0.55
1:B:90:ALA:O	1:B:94:TYR:HD1	1.89	0.55
1:A:430:LEU:CD2	1:B:223:ILE:HD12	2.34	0.55
2:E:213:LYS:HD3	5:E:226:HOH:O	2.05	0.55
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.42	0.55
2:E:6:GLU:HA	2:E:22:CYS:HA	1.88	0.55
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.71	0.55
2:C:7:SER:CA	2:C:115:THR:HG21	2.35	0.55
1:A:211:THR:HG22	1:A:213:ILE:HG13	1.89	0.55
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.89	0.55
1:A:455:LYS:O	1:A:459:GLU:HG2	2.07	0.55
1:B:147:ARG:N	1:B:148:GLU:OE2	2.40	0.55
2:C:32:TYR:CD2	2:C:98:ARG:HG3	2.41	0.55
2:E:144:VAL:O	2:E:144:VAL:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:TYR:HB3	1:A:384:LEU:CD2	2.37	0.54
1:B:68:LEU:HD22	1:B:78:LEU:HB2	1.89	0.54
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.22	0.54
1:B:197:ILE:HD13	1:B:219:PHE:CD1	2.42	0.54
1:A:192:ALA:HB1	1:A:414:GLU:OE2	2.07	0.54
1:A:241:VAL:CG1	1:A:324:THR:HG21	2.37	0.54
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.90	0.54
1:A:154:ILE:O	1:A:158:ILE:HG12	2.06	0.54
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.88	0.54
3:D:192:THR:HG22	3:D:207:SER:HB2	1.88	0.54
1:A:216:LYS:HZ1	1:B:437:GLN:HE21	1.55	0.54
1:A:98:ARG:HD2	1:A:291:TRP:CD2	2.42	0.54
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.30	0.54
1:B:148:GLU:HG2	1:B:357:PHE:HB3	1.89	0.54
3:D:164:ASP:HB3	5:D:226:HOH:O	2.08	0.54
1:A:433:THR:HG22	1:B:216:LYS:NZ	2.23	0.54
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.90	0.54
3:F:22:THR:HG23	5:F:268:HOH:O	2.08	0.54
1:A:398:LEU:O	1:A:402:ILE:HB	2.07	0.54
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.73	0.54
3:D:162:TRP:HE3	5:D:221:HOH:O	1.90	0.54
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.08	0.53
2:E:46:LYS:HB3	5:E:225:HOH:O	2.06	0.53
1:A:197:ILE:HD13	1:A:219:PHE:CD1	2.43	0.53
1:A:227:ILE:O	1:A:231:ILE:HG12	2.07	0.53
1:A:413:LEU:HD13	1:A:425:MET:HE1	1.89	0.53
1:B:148:GLU:HG3	1:B:190:PHE:CZ	2.43	0.53
2:E:86:VAL:HG12	2:E:119:VAL:CG1	2.38	0.53
1:A:119:GLN:HE21	1:A:119:GLN:CA	1.90	0.53
1:B:191:ASN:HB2	1:B:229:TYR:CE2	2.44	0.53
2:C:17:SER:HB3	5:C:238:HOH:O	2.08	0.53
3:D:21:MET:HB2	5:D:224:HOH:O	2.08	0.53
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.89	0.53
2:E:10:GLY:N	2:E:116:THR:O	2.40	0.53
1:A:148:GLU:CG	1:A:357:PHE:HB3	2.39	0.53
1:B:155:GLY:HA3	1:B:181:GLY:O	2.09	0.53
1:B:226:THR:O	1:B:230:ARG:HG2	2.09	0.53
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.43	0.53
1:B:218:VAL:O	1:B:222:VAL:HG23	2.08	0.53
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.91	0.53
1:A:340:ARG:HA	1:A:343:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD22	1:B:294:MET:SD	2.49	0.53
2:E:30:SER:O	2:E:32:TYR:N	2.42	0.53
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.44	0.52
1:B:61:GLN:HA	1:B:64:ARG:HE	1.74	0.52
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.90	0.52
2:C:86:VAL:HG12	2:C:119:VAL:CG1	2.38	0.52
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.73	0.52
1:A:275:GLY:HA2	5:A:486:HOH:O	2.08	0.52
3:D:75:ASN:O	3:D:76:THR:HB	2.09	0.52
2:E:9:GLY:CA	2:E:115:THR:CG2	2.86	0.52
1:A:226:THR:CG2	1:B:423:LEU:HD11	2.39	0.52
2:C:6:GLU:HA	2:C:22:CYS:HA	1.92	0.52
1:A:451:ARG:HH11	1:A:451:ARG:CB	2.22	0.52
1:B:379:PHE:HA	1:B:381:GLN:HE22	1.74	0.52
2:C:113:ALA:HA	3:D:42:SER:HG	1.72	0.52
2:E:35:SER:HB3	2:E:99:LEU:HD21	1.91	0.52
2:E:106:TRP:CD1	2:E:106:TRP:H	2.28	0.52
2:C:141:ALA:O	2:C:193:SER:HB2	2.10	0.52
3:D:82:ALA:HB2	3:D:105:ILE:HG13	1.91	0.52
3:D:189:ASN:ND2	3:D:210:ARG:HB2	2.25	0.52
1:A:91:MET:HG2	1:A:292:VAL:O	2.09	0.52
1:B:356:ILE:O	1:B:360:MET:HG3	2.09	0.52
3:F:189:ASN:HD22	3:F:210:ARG:HB2	1.74	0.52
3:F:60:ARG:NH2	3:F:81:ASP:CG	2.68	0.52
3:F:93:HIS:CG	3:F:94:PRO:HA	2.45	0.52
1:A:78:LEU:HD23	1:A:78:LEU:C	2.36	0.51
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.35	0.51
1:A:379:PHE:HA	1:A:381:GLN:NE2	2.25	0.51
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.24	0.51
1:B:248:PRO:O	1:B:251:THR:HB	2.10	0.51
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.44	0.51
2:E:30:SER:C	2:E:32:TYR:N	2.64	0.51
1:B:182:ALA:HB1	1:B:204:MET:HE2	1.91	0.51
2:E:185:LEU:C	2:E:185:LEU:HD12	2.36	0.51
1:A:18:ARG:O	1:A:22:ILE:HG13	2.09	0.51
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.92	0.51
1:A:423:LEU:HD11	1:B:226:THR:CG2	2.40	0.51
1:A:208:PHE:CE2	1:B:24:GLN:HB3	2.45	0.51
2:C:31:ARG:HD2	5:C:289:HOH:O	2.11	0.51
3:D:78:GLU:O	3:D:81:ASP:HB2	2.10	0.51
1:B:93:GLY:O	1:B:97:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.45	0.51
2:E:2:VAL:HG23	2:E:2:VAL:O	2.11	0.51
1:A:38:MET:HA	1:A:41:VAL:HG12	1.92	0.51
1:B:263:GLY:HA3	1:B:435:LEU:HB2	1.92	0.51
1:A:17:ARG:HG3	1:A:18:ARG:N	2.26	0.51
1:B:20:GLN:O	1:B:23:ARG:HB3	2.10	0.51
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.45	0.51
1:B:77:LEU:O	1:B:80:THR:HB	2.11	0.51
1:B:103:GLU:OE2	5:B:531:HOH:O	2.18	0.51
2:C:185:LEU:HD12	2:C:185:LEU:O	2.09	0.51
1:A:80:THR:O	1:A:84:LEU:HG	2.11	0.51
1:A:159:GLY:O	1:A:162:VAL:HG22	2.11	0.51
1:A:226:THR:HG21	1:B:423:LEU:HD11	1.93	0.51
1:B:180:THR:HG22	1:B:218:VAL:CA	2.37	0.51
1:A:356:ILE:O	1:A:360:MET:HG3	2.10	0.50
1:B:260:ILE:O	1:B:264:ILE:HG23	2.11	0.50
3:D:15:PRO:HA	3:D:77:MET:O	2.11	0.50
2:E:39:GLN:O	2:E:92:ALA:HB1	2.11	0.50
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.41	0.50
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.93	0.50
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.93	0.50
3:D:20:THR:HG23	3:D:73:THR:OG1	2.11	0.50
2:E:135:GLY:C	2:E:137:ALA:H	2.19	0.50
3:F:23:CYS:HB2	5:F:223:HOH:O	2.10	0.50
1:B:110:PRO:HG2	4:B:467:CL:CL	2.48	0.50
1:B:182:ALA:HB1	1:B:204:MET:CE	2.41	0.50
2:E:197:PRO:HD3	5:E:247:HOH:O	2.12	0.50
2:E:51:ILE:HG23	2:E:51:ILE:O	2.11	0.50
3:F:31:TYR:HB3	3:F:49:ASP:HA	1.93	0.50
2:C:30:SER:O	2:C:32:TYR:N	2.45	0.50
1:A:202:GLU:O	1:A:202:GLU:HG2	2.10	0.50
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.76	0.50
2:E:188:SER:HB3	3:F:134:PHE:CE2	2.46	0.50
1:A:91:MET:CG	1:A:296:GLY:HA3	2.42	0.50
1:A:410:ILE:O	1:A:414:GLU:HG3	2.11	0.50
1:A:447:ALA:O	1:A:451:ARG:HG2	2.11	0.50
1:B:180:THR:CG2	1:B:218:VAL:HA	2.37	0.50
3:F:77:MET:CE	3:F:103:LEU:HD11	2.42	0.50
1:B:243:LYS:HD2	5:B:482:HOH:O	2.10	0.50
2:C:30:SER:C	2:C:32:TYR:N	2.70	0.50
1:A:33:LEU:HD23	1:A:33:LEU:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.47	0.50
2:C:167:LEU:HD21	2:C:191:VAL:HG11	1.94	0.49
2:E:32:TYR:HA	5:E:223:HOH:O	2.12	0.49
1:A:235:GLU:O	1:A:236:VAL:CG2	2.51	0.49
1:A:449:LEU:O	1:A:453:LEU:HB2	2.12	0.49
1:B:323:ALA:HA	5:B:503:HOH:O	2.11	0.49
3:D:38:LYS:O	3:D:41:THR:HG22	2.11	0.49
1:A:59:TRP:O	1:A:62:ASN:HB3	2.13	0.49
1:B:33:LEU:HD23	1:B:33:LEU:C	2.37	0.49
1:B:382:TYR:HB3	1:B:384:LEU:HD21	1.95	0.49
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.93	0.49
1:B:41:VAL:O	1:B:45:LEU:HG	2.11	0.49
2:C:12:VAL:HG11	2:C:18:LEU:HB3	1.94	0.49
1:A:213:ILE:HB	5:A:498:HOH:O	2.12	0.49
3:D:82:ALA:HA	3:D:103:LEU:O	2.12	0.49
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.48	0.49
1:A:420:GLN:NE2	5:A:516:HOH:O	2.45	0.49
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.37	0.49
3:D:2:ILE:O	3:D:96:THR:HG21	2.13	0.49
3:F:13:ALA:HB3	3:F:77:MET:HE1	1.93	0.49
1:A:416:THR:O	1:A:418:ASN:ND2	2.41	0.49
2:E:71:SER:O	2:E:79:LEU:HD12	2.13	0.49
1:A:41:VAL:O	1:A:45:LEU:HG	2.13	0.48
1:B:200:ILE:CD1	1:B:204:MET:HG3	2.31	0.48
1:B:336:ILE:O	1:B:340:ARG:HG3	2.13	0.48
2:E:159:THR:OG1	2:E:206:ALA:HB3	2.13	0.48
3:F:15:PRO:HD3	3:F:105:ILE:HG23	1.95	0.48
1:A:68:LEU:HD23	1:A:81:VAL:HG23	1.95	0.48
1:B:109:ILE:HD12	1:B:445:TYR:OH	2.12	0.48
1:B:387:GLY:N	5:B:502:HOH:O	2.36	0.48
2:C:6:GLU:CG	2:C:114:GLY:HA2	2.43	0.48
2:C:12:VAL:HG11	2:C:18:LEU:HD13	1.94	0.48
2:E:9:GLY:N	2:E:115:THR:CG2	2.68	0.48
2:E:221:ARG:HH11	3:F:118:PRO:HD2	1.79	0.48
3:F:7:SER:CB	3:F:22:THR:HB	2.43	0.48
1:A:78:LEU:C	1:A:80:THR:N	2.70	0.48
1:A:423:LEU:HD11	1:B:226:THR:HG21	1.94	0.48
1:B:330:MET:HE1	1:B:370:ALA:CB	2.42	0.48
2:E:18:LEU:HD11	2:E:117:VAL:CG2	2.43	0.48
2:E:61:THR:O	2:E:63:SER:N	2.46	0.48
2:E:86:VAL:HG13	2:E:90:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD12	1:A:445:TYR:OH	2.13	0.48
1:A:224:MET:O	1:A:228:MET:HG2	2.14	0.48
1:A:330:MET:HE1	1:A:370:ALA:CB	2.42	0.48
1:A:336:ILE:O	1:A:340:ARG:HG3	2.11	0.48
1:A:409:ILE:HD12	1:A:426:ILE:HA	1.94	0.48
3:D:93:HIS:CG	3:D:94:PRO:HA	2.49	0.48
1:B:78:LEU:HD12	1:B:78:LEU:C	2.38	0.48
1:B:144:VAL:HG21	1:B:343:THR:CB	2.40	0.48
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.49	0.48
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.96	0.48
1:A:305:LEU:C	1:A:307:PHE:H	2.21	0.48
1:A:442:LYS:HZ3	1:B:26:LEU:HB3	1.79	0.48
1:B:163:LEU:HD22	1:B:174:ARG:HA	1.95	0.48
2:E:29:TYR:HB2	2:E:77:ASP:OD2	2.14	0.48
1:A:78:LEU:C	1:A:80:THR:H	2.21	0.48
1:B:111:GLU:OE2	1:B:120:ARG:NE	2.45	0.48
3:F:2:ILE:CD1	3:F:27:SER:HB2	2.43	0.48
1:B:71:THR:O	1:B:78:LEU:HB3	2.13	0.48
1:B:148:GLU:CD	1:B:357:PHE:HB3	2.38	0.48
2:C:51:ILE:CD1	2:C:72:ARG:HG2	2.44	0.48
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.96	0.47
2:E:141:ALA:O	2:E:193:SER:HB2	2.15	0.47
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.96	0.47
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.97	0.47
1:B:186:LEU:HD22	1:B:199:PHE:CD2	2.49	0.47
2:E:104:GLY:O	2:E:106:TRP:HD1	1.97	0.47
1:A:74:ASN:HD22	1:A:74:ASN:C	2.21	0.47
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.95	0.47
2:E:12:VAL:HG11	2:E:18:LEU:HD13	1.96	0.47
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.29	0.47
1:A:457:GLU:O	1:A:459:GLU:N	2.46	0.47
1:B:270:ASN:O	1:B:273:VAL:CG1	2.61	0.47
1:A:20:GLN:O	1:A:23:ARG:HB3	2.14	0.47
1:B:241:VAL:HG12	1:B:241:VAL:O	2.14	0.47
1:B:245:SER:HB2	5:B:550:HOH:O	2.13	0.47
1:A:73:ASP:CG	1:A:74:ASN:N	2.72	0.47
1:A:123:ARG:HA	1:A:125:TRP:CH2	2.50	0.47
1:B:91:MET:CG	1:B:296:GLY:HA3	2.44	0.47
1:B:190:PHE:HA	1:B:238:LEU:CD1	2.45	0.47
1:B:239:ILE:CD1	1:B:394:MET:HE1	2.44	0.47
3:D:12:SER:HA	3:D:104:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:151:LYS:HB2	2:E:184:THR:OG1	2.15	0.47
3:F:11:MET:HE2	3:F:19:VAL:HG13	1.97	0.47
1:A:144:VAL:HG12	1:A:144:VAL:O	2.15	0.47
1:A:239:ILE:HG22	1:A:241:VAL:HG23	1.97	0.47
1:B:74:ASN:C	1:B:74:ASN:HD22	2.22	0.47
1:B:109:ILE:N	1:B:110:PRO:CD	2.78	0.47
2:E:16:GLY:O	2:E:86:VAL:HG23	2.15	0.47
2:E:94:TYR:O	2:E:114:GLY:HA2	2.14	0.47
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.30	0.47
1:B:148:GLU:CG	1:B:357:PHE:HB3	2.45	0.47
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.97	0.47
1:A:109:ILE:O	1:A:113:GLU:HG3	2.15	0.47
1:B:374:VAL:O	1:B:378:LEU:HG	2.14	0.47
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.97	0.47
1:A:75:TYR:CZ	1:A:79:LEU:HD11	2.50	0.46
1:B:305:LEU:C	1:B:307:PHE:H	2.22	0.46
3:F:139:TYR:HA	3:F:140:PRO:C	2.40	0.46
1:A:413:LEU:HD11	1:A:419:TYR:HA	1.98	0.46
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.97	0.46
2:C:2:VAL:HG23	2:C:2:VAL:O	2.15	0.46
2:C:6:GLU:CD	2:C:114:GLY:H	2.24	0.46
2:C:189:VAL:O	2:C:189:VAL:HG13	2.14	0.46
1:A:260:ILE:O	1:A:264:ILE:HG23	2.15	0.46
3:F:192:THR:HG22	3:F:207:SER:HB2	1.97	0.46
3:D:13:ALA:O	3:D:77:MET:HE1	2.15	0.46
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.16	0.46
1:A:457:GLU:O	1:A:458:ALA:C	2.59	0.46
1:B:107:SER:HB3	4:B:467:CL:CL	2.53	0.46
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.98	0.46
1:B:273:VAL:HG11	1:B:444:LEU:HD21	1.98	0.46
1:A:144:VAL:HG21	1:A:343:THR:CB	2.41	0.46
1:A:144:VAL:CG2	1:A:343:THR:HB	2.41	0.46
1:B:456:GLN:C	1:B:458:ALA:H	2.24	0.46
2:E:105:TYR:CD1	2:E:105:TYR:N	2.83	0.46
3:F:6:GLN:HG2	5:F:223:HOH:O	2.14	0.46
1:B:253:TRP:CZ2	1:B:254:LEU:HD21	2.51	0.46
1:B:274:LEU:O	1:B:277:GLN:HB2	2.16	0.46
2:C:122:ALA:HB1	2:C:181:ALA:HB1	1.98	0.46
3:F:90:TRP:CE3	3:F:95:GLN:HG3	2.51	0.46
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.81	0.46
2:C:185:LEU:C	2:C:185:LEU:CD1	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:75:ASN:O	3:F:76:THR:HB	2.16	0.46
3:F:169:ASP:HA	5:F:227:HOH:O	2.16	0.46
3:D:149:ILE:HD11	3:D:178:LEU:HD21	1.97	0.45
3:D:210:ARG:HG2	3:D:210:ARG:HH11	1.80	0.45
2:E:70:ILE:HG12	2:E:81:LEU:HD13	1.98	0.45
2:E:167:LEU:HD21	2:E:191:VAL:HG11	1.98	0.45
3:D:17:ASP:OD1	3:D:18:LYS:N	2.50	0.45
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.51	0.45
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.50	0.45
3:F:78:GLU:O	3:F:81:ASP:HB2	2.15	0.45
1:A:147:ARG:N	1:A:148:GLU:OE2	2.50	0.45
1:A:155:GLY:HA3	1:A:181:GLY:O	2.16	0.45
1:A:146:GLY:HA3	1:A:148:GLU:OE2	2.16	0.45
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.51	0.45
1:B:454:ALA:C	1:B:456:GLN:H	2.24	0.45
1:A:73:ASP:CG	1:A:74:ASN:H	2.23	0.45
1:B:209:ARG:HG2	1:B:209:ARG:HH11	1.82	0.45
1:B:379:PHE:HA	1:B:381:GLN:NE2	2.32	0.45
2:C:86:VAL:CG1	2:C:119:VAL:CG2	2.95	0.45
3:D:111:ALA:HA	3:D:199:THR:OG1	2.16	0.45
2:E:207:HIS:CE1	2:E:209:ALA:HB3	2.51	0.45
3:F:154:ARG:HE	3:F:156:ASN:HB2	1.81	0.45
1:A:26:LEU:HD21	5:B:545:HOH:O	2.17	0.45
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.13	0.45
3:D:145:VAL:HA	3:D:194:GLU:O	2.17	0.45
2:E:113:ALA:HA	3:F:42:SER:OG	2.15	0.45
2:C:86:VAL:HG11	2:C:119:VAL:HG22	1.99	0.45
2:E:9:GLY:CA	2:E:115:THR:HG21	2.45	0.45
3:F:7:SER:HB2	3:F:22:THR:HB	1.99	0.45
1:A:255:TYR:CE2	1:A:424:PRO:HB3	2.51	0.45
1:A:270:ASN:HD21	1:A:401:SER:HB3	1.81	0.45
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.32	0.45
1:B:241:VAL:HG11	1:B:324:THR:HG21	1.99	0.45
3:D:192:THR:HG22	3:D:207:SER:HB3	1.98	0.45
1:A:332:MET:O	1:A:336:ILE:HG13	2.17	0.45
1:B:72:ALA:HA	1:B:78:LEU:HD23	1.98	0.45
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.99	0.45
1:A:148:GLU:CG	1:A:190:PHE:CZ	3.00	0.45
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.99	0.45
1:B:126:ARG:O	1:B:130:VAL:HG23	2.17	0.45
1:B:239:ILE:HG22	1:B:241:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:THR:HG22	1:B:255:TYR:HE1	1.81	0.45
2:E:61:THR:O	2:E:62:PRO:C	2.60	0.45
2:E:110:VAL:HA	5:E:281:HOH:O	2.16	0.45
1:A:90:ALA:O	1:A:94:TYR:HD1	2.01	0.44
1:B:229:TYR:CE1	1:B:233:ASN:ND2	2.86	0.44
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.87	0.44
1:A:434:LEU:HD23	1:B:216:LYS:HD3	2.00	0.44
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.99	0.44
2:C:86:VAL:HG12	2:C:119:VAL:HG11	1.99	0.44
3:F:7:SER:CB	3:F:8:PRO:CD	2.94	0.44
1:A:216:LYS:NZ	1:B:433:THR:HG22	2.31	0.44
1:A:218:VAL:O	1:A:222:VAL:HG23	2.17	0.44
1:A:241:VAL:HG12	1:A:241:VAL:O	2.17	0.44
1:A:249:LEU:C	1:A:251:THR:H	2.25	0.44
2:E:177:VAL:HG13	5:E:254:HOH:O	2.16	0.44
1:A:187:ALA:HB2	1:A:222:VAL:HG13	1.99	0.44
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.83	0.44
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.98	0.44
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.99	0.44
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.50	0.44
3:F:179:THR:O	3:F:180:LEU:HD23	2.18	0.44
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.86	0.44
1:A:24:GLN:HB3	1:B:208:PHE:CE2	2.53	0.44
1:A:109:ILE:N	1:A:110:PRO:CD	2.80	0.44
1:A:198:LEU:HG	1:A:410:ILE:CD1	2.48	0.44
1:A:402:ILE:HD13	1:A:445:TYR:CE1	2.53	0.44
1:B:148:GLU:O	1:B:152:VAL:HG23	2.18	0.44
1:B:402:ILE:HD12	1:B:445:TYR:HE1	1.82	0.44
1:B:451:ARG:HH11	1:B:451:ARG:CG	2.30	0.44
1:A:67:ALA:C	1:A:69:VAL:H	2.26	0.44
1:A:148:GLU:CD	1:A:148:GLU:N	2.76	0.44
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.85	0.44
2:C:42:GLY:N	5:C:276:HOH:O	2.51	0.44
2:C:43:LYS:HB3	2:C:43:LYS:NZ	2.32	0.44
3:D:20:THR:HG23	3:D:73:THR:HG1	1.82	0.44
1:B:148:GLU:CG	1:B:190:PHE:CZ	3.00	0.44
1:B:280:LEU:HD13	1:B:350:SER:HA	2.00	0.44
3:D:6:GLN:HA	3:D:22:THR:O	2.17	0.44
3:D:184:GLU:HG2	5:D:239:HOH:O	2.18	0.44
2:E:51:ILE:HG13	2:E:58:ILE:HG12	2.00	0.44
3:F:6:GLN:CG	5:F:223:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:11:MET:CE	3:F:19:VAL:HG13	2.48	0.44
1:A:75:TYR:CZ	1:A:79:LEU:HD21	2.53	0.43
1:A:83:PHE:CD1	1:A:83:PHE:C	2.96	0.43
1:A:100:TYR:O	1:A:126:ARG:NH1	2.48	0.43
1:A:162:VAL:HG23	1:A:163:LEU:N	2.33	0.43
1:B:148:GLU:O	1:B:149:GLY:C	2.61	0.43
1:B:38:MET:O	1:B:41:VAL:HG12	2.18	0.43
1:B:187:ALA:HB2	1:B:222:VAL:HG13	1.99	0.43
1:B:255:TYR:CE2	1:B:424:PRO:HB3	2.53	0.43
1:B:382:TYR:HB3	1:B:384:LEU:CD2	2.48	0.43
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.53	0.43
2:E:188:SER:HB3	3:F:134:PHE:CZ	2.53	0.43
3:F:2:ILE:O	3:F:96:THR:HG21	2.18	0.43
3:F:189:ASN:ND2	3:F:210:ARG:HB2	2.33	0.43
1:B:309:ALA:N	1:B:310:PRO:HD3	2.33	0.43
2:C:159:THR:OG1	2:C:206:ALA:HB3	2.18	0.43
2:E:86:VAL:HG12	2:E:119:VAL:HG13	1.98	0.43
1:B:74:ASN:HD22	1:B:76:PRO:HD2	1.83	0.43
3:D:7:SER:CB	3:D:8:PRO:CD	2.95	0.43
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.32	0.43
3:F:210:ARG:HH11	3:F:210:ARG:HG2	1.82	0.43
1:A:180:THR:CG2	1:A:218:VAL:HA	2.32	0.43
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.44	0.43
1:B:194:LEU:O	1:B:198:LEU:HD23	2.19	0.43
1:B:231:ILE:O	1:B:231:ILE:HG22	2.17	0.43
1:B:422:ILE:CG2	1:B:423:LEU:N	2.81	0.43
1:B:447:ALA:O	1:B:451:ARG:HG2	2.18	0.43
3:D:17:ASP:OD1	3:D:17:ASP:C	2.61	0.43
3:F:13:ALA:HB3	3:F:77:MET:HE3	2.00	0.43
3:F:149:ILE:HD11	3:F:178:LEU:HD21	2.01	0.43
1:A:193:PRO:HA	1:A:222:VAL:CG1	2.49	0.43
1:A:200:ILE:CD1	1:A:204:MET:HG3	2.29	0.43
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.19	0.43
2:E:139:ALA:O	2:E:141:ALA:N	2.52	0.43
1:A:91:MET:HG3	1:A:296:GLY:CA	2.48	0.43
1:A:94:TYR:OH	1:A:352:ALA:HB2	2.19	0.43
1:B:73:ASP:O	1:B:74:ASN:HB3	2.19	0.43
1:B:123:ARG:HA	1:B:125:TRP:CH2	2.54	0.43
1:B:198:LEU:HG	1:B:410:ILE:CD1	2.49	0.43
2:E:178:LEU:HB2	2:E:183:TYR:CE2	2.54	0.43
3:F:141:LYS:HB3	3:F:172:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLY:HA3	1:A:435:LEU:CB	2.48	0.43
1:B:124:TRP:CA	1:B:157:ASN:HD22	2.23	0.43
2:C:33:TRP:CZ2	2:C:52:ASN:HB3	2.53	0.43
2:C:139:ALA:O	2:C:141:ALA:N	2.52	0.43
2:E:35:SER:CB	2:E:99:LEU:HD21	2.49	0.43
3:F:90:TRP:CD2	3:F:95:GLN:HG3	2.54	0.43
3:F:124:LEU:O	3:F:182:LYS:HD2	2.19	0.43
1:A:421:LEU:C	1:A:424:PRO:HD2	2.43	0.43
1:B:144:VAL:CG2	1:B:343:THR:HB	2.44	0.43
1:B:241:VAL:CG1	1:B:324:THR:HG21	2.49	0.43
1:B:349:SER:C	1:B:351:GLY:H	2.27	0.43
3:D:104:GLU:CD	3:D:172:TYR:HH	2.26	0.43
3:F:14:ALA:O	3:F:15:PRO:C	2.61	0.43
1:A:314:GLY:O	1:A:340:ARG:NH2	2.52	0.42
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.86	0.42
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.54	0.42
3:D:2:ILE:CD1	3:D:27:SER:HB2	2.48	0.42
1:B:91:MET:HG3	1:B:296:GLY:CA	2.50	0.42
1:B:248:PRO:HB3	2:E:104:GLY:HA2	1.99	0.42
1:B:313:SER:OG	1:B:314:GLY:N	2.52	0.42
2:C:86:VAL:CG1	2:C:119:VAL:HG22	2.48	0.42
3:D:166:ASP:O	3:D:170:SER:HA	2.18	0.42
1:A:190:PHE:HA	1:A:238:LEU:CD1	2.49	0.42
1:A:288:ILE:O	1:A:292:VAL:HG23	2.19	0.42
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.84	0.42
2:C:135:GLY:C	2:C:137:ALA:N	2.78	0.42
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.54	0.42
2:E:106:TRP:CD1	2:E:106:TRP:N	2.86	0.42
3:F:185:TYR:HA	3:F:191:TYR:OH	2.19	0.42
1:B:200:ILE:HD12	1:B:204:MET:CG	2.35	0.42
2:C:6:GLU:O	2:C:115:THR:CG2	2.66	0.42
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.01	0.42
1:B:123:ARG:NH1	5:B:491:HOH:O	2.52	0.42
1:B:59:TRP:O	1:B:62:ASN:HB3	2.19	0.42
1:B:91:MET:HG3	1:B:296:GLY:HA3	2.00	0.42
3:D:82:ALA:O	3:D:83:ALA:HB2	2.19	0.42
3:D:107:ARG:NE	3:D:108:ALA:O	2.44	0.42
2:E:105:TYR:HD2	3:F:91:SER:HA	1.85	0.42
2:E:143:MET:HE3	2:E:190:THR:HG22	2.01	0.42
3:F:168:LYS:HD3	3:F:168:LYS:N	2.34	0.42
1:A:75:TYR:CE1	1:A:79:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:CD1	1:B:83:PHE:C	2.97	0.42
1:B:267:PRO:O	1:B:270:ASN:HB2	2.19	0.42
1:B:348:PHE:CD1	1:B:356:ILE:HB	2.54	0.42
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.55	0.42
2:E:29:TYR:HB3	5:E:265:HOH:O	2.19	0.42
1:A:216:LYS:NZ	1:B:437:GLN:NE2	2.67	0.42
1:B:272:TRP:O	1:B:276:MET:HB2	2.19	0.42
2:C:84:SER:O	2:C:85:LYS:C	2.62	0.42
1:B:61:GLN:HG2	1:B:64:ARG:HH21	1.84	0.42
1:B:454:ALA:C	1:B:456:GLN:N	2.76	0.42
2:C:105:TYR:HD2	3:D:91:SER:HA	1.85	0.42
3:D:78:GLU:OE2	3:D:78:GLU:HA	2.20	0.42
2:E:38:ARG:HD3	2:E:48:ILE:HD11	2.02	0.42
2:E:111:TRP:CD1	2:E:111:TRP:N	2.87	0.42
1:B:123:ARG:HH21	1:B:126:ARG:HD3	1.85	0.41
1:B:272:TRP:HZ3	1:B:341:VAL:HG11	1.85	0.41
2:C:47:TRP:O	2:C:61:THR:HB	2.19	0.41
2:E:106:TRP:H	2:E:106:TRP:HD1	1.67	0.41
2:E:189:VAL:HG13	2:E:189:VAL:O	2.20	0.41
1:A:107:SER:HB3	4:A:467:CL:CL	2.57	0.41
1:B:38:MET:O	1:B:42:VAL:HG23	2.21	0.41
3:F:114:VAL:HA	3:F:134:PHE:O	2.19	0.41
1:A:357:PHE:HE2	1:A:411:LEU:HD22	1.85	0.41
1:B:64:ARG:NH1	1:B:141:GLY:O	2.53	0.41
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.55	0.41
2:C:147:GLY:HA2	2:C:162:TRP:CH2	2.55	0.41
2:C:172:HIS:O	2:C:187:SER:HA	2.21	0.41
3:F:77:MET:HE2	3:F:103:LEU:HD11	2.01	0.41
1:A:422:ILE:CG2	1:A:423:LEU:N	2.84	0.41
1:B:383:HIS:HB3	2:E:33:TRP:CZ2	2.55	0.41
2:C:106:TRP:H	2:C:106:TRP:HD1	1.68	0.41
2:E:185:LEU:HD12	2:E:185:LEU:O	2.21	0.41
1:A:71:THR:O	1:A:78:LEU:HB2	2.20	0.41
1:A:91:MET:HG3	1:A:296:GLY:HA3	2.01	0.41
1:A:200:ILE:HA	1:A:204:MET:HB2	2.01	0.41
1:A:272:TRP:O	1:A:276:MET:HB2	2.19	0.41
1:B:119:GLN:NE2	1:B:119:GLN:HA	2.36	0.41
1:B:195:ALA:N	1:B:414:GLU:OE2	2.53	0.41
3:D:79:ALA:O	3:D:81:ASP:N	2.49	0.41
2:E:154:PHE:HA	2:E:155:PRO:HA	1.82	0.41
2:E:221:ARG:NH1	3:F:118:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:O	1:A:273:VAL:CG1	2.69	0.41
1:A:280:LEU:HD22	1:A:294:MET:SD	2.60	0.41
1:A:305:LEU:HA	1:A:308:VAL:HG22	2.03	0.41
1:A:421:LEU:O	1:A:424:PRO:HD2	2.21	0.41
1:B:239:ILE:HD13	1:B:394:MET:HE1	2.02	0.41
3:D:84:THR:HA	3:D:101:THR:O	2.19	0.41
3:D:168:LYS:O	3:D:169:ASP:HB3	2.19	0.41
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.50	0.41
3:F:95:GLN:OE1	3:F:95:GLN:O	2.38	0.41
3:F:89:GLN:C	3:F:89:GLN:CD	2.88	0.41
3:F:161:SER:HA	5:F:237:HOH:O	2.20	0.41
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.36	0.41
2:C:2:VAL:N	5:C:252:HOH:O	2.54	0.41
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.56	0.41
3:F:36:GLN:HG3	3:F:85:TYR:CE2	2.56	0.41
3:F:105:ILE:O	3:F:165:GLN:NE2	2.45	0.41
1:A:145:LEU:HB3	1:A:354:GLY:HA3	2.03	0.41
1:B:193:PRO:HA	1:B:222:VAL:CG1	2.51	0.41
1:B:207:GLN:HB3	1:B:208:PHE:CE1	2.56	0.41
2:C:6:GLU:HA	2:C:21:SER:O	2.20	0.41
2:C:124:THR:HA	2:C:154:PHE:O	2.21	0.41
2:E:30:SER:O	2:E:31:ARG:HB2	2.21	0.41
2:E:33:TRP:CZ2	2:E:52:ASN:HB3	2.56	0.41
1:A:198:LEU:HG	1:A:410:ILE:HD13	2.03	0.41
1:B:35:ILE:HD13	1:B:172:GLU:HG2	2.03	0.41
2:C:106:TRP:CD1	2:C:106:TRP:N	2.89	0.41
2:C:172:HIS:HB2	2:C:188:SER:OG	2.21	0.41
2:C:176:ALA:HA	2:C:185:LEU:HB3	2.03	0.41
3:D:166:ASP:OD1	3:D:167:SER:N	2.54	0.41
3:F:21:MET:HE1	3:F:85:TYR:CD1	2.56	0.41
1:A:236:VAL:O	1:A:236:VAL:HG12	2.19	0.40
1:B:86:SER:HB2	1:B:300:GLY:HA2	2.02	0.40
1:B:98:ARG:HA	1:B:98:ARG:NE	2.37	0.40
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.51	0.40
1:B:328:PHE:HB2	1:B:333:LEU:HD21	2.02	0.40
2:C:105:TYR:CD1	2:C:105:TYR:N	2.88	0.40
2:C:144:VAL:O	2:C:144:VAL:HG13	2.20	0.40
3:D:11:MET:CE	3:D:19:VAL:HG13	2.49	0.40
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.21	0.40
2:E:18:LEU:HD23	2:E:18:LEU:H	1.86	0.40
1:A:22:ILE:HD13	1:B:454:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TRP:CA	1:A:157:ASN:HD22	2.22	0.40
1:A:219:PHE:CE1	1:B:406:LEU:HD13	2.56	0.40
1:B:148:GLU:CD	1:B:148:GLU:N	2.76	0.40
3:D:90:TRP:CD2	3:D:95:GLN:HB3	2.56	0.40
3:D:124:LEU:O	3:D:182:LYS:HD2	2.22	0.40
3:F:169:ASP:OD1	3:F:169:ASP:C	2.63	0.40
1:A:87:ALA:O	1:A:91:MET:HG3	2.21	0.40
1:A:287:ASN:ND2	1:A:290:LYS:H	2.19	0.40
1:A:423:LEU:CB	1:A:424:PRO:HD3	2.51	0.40
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.56	0.40
1:A:148:GLU:O	1:A:149:GLY:C	2.64	0.40
1:A:148:GLU:O	1:A:152:VAL:HG23	2.20	0.40
1:A:442:LYS:NZ	1:B:26:LEU:HB3	2.36	0.40
2:C:6:GLU:CD	2:C:114:GLY:HA2	2.47	0.40
1:B:127:VAL:O	1:B:128:LEU:C	2.65	0.40
2:C:22:CYS:O	2:C:78:THR:HG23	2.22	0.40
2:C:38:ARG:CD	2:C:48:ILE:HD11	2.42	0.40
2:E:11:LEU:CD1	2:E:120:SER:HB3	2.51	0.40
2:E:32:TYR:CD2	2:E:98:ARG:HG3	2.56	0.40
3:F:139:TYR:HA	3:F:140:PRO:O	2.21	0.40
3:F:145:VAL:HA	3:F:194:GLU:O	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	442/465 (95%)	404 (91%)	32 (7%)	6 (1%)	9	17
1	B	439/465 (94%)	396 (90%)	39 (9%)	4 (1%)	14	27
2	C	219/222 (99%)	195 (89%)	18 (8%)	6 (3%)	4	6
2	E	219/222 (99%)	194 (89%)	18 (8%)	7 (3%)	3	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	209/211 (99%)	187 (90%)	16 (8%)	6 (3%)	3	5
3	F	209/211 (99%)	191 (91%)	16 (8%)	2 (1%)	12	24
All	All	1737/1796 (97%)	1567 (90%)	139 (8%)	31 (2%)	6	12

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	VAL
2	C	140	ALA
3	D	7	SER
3	D	169	ASP
2	E	140	ALA
3	F	7	SER
1	A	458	ALA
2	C	65	LYS
3	D	67	GLY
3	D	80	GLU
2	E	122	ALA
1	A	171	ASP
2	C	136	SER
3	D	126	SER
2	E	65	LYS
1	A	107	SER
1	A	386	ALA
1	B	107	SER
3	F	126	SER
1	A	307	PHE
1	B	307	PHE
1	B	309	ALA
1	B	365	THR
2	C	31	ARG
2	C	109	ASP
2	E	136	SER
2	E	9	GLY
2	E	31	ARG
3	D	105	ILE
2	C	157	PRO
2	E	157	PRO

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	108/353 (31%)	101 (94%)	7 (6%)	15	32
1	B	332/353 (94%)	311 (94%)	21 (6%)	16	34
2	C	181/182 (100%)	173 (96%)	8 (4%)	25	50
2	E	181/182 (100%)	172 (95%)	9 (5%)	22	44
3	D	185/185 (100%)	183 (99%)	2 (1%)	65	84
3	F	185/185 (100%)	181 (98%)	4 (2%)	45	73
All	All	1172/1440 (81%)	1121 (96%)	51 (4%)	25	50

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	LEU
1	A	381	GLN
1	A	397	LEU
1	A	409	ILE
1	A	420	GLN
1	A	451	ARG
1	A	453	LEU
1	B	103	GLU
1	B	148	GLU
1	B	168	LEU
1	B	200	ILE
1	B	219	PHE
1	B	244	LEU
1	B	245	SER
1	B	251	THR
1	B	277	GLN
1	B	340	ARG
1	B	346	LEU
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN

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Mol	Chain	Res	Type
1	B	423	LEU
1	B	444	LEU
1	B	451	ARG
1	B	452	THR
1	B	453	LEU
1	B	457	GLU
2	C	66	ASP
2	C	98	ARG
2	C	151	LYS
2	C	155	PRO
2	C	157	PRO
2	C	185	LEU
2	C	203	CYS
2	C	204	ASN
3	D	81	ASP
3	D	95	GLN
2	E	91	THR
2	E	118	THR
2	E	119	VAL
2	E	151	LYS
2	E	157	PRO
2	E	184	THR
2	E	185	LEU
2	E	203	CYS
2	E	204	ASN
3	F	15	PRO
3	F	74	ILE
3	F	77	MET
3	F	95	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	B	62	ASN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	207	GLN
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	437	GLN
1	B	456	GLN
2	C	172	HIS
3	D	6	GLN
3	D	136	ASN
3	D	189	ASN
3	D	209	ASN
2	E	172	HIS
3	F	6	GLN
3	F	36	GLN
3	F	89	GLN
3	F	189	ASN
3	F	209	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 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

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, 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	444/465 (95%)	0.69	27 (6%)	27	23	44, 67, 95, 113	0
1	B	441/465 (94%)	0.72	22 (4%)	34	30	44, 66, 95, 112	0
2	C	221/222 (99%)	0.80	21 (9%)	14	12	40, 67, 92, 112	0
2	E	221/222 (99%)	0.82	17 (7%)	19	17	42, 67, 93, 112	0
3	D	211/211 (100%)	1.13	24 (11%)	10	8	46, 76, 95, 103	0
3	F	211/211 (100%)	0.59	6 (2%)	55	50	31, 62, 94, 104	0
All	All	1749/1796 (97%)	0.77	117 (6%)	24	21	31, 68, 95, 113	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	140	ALA	5.3
1	B	235	GLU	5.0
3	D	16	GLY	4.6
1	B	72	ALA	4.5
1	A	168	LEU	4.2
3	D	1	ASP	4.2
3	D	22	THR	4.2
1	B	69	VAL	4.0
2	C	139	ALA	3.8
2	C	29	TYR	3.8
2	E	31	ARG	3.8
1	B	212	LEU	3.8
1	A	234	HIS	3.6
3	D	95	GLN	3.5
3	F	7	SER	3.5
3	D	15	PRO	3.5
2	E	29	TYR	3.4
1	B	73	ASP	3.3
1	A	17	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	140	ALA	3.3
1	A	458	ALA	3.2
1	A	285	GLY	3.2
1	B	307	PHE	3.1
3	D	86	TYR	3.1
1	B	67	ALA	3.1
1	A	72	ALA	3.1
1	A	73	ASP	3.1
2	E	59	ASN	3.0
1	B	18	ARG	3.0
3	D	201	THR	3.0
1	B	458	ALA	3.0
2	C	222	ALA	3.0
2	E	2	VAL	2.9
2	E	65	LYS	2.9
2	E	64	LEU	2.9
1	A	402	ILE	2.9
1	B	71	THR	2.9
2	C	41	PRO	2.9
2	E	13	GLN	2.8
2	E	211	SER	2.8
1	A	101	ALA	2.8
2	C	172	HIS	2.8
2	C	135	GLY	2.7
3	F	152	SER	2.7
2	C	141	ALA	2.7
2	E	96	CYS	2.7
1	A	438	PHE	2.6
2	C	214	VAL	2.6
2	C	136	SER	2.6
3	D	39	SER	2.6
3	D	14	ALA	2.6
3	D	204	ILE	2.6
2	C	138	ALA	2.6
1	B	66	GLY	2.5
1	B	22	ILE	2.5
3	D	138	PHE	2.5
1	A	71	THR	2.5
1	B	75	TYR	2.5
3	F	8	PRO	2.5
2	E	44	GLY	2.5
1	A	169	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	201	VAL	2.5
2	C	31	ARG	2.5
2	C	137	ALA	2.5
1	B	234	HIS	2.4
1	A	69	VAL	2.4
2	E	168	ALA	2.4
3	D	59	VAL	2.4
2	C	44	GLY	2.3
1	A	450	ALA	2.3
2	E	181	ALA	2.3
2	C	221	ARG	2.3
1	A	212	LEU	2.3
3	D	103	LEU	2.3
1	B	103	GLU	2.3
3	D	70	TYR	2.3
1	B	237	ALA	2.3
3	D	8	PRO	2.3
2	E	212	THR	2.3
2	C	133	ALA	2.2
2	C	42	GLY	2.2
1	A	436	ALA	2.2
1	A	61	GLN	2.2
3	D	41	THR	2.2
1	A	264	ILE	2.2
1	A	308	VAL	2.2
1	A	377	GLU	2.2
1	A	282	ARG	2.2
2	C	2	VAL	2.2
3	D	205	VAL	2.2
1	A	82	ALA	2.2
2	C	5	LEU	2.2
2	C	170	GLY	2.2
1	A	235	GLU	2.2
3	D	11	MET	2.1
2	C	64	LEU	2.1
3	D	76	THR	2.1
3	D	17	ASP	2.1
1	B	310	PRO	2.1
2	E	213	LYS	2.1
3	F	162	TRP	2.1
1	A	460	GLN	2.1
1	B	104	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	211	ALA	2.1
2	E	105	TYR	2.1
1	A	70	HIS	2.1
1	B	70	HIS	2.1
3	D	108	ALA	2.1
1	A	27	GLU	2.1
3	D	7	SER	2.1
1	B	116	LEU	2.0
1	B	301	LEU	2.0
3	D	18	LYS	2.0
3	D	20	THR	2.0
1	B	438	PHE	2.0
1	A	66	GLY	2.0
3	F	209	ASN	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	CL	B	466	1/1	0.83	0.18	52,52,52,52	0
4	CL	B	467	1/1	0.91	0.09	60,60,60,60	0
4	CL	A	467	1/1	0.94	0.13	63,63,63,63	0
4	CL	A	466	1/1	0.95	0.14	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.