



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:20 AM GMT

PDB ID : 3ORG  
Title : Crystal Structure of a eukaryotic CLC transporter  
Authors : Feng, L.; MacKinnon, R.  
Deposited on : 2010-09-07  
Resolution : 3.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

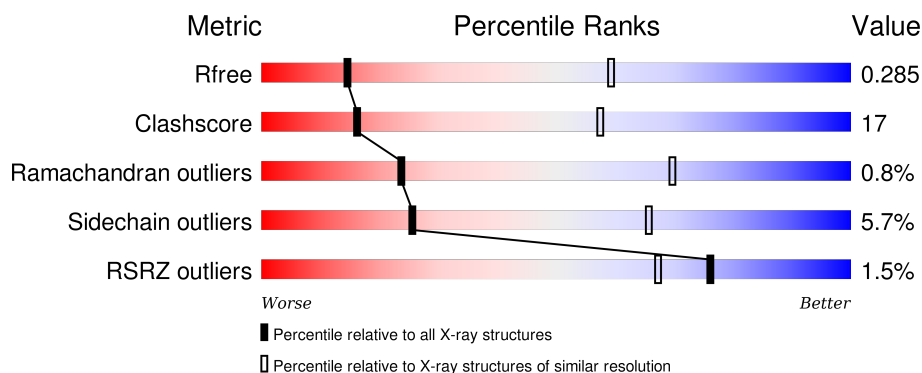
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	632	<div> <div> <div></div> <div>54%</div> <div>28%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	632	<div> <div> <div></div> <div>56%</div> <div>27%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	632	<div> <div> <div></div> <div>51%</div> <div>31%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	632	<div> <div> <div></div> <div>53%</div> <div>30%</div> <div>•</div> <div>16%</div> </div> </div>

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
2	CL	A	802	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16236 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.

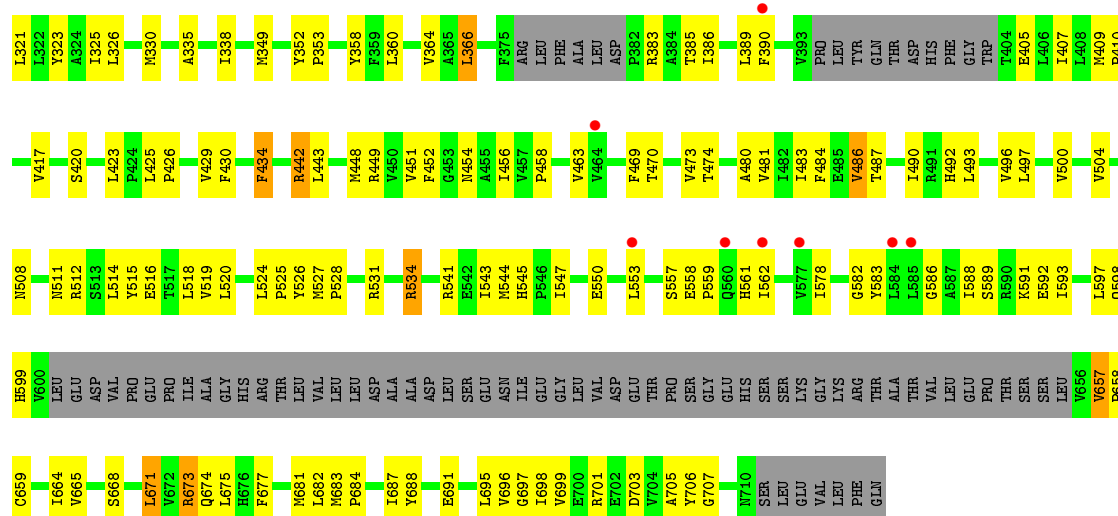
- Molecule 1 is a protein called CmCLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			
1	B	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			
1	C	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			
1	D	534	Total	C	N	O	S	0	0	0
			4057	2669	675	688	25			

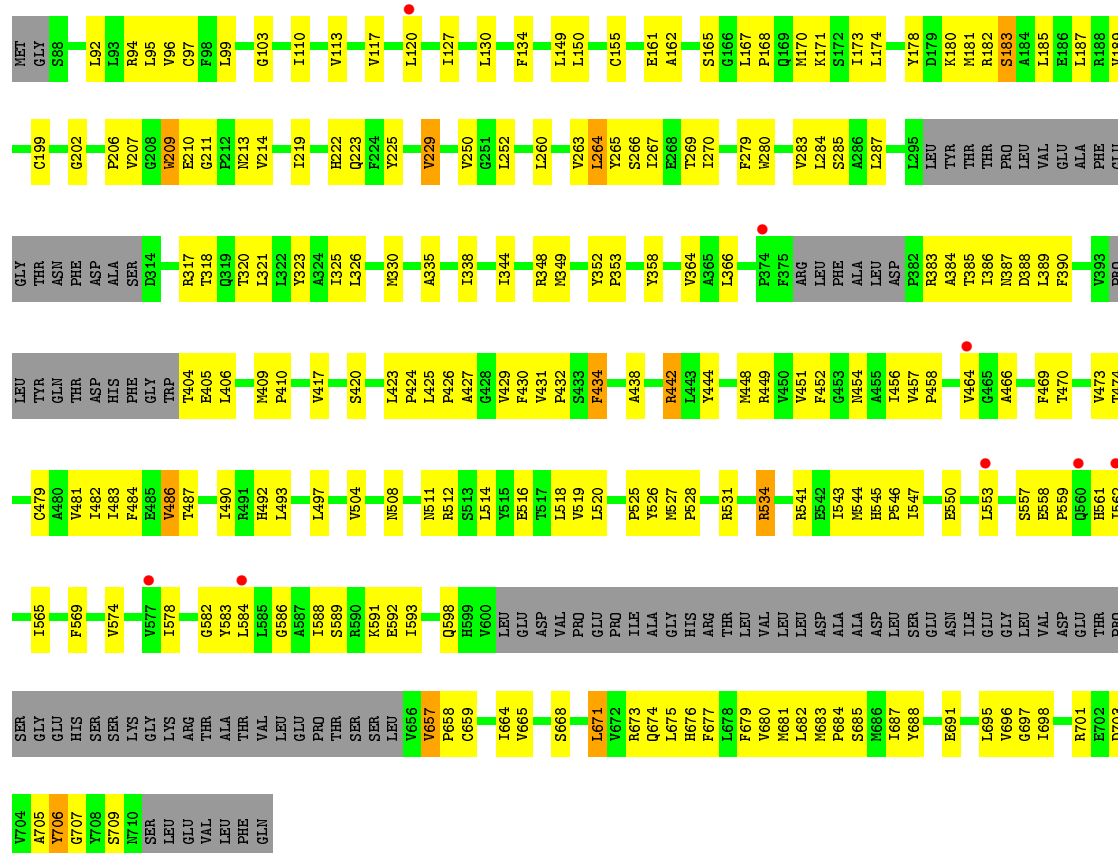
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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





• Molecule 1: CmCLC



• Molecule 1: CmCLC





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	229.63Å 178.27Å 145.13Å 90.00° 129.21° 90.00°	Depositor
Resolution (Å)	29.66 – 3.50 28.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.66-3.50) 97.1 (28.88-3.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.259 , 0.284 0.259 , 0.285	Depositor DCC
$R_{free}$ test set	2774 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	111.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.429 for -k+l,-h-l,-l 0.418 for k+l,h+l,-l 0.428 for -h-2*l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55484 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:  
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	0.43	0/4142	0.60	2/5626 (0.0%)
1	B	0.43	0/4142	0.61	2/5626 (0.0%)
1	C	0.43	0/4142	0.60	1/5626 (0.0%)
1	D	0.43	0/4142	0.60	1/5626 (0.0%)
All	All	0.43	0/16568	0.60	6/22504 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	95	LEU	CA-CB-CG	5.44	127.81	115.30
1	D	95	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	366	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	95	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	582	GLY	N-CA-C	5.00	125.61	113.10

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	4057	0	4215	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4057	0	4215	136	0
1	C	4057	0	4215	151	0
1	D	4057	0	4215	146	0
2	A	2	0	0	1	0
2	B	2	0	0	1	0
2	C	2	0	0	1	0
2	D	2	0	0	0	0
All	All	16236	0	16860	556	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 17.

All (556) 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:B:664:ILE:HD11	1:B:684:PRO:HG3	1.29	1.08
1:A:664:ILE:HD11	1:A:684:PRO:HG3	1.35	1.08
1:A:317:ARG:HD3	1:A:318:THR:H	1.17	1.07
1:D:664:ILE:HD11	1:D:684:PRO:HG3	1.37	1.07
1:D:317:ARG:HD3	1:D:318:THR:H	1.22	1.02
1:B:317:ARG:HD3	1:B:318:THR:H	1.20	1.02
1:C:664:ILE:HD11	1:C:684:PRO:HG3	1.40	0.99
1:C:317:ARG:HD3	1:C:318:THR:H	1.24	0.98
1:C:504:VAL:O	1:C:508:ASN:HB2	1.64	0.97
1:A:504:VAL:O	1:A:508:ASN:HB2	1.66	0.96
1:B:504:VAL:O	1:B:508:ASN:HB2	1.66	0.95
1:A:317:ARG:HD3	1:A:318:THR:N	1.84	0.91
1:D:317:ARG:HD3	1:D:318:THR:N	1.87	0.90
1:A:671:LEU:CD1	1:A:673:ARG:HG2	2.01	0.90
1:B:671:LEU:CD1	1:B:673:ARG:HG2	2.03	0.89
1:B:317:ARG:HD3	1:B:318:THR:N	1.87	0.88
1:A:383:ARG:HA	1:A:386:ILE:HD12	1.56	0.88
1:C:317:ARG:HD3	1:C:318:THR:N	1.88	0.86
1:B:664:ILE:CD1	1:B:684:PRO:HG3	2.07	0.84
1:D:504:VAL:O	1:D:508:ASN:HB2	1.78	0.84
1:D:671:LEU:CD1	1:D:673:ARG:HG2	2.11	0.81
1:B:541:ARG:HG3	1:B:668:SER:HB2	1.63	0.81
1:A:338:ILE:HB	1:A:511:ASN:ND2	1.96	0.81
1:A:349:MET:O	1:A:353:PRO:HB3	1.82	0.80
1:C:588:ILE:HG12	1:C:589:SER:N	1.95	0.79
1:A:588:ILE:HG12	1:A:589:SER:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ILE:HB	1:D:511:ASN:ND2	1.97	0.78
1:D:349:MET:O	1:D:353:PRO:HB3	1.83	0.78
1:C:671:LEU:HD12	1:C:673:ARG:HG2	1.64	0.78
1:C:338:ILE:HB	1:C:511:ASN:ND2	1.99	0.77
1:A:671:LEU:HD12	1:A:673:ARG:HG2	1.65	0.76
1:D:541:ARG:HG3	1:D:668:SER:HB2	1.66	0.76
1:B:383:ARG:HA	1:B:386:ILE:HD12	1.67	0.75
1:A:665:VAL:HG23	1:D:665:VAL:HG23	1.68	0.75
1:A:525:PRO:HA	1:A:707:GLY:HA2	1.69	0.75
1:C:527:MET:CE	1:C:705:ALA:HB2	2.18	0.74
1:C:349:MET:O	1:C:353:PRO:HB3	1.87	0.74
1:C:383:ARG:HA	1:C:386:ILE:HD12	1.70	0.74
1:C:209:TRP:O	1:C:213:ASN:HB2	1.87	0.74
1:D:671:LEU:HD12	1:D:673:ARG:HG2	1.69	0.73
1:B:338:ILE:HB	1:B:511:ASN:ND2	2.03	0.72
1:D:657:VAL:HG22	1:D:658:PRO:HA	1.69	0.72
1:A:451:VAL:HG23	1:A:452:PHE:HD2	1.55	0.72
1:C:541:ARG:HG3	1:C:668:SER:HB2	1.72	0.72
1:B:209:TRP:O	1:B:213:ASN:HB2	1.90	0.71
1:A:209:TRP:O	1:A:213:ASN:HB2	1.90	0.71
1:B:484:PHE:HB3	1:B:490:ILE:HG13	1.71	0.71
1:B:664:ILE:HD11	1:B:684:PRO:CG	2.15	0.71
1:C:589:SER:O	1:C:593:ILE:HB	1.91	0.71
1:D:484:PHE:HB3	1:D:490:ILE:HG13	1.71	0.71
1:A:657:VAL:HG22	1:A:658:PRO:HA	1.72	0.71
1:D:209:TRP:O	1:D:213:ASN:HB2	1.91	0.70
1:A:541:ARG:HG3	1:A:668:SER:HB2	1.71	0.70
1:C:484:PHE:HB3	1:C:490:ILE:HG13	1.73	0.70
1:B:588:ILE:HG12	1:B:589:SER:N	2.07	0.70
1:D:588:ILE:HG12	1:D:589:SER:N	2.06	0.70
1:B:525:PRO:HA	1:B:707:GLY:HA2	1.72	0.70
1:A:664:ILE:CD1	1:A:684:PRO:HG3	2.17	0.69
1:B:671:LEU:HD12	1:B:673:ARG:HG2	1.74	0.69
1:C:671:LEU:O	1:C:674:GLN:HG2	1.91	0.69
1:A:527:MET:CE	1:A:705:ALA:HB2	2.22	0.69
1:C:657:VAL:HG22	1:C:658:PRO:HA	1.72	0.69
1:A:110:ILE:HG23	1:A:213:ASN:HD21	1.57	0.69
1:B:349:MET:O	1:B:353:PRO:HB3	1.93	0.69
1:C:110:ILE:HG23	1:C:213:ASN:HD21	1.57	0.69
1:D:531:ARG:HB2	1:D:534:ARG:HG3	1.75	0.69
1:C:671:LEU:CD1	1:C:673:ARG:HG2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ARG:NH1	1:A:454:ASN:HA	2.08	0.68
1:D:527:MET:HE2	1:D:705:ALA:HB2	1.76	0.68
1:A:665:VAL:HG23	1:D:665:VAL:CG2	2.24	0.68
1:B:451:VAL:HG23	1:B:452:PHE:HD2	1.57	0.68
1:D:525:PRO:HA	1:D:707:GLY:HA2	1.77	0.67
1:A:484:PHE:HB3	1:A:490:ILE:HG13	1.74	0.67
1:A:665:VAL:HG12	1:A:688:TYR:HB2	1.76	0.67
1:D:664:ILE:CD1	1:D:684:PRO:HG3	2.19	0.67
1:A:171:LYS:HE2	1:A:526:TYR:OH	1.94	0.67
1:B:210:GLU:HG2	1:B:430:PHE:HB2	1.75	0.67
1:D:390:PHE:HE2	1:D:483:ILE:HD11	1.59	0.67
1:A:665:VAL:CG2	1:D:665:VAL:HG23	2.25	0.66
1:C:525:PRO:HA	1:C:707:GLY:HA2	1.77	0.66
1:D:171:LYS:HE2	1:D:526:TYR:OH	1.95	0.66
1:A:588:ILE:HG12	1:A:589:SER:H	1.60	0.66
1:C:665:VAL:HG12	1:C:688:TYR:HB2	1.78	0.66
1:B:449:ARG:NH1	1:B:454:ASN:HA	2.11	0.66
1:C:588:ILE:HG12	1:C:589:SER:H	1.61	0.65
1:D:383:ARG:HA	1:D:386:ILE:HD12	1.76	0.65
1:C:527:MET:HE2	1:C:705:ALA:HB2	1.76	0.65
1:A:486:VAL:HG23	1:A:487:THR:H	1.61	0.65
1:C:448:MET:HA	1:C:451:VAL:HG22	1.78	0.65
1:B:206:PRO:HB2	1:B:417:VAL:HG22	1.79	0.65
1:D:589:SER:O	1:D:593:ILE:HB	1.96	0.65
1:D:588:ILE:CG2	1:D:592:GLU:HB2	2.26	0.65
1:D:434:PHE:CZ	1:D:483:ILE:HD13	2.31	0.65
1:A:589:SER:O	1:A:593:ILE:HB	1.97	0.65
1:D:665:VAL:HG12	1:D:688:TYR:HB2	1.78	0.65
1:B:287:LEU:HD21	1:C:497:LEU:HD23	1.78	0.65
1:B:586:GLY:O	1:B:659:CYS:HB3	1.96	0.65
1:D:527:MET:CE	1:D:701:ARG:HG3	2.28	0.64
1:B:657:VAL:HG22	1:B:658:PRO:HA	1.80	0.64
1:C:434:PHE:CZ	1:C:483:ILE:HD13	2.32	0.64
1:A:664:ILE:O	1:A:687:ILE:HG23	1.98	0.64
1:A:434:PHE:CZ	1:A:483:ILE:HD13	2.33	0.63
1:A:338:ILE:HB	1:A:511:ASN:HD22	1.61	0.63
1:D:527:MET:CE	1:D:705:ALA:HB2	2.28	0.63
1:A:484:PHE:HB3	1:A:490:ILE:CG1	2.28	0.63
1:C:451:VAL:HG23	1:C:452:PHE:HD2	1.64	0.63
1:D:174:LEU:HD22	1:D:270:ILE:HG22	1.81	0.63
1:B:110:ILE:HG23	1:B:213:ASN:HD21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:HD11	1:C:264:LEU:HD21	1.80	0.63
1:C:434:PHE:HZ	1:C:483:ILE:HD13	1.63	0.62
1:C:167:LEU:HB3	1:C:168:PRO:HD3	1.81	0.62
1:A:527:MET:HE3	1:A:705:ALA:HB2	1.82	0.62
1:B:589:SER:O	1:B:593:ILE:HB	1.99	0.62
1:A:103:GLY:HA2	1:A:250:VAL:HG21	1.81	0.62
1:B:588:ILE:CG2	1:B:592:GLU:HB2	2.30	0.62
1:D:321:LEU:O	1:D:325:ILE:HG12	2.00	0.62
1:A:264:LEU:HD21	1:D:264:LEU:HD11	1.82	0.61
1:D:110:ILE:HG23	1:D:213:ASN:HD21	1.62	0.61
1:B:531:ARG:HB2	1:B:534:ARG:HG3	1.82	0.61
1:A:448:MET:HA	1:A:451:VAL:HG22	1.82	0.61
1:C:155:CYS:SG	1:C:426:PRO:HD3	2.40	0.61
1:D:434:PHE:HZ	1:D:483:ILE:HD13	1.65	0.61
1:D:484:PHE:HB3	1:D:490:ILE:CG1	2.31	0.61
1:C:390:PHE:HE2	1:C:483:ILE:HD11	1.66	0.61
1:D:103:GLY:HA2	1:D:250:VAL:HG21	1.83	0.61
1:D:586:GLY:O	1:D:659:CYS:HB3	2.01	0.60
1:B:484:PHE:HB3	1:B:490:ILE:CG1	2.32	0.60
1:D:449:ARG:NH1	1:D:454:ASN:HA	2.16	0.60
1:B:103:GLY:HA2	1:B:250:VAL:HG21	1.83	0.60
1:B:527:MET:CE	1:B:705:ALA:HB2	2.31	0.60
1:D:210:GLU:HG2	1:D:430:PHE:HB2	1.84	0.60
1:C:588:ILE:CG2	1:C:592:GLU:HB2	2.32	0.59
1:B:665:VAL:CG2	1:C:665:VAL:HG23	2.32	0.59
1:B:706:TYR:CD2	1:B:706:TYR:O	2.55	0.59
1:B:496:VAL:O	1:B:500:VAL:HG23	2.02	0.59
1:D:338:ILE:HB	1:D:511:ASN:HD22	1.65	0.59
1:C:676:HIS:O	1:C:680:VAL:HG23	2.03	0.59
1:C:484:PHE:HB3	1:C:490:ILE:CG1	2.33	0.58
1:D:469:PHE:O	1:D:473:VAL:HG12	2.03	0.58
1:B:155:CYS:SG	1:B:426:PRO:HD3	2.43	0.58
1:D:409:MET:HB3	1:D:410:PRO:HD3	1.84	0.58
1:A:586:GLY:O	1:A:659:CYS:HB3	2.03	0.58
1:B:171:LYS:HE2	1:B:526:TYR:OH	2.04	0.58
1:B:92:LEU:O	1:B:96:VAL:HG23	2.02	0.58
1:A:434:PHE:HZ	1:A:483:ILE:HD13	1.67	0.58
1:B:214:VAL:HG23	1:B:248:CYS:HA	1.86	0.58
1:B:682:LEU:HD11	1:C:682:LEU:HD11	1.84	0.57
1:C:531:ARG:HB2	1:C:534:ARG:HG3	1.86	0.57
1:B:469:PHE:O	1:B:473:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LEU:HD23	1:D:287:LEU:HD21	1.86	0.57
1:A:206:PRO:HB2	1:A:417:VAL:HG22	1.85	0.57
1:C:664:ILE:CD1	1:C:684:PRO:HG3	2.25	0.57
1:A:671:LEU:O	1:A:674:GLN:HG2	2.04	0.57
1:D:206:PRO:HB2	1:D:417:VAL:HG22	1.86	0.57
1:B:390:PHE:HE2	1:B:483:ILE:HD11	1.69	0.57
1:A:210:GLU:HG2	1:A:430:PHE:HB2	1.87	0.57
1:B:664:ILE:HG21	1:B:682:LEU:HD13	1.86	0.57
1:A:531:ARG:HB2	1:A:534:ARG:HG3	1.86	0.57
1:A:706:TYR:CD2	1:A:706:TYR:O	2.58	0.57
1:A:588:ILE:CG2	1:A:592:GLU:HB2	2.35	0.57
1:C:449:ARG:NH1	1:C:454:ASN:HA	2.20	0.57
1:A:390:PHE:HE2	1:A:483:ILE:HD11	1.70	0.57
1:D:677:PHE:CZ	1:D:681:MET:HG3	2.39	0.57
1:C:409:MET:HB3	1:C:410:PRO:HD3	1.87	0.56
1:B:665:VAL:HG12	1:B:688:TYR:HB2	1.86	0.56
1:D:92:LEU:O	1:D:96:VAL:HG23	2.05	0.56
1:C:210:GLU:HG2	1:C:430:PHE:HB2	1.86	0.56
1:A:264:LEU:HD11	1:D:264:LEU:HD21	1.87	0.56
1:D:706:TYR:CD2	1:D:706:TYR:O	2.59	0.56
1:D:174:LEU:HD22	1:D:270:ILE:CG2	2.36	0.56
1:A:167:LEU:HB3	1:A:168:PRO:HD3	1.87	0.56
1:A:358:TYR:CD2	1:A:358:TYR:N	2.74	0.55
1:A:682:LEU:HD11	1:D:682:LEU:HD11	1.88	0.55
1:B:434:PHE:CZ	1:B:483:ILE:HD13	2.40	0.55
1:C:527:MET:HE3	1:C:705:ALA:HB2	1.88	0.55
1:C:543:ILE:HD11	1:C:675:LEU:HD12	1.88	0.55
1:D:448:MET:HA	1:D:451:VAL:HG22	1.87	0.55
1:D:451:VAL:HG23	1:D:452:PHE:HD2	1.72	0.55
1:A:326:LEU:HD22	1:A:464:VAL:HG12	1.88	0.55
1:B:321:LEU:O	1:B:325:ILE:HG12	2.07	0.55
1:C:206:PRO:HB2	1:C:417:VAL:HG22	1.89	0.55
1:C:335:ALA:O	1:C:511:ASN:ND2	2.39	0.55
1:C:586:GLY:O	1:C:659:CYS:HB3	2.06	0.55
1:C:664:ILE:HG21	1:C:682:LEU:HD13	1.88	0.54
1:B:486:VAL:HG23	1:B:487:THR:H	1.71	0.54
1:D:155:CYS:SG	1:D:426:PRO:HD3	2.46	0.54
1:B:320:THR:HA	1:B:323:TYR:HD2	1.73	0.54
1:B:442:ARG:NH1	1:B:458:PRO:HB2	2.22	0.54
1:B:671:LEU:O	1:B:674:GLN:HG2	2.07	0.54
1:C:222:HIS:O	1:C:225:TYR:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LEU:O	1:C:325:ILE:HG12	2.07	0.54
1:A:222:HIS:HA	1:A:225:TYR:CD1	2.42	0.54
1:C:326:LEU:HD22	1:C:464:VAL:HG12	1.90	0.54
1:B:578:ILE:HD12	1:B:582:GLY:HA3	1.89	0.54
1:A:321:LEU:O	1:A:325:ILE:HG12	2.08	0.54
1:C:484:PHE:CZ	1:C:493:LEU:HA	2.43	0.54
1:B:364:VAL:HG21	1:B:423:LEU:HD11	1.90	0.54
1:D:671:LEU:O	1:D:674:GLN:HG2	2.07	0.54
1:A:691:GLU:HB3	1:A:696:VAL:HG21	1.89	0.54
1:A:449:ARG:HD3	1:A:458:PRO:HG3	1.89	0.54
1:A:545:HIS:O	1:A:697:GLY:HA2	2.08	0.53
1:C:103:GLY:HA2	1:C:250:VAL:HG21	1.89	0.53
1:A:364:VAL:HG21	1:A:423:LEU:HD11	1.91	0.53
1:D:484:PHE:CZ	1:D:493:LEU:HA	2.43	0.53
1:A:214:VAL:HG23	1:A:248:CYS:HA	1.90	0.53
1:A:174:LEU:HD22	1:A:270:ILE:HG22	1.89	0.53
1:C:161:GLU:OE1	1:C:183:SER:HB2	2.08	0.53
1:C:486:VAL:HG23	1:C:487:THR:H	1.74	0.53
1:D:527:MET:HE1	1:D:701:ARG:HG3	1.89	0.53
1:D:211:GLY:O	1:D:214:VAL:HG12	2.08	0.53
1:D:512:ARG:HD3	1:D:516:GLU:HB3	1.90	0.53
1:C:211:GLY:O	1:C:214:VAL:HG12	2.09	0.53
1:B:664:ILE:O	1:B:687:ILE:HG23	2.08	0.53
1:B:480:ALA:HB2	1:B:500:VAL:HG21	1.91	0.53
1:B:518:LEU:HD22	2:B:801:CL:CL	2.46	0.53
1:C:171:LYS:HE2	1:C:526:TYR:OH	2.09	0.53
1:B:665:VAL:HG23	1:C:665:VAL:CG2	2.39	0.53
1:C:92:LEU:O	1:C:96:VAL:HG23	2.08	0.53
1:C:691:GLU:HB3	1:C:696:VAL:HG21	1.90	0.53
1:B:527:MET:CE	1:B:701:ARG:HG3	2.39	0.53
1:C:222:HIS:HA	1:C:225:TYR:CD1	2.43	0.53
1:C:320:THR:HA	1:C:323:TYR:HD2	1.74	0.53
1:C:174:LEU:HD22	1:C:270:ILE:HG22	1.91	0.53
1:A:484:PHE:CZ	1:A:493:LEU:HA	2.44	0.53
1:C:364:VAL:HG21	1:C:423:LEU:HD11	1.90	0.53
1:B:481:VAL:CG2	1:C:260:LEU:HD21	2.39	0.53
1:D:486:VAL:HG23	1:D:487:THR:H	1.74	0.53
1:B:448:MET:HA	1:B:451:VAL:HG22	1.91	0.52
1:B:550:GLU:OE2	1:B:550:GLU:HA	2.09	0.52
1:A:664:ILE:HG21	1:A:682:LEU:HD13	1.90	0.52
1:D:167:LEU:HB3	1:D:168:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ILE:HG21	1:D:682:LEU:HD13	1.91	0.52
1:B:264:LEU:HD21	1:C:264:LEU:HD11	1.92	0.52
1:C:677:PHE:CZ	1:C:681:MET:HG3	2.45	0.52
1:D:326:LEU:O	1:D:330:MET:HB2	2.10	0.52
1:B:338:ILE:HB	1:B:511:ASN:HD22	1.74	0.52
1:A:527:MET:HE2	1:A:705:ALA:HB2	1.90	0.52
1:B:534:ARG:HD2	1:B:703:ASP:O	2.10	0.52
1:A:385:THR:O	1:A:389:LEU:HD12	2.10	0.52
1:D:588:ILE:HG12	1:D:589:SER:H	1.75	0.52
1:B:260:LEU:HD21	1:C:481:VAL:CG2	2.40	0.52
1:C:578:ILE:HD12	1:C:582:GLY:HA3	1.91	0.52
1:D:326:LEU:HD12	1:D:444:TYR:CD2	2.45	0.51
1:A:442:ARG:NH1	1:A:458:PRO:HB2	2.25	0.51
1:A:222:HIS:O	1:A:225:TYR:HB2	2.11	0.51
1:D:222:HIS:HA	1:D:225:TYR:CD1	2.45	0.51
1:D:279:PHE:O	1:D:283:VAL:HG23	2.10	0.51
1:C:534:ARG:HD2	1:C:703:ASP:O	2.11	0.51
1:C:526:TYR:CD2	1:C:528:PRO:HD2	2.46	0.51
1:A:335:ALA:O	1:A:511:ASN:ND2	2.44	0.51
1:D:691:GLU:HB3	1:D:696:VAL:HG21	1.92	0.51
1:D:588:ILE:CG1	1:D:589:SER:N	2.72	0.51
1:B:434:PHE:HZ	1:B:483:ILE:HD13	1.76	0.51
1:D:326:LEU:HD22	1:D:464:VAL:HG12	1.92	0.51
1:D:364:VAL:HG21	1:D:423:LEU:HD11	1.93	0.51
1:B:588:ILE:HG12	1:B:589:SER:H	1.76	0.51
1:B:385:THR:O	1:B:389:LEU:HD12	2.11	0.51
1:A:409:MET:HB3	1:A:410:PRO:HD3	1.93	0.50
1:B:165:SER:HB3	1:B:168:PRO:HD2	1.93	0.50
1:B:512:ARG:HD3	1:B:516:GLU:HB3	1.93	0.50
1:A:512:ARG:HD3	1:A:516:GLU:HB3	1.93	0.50
1:C:358:TYR:N	1:C:358:TYR:CD2	2.77	0.50
1:B:167:LEU:HB3	1:B:168:PRO:HD3	1.93	0.50
1:D:588:ILE:HD13	1:D:591:LYS:HB2	1.94	0.50
1:B:409:MET:HB3	1:B:410:PRO:HD3	1.93	0.50
1:B:558:GLU:HB3	1:B:559:PRO:HD2	1.94	0.50
1:C:120:LEU:HD23	1:C:202:GLY:HA3	1.92	0.50
1:B:452:PHE:HB2	1:B:456:ILE:HD12	1.94	0.50
1:A:534:ARG:HD2	1:A:703:ASP:O	2.12	0.50
1:B:407:ILE:HG23	1:B:443:LEU:HD11	1.94	0.50
1:A:677:PHE:CZ	1:A:681:MET:HG3	2.47	0.50
1:A:493:LEU:H	1:A:493:LEU:HD12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD22	1:A:270:ILE:CG2	2.41	0.50
1:D:496:VAL:O	1:D:500:VAL:HG23	2.12	0.50
1:A:470:THR:O	1:A:474:THR:HB	2.11	0.50
1:C:545:HIS:O	1:C:697:GLY:HA2	2.11	0.50
1:D:385:THR:O	1:D:389:LEU:HD12	2.12	0.50
1:B:484:PHE:CZ	1:B:493:LEU:HA	2.47	0.50
1:A:578:ILE:HD12	1:A:582:GLY:HA3	1.94	0.50
1:A:155:CYS:SG	1:A:426:PRO:HD3	2.52	0.50
1:D:442:ARG:NH1	1:D:458:PRO:HB2	2.27	0.49
1:A:120:LEU:HD23	1:A:202:GLY:HA3	1.94	0.49
1:B:545:HIS:O	1:B:697:GLY:HA2	2.12	0.49
1:B:558:GLU:HB3	1:B:559:PRO:CD	2.42	0.49
1:B:358:TYR:N	1:B:358:TYR:CD2	2.77	0.49
1:C:706:TYR:CD2	1:C:706:TYR:O	2.66	0.49
1:B:279:PHE:O	1:B:283:VAL:HG23	2.13	0.49
1:A:326:LEU:O	1:A:330:MET:HB2	2.13	0.49
1:A:519:VAL:HG11	1:A:526:TYR:HB2	1.94	0.49
1:A:190:LEU:HB2	1:A:219:ILE:HG21	1.94	0.49
1:A:287:LEU:HD21	1:D:497:LEU:HD23	1.95	0.49
1:B:222:HIS:O	1:B:225:TYR:HB2	2.13	0.49
1:B:515:TYR:O	1:B:519:VAL:HG23	2.13	0.49
1:C:326:LEU:HD12	1:C:444:TYR:CD2	2.47	0.49
1:D:320:THR:HA	1:D:323:TYR:HD2	1.78	0.49
1:C:252:LEU:HD13	1:C:265:TYR:HD2	1.76	0.49
1:B:420:SER:HA	1:B:423:LEU:HD13	1.95	0.49
1:C:565:ILE:HG23	1:C:569:PHE:HD1	1.77	0.49
1:A:106:ALA:O	1:A:110:ILE:HG12	2.12	0.49
1:A:110:ILE:HG13	1:A:213:ASN:OD1	2.13	0.49
1:B:120:LEU:HD23	1:B:202:GLY:HA3	1.95	0.49
1:B:665:VAL:HG23	1:C:665:VAL:HG23	1.95	0.48
1:B:701:ARG:HB3	1:B:701:ARG:HE	1.48	0.48
1:B:526:TYR:CD2	1:B:528:PRO:HD2	2.47	0.48
1:D:214:VAL:HG23	1:D:248:CYS:HA	1.94	0.48
1:B:326:LEU:O	1:B:330:MET:HB2	2.13	0.48
1:D:517:THR:O	1:D:521:MET:HB2	2.13	0.48
1:C:679:PHE:HA	1:C:684:PRO:HD2	1.96	0.48
1:B:527:MET:HE3	1:B:705:ALA:HB2	1.94	0.48
1:A:320:THR:HA	1:A:323:TYR:HD2	1.78	0.48
1:A:260:LEU:HD21	1:D:481:VAL:CG2	2.43	0.48
1:B:449:ARG:HD3	1:B:458:PRO:HG3	1.95	0.48
1:B:527:MET:HE2	1:B:705:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:VAL:O	1:C:266:SER:HB3	2.14	0.48
1:D:578:ILE:HD12	1:D:582:GLY:HA3	1.96	0.48
1:B:280:TRP:HZ3	1:B:284:LEU:HD22	1.78	0.48
1:A:584:LEU:HD21	1:A:695:LEU:HG	1.95	0.48
1:C:544:MET:HE1	1:C:696:VAL:HG12	1.96	0.48
1:B:149:LEU:HD22	1:B:358:TYR:HB3	1.95	0.48
1:D:120:LEU:HD23	1:D:202:GLY:HA3	1.95	0.48
1:A:384:ALA:O	1:A:387:ASN:ND2	2.47	0.48
1:D:519:VAL:HG11	1:D:526:TYR:HB2	1.95	0.48
1:D:404:THR:C	1:D:406:LEU:H	2.17	0.48
1:A:526:TYR:CD2	1:A:528:PRO:HD2	2.49	0.48
1:A:527:MET:CE	1:A:701:ARG:HG3	2.44	0.48
1:D:335:ALA:O	1:D:511:ASN:ND2	2.47	0.48
1:B:588:ILE:CG1	1:B:589:SER:N	2.77	0.48
1:C:170:MET:SD	1:C:173:ILE:HD12	2.53	0.48
1:B:553:LEU:HD11	1:B:562:ILE:HG22	1.96	0.48
1:A:550:GLU:HG2	1:A:698:ILE:HG13	1.96	0.48
1:B:222:HIS:HA	1:B:225:TYR:CD1	2.49	0.47
1:C:470:THR:O	1:C:474:THR:HB	2.14	0.47
1:D:149:LEU:HD22	1:D:358:TYR:HB3	1.96	0.47
1:B:470:THR:O	1:B:474:THR:HB	2.14	0.47
1:A:92:LEU:O	1:A:96:VAL:HG23	2.13	0.47
1:B:94:ARG:HD2	1:B:229:VAL:HB	1.96	0.47
1:B:691:GLU:HB3	1:B:696:VAL:HG21	1.96	0.47
1:A:452:PHE:HB2	1:A:456:ILE:HD12	1.95	0.47
1:D:545:HIS:O	1:D:697:GLY:HA2	2.14	0.47
1:A:410:PRO:HB2	1:A:440:PHE:CE2	2.49	0.47
1:C:550:GLU:HG2	1:C:698:ILE:HG13	1.95	0.47
1:D:352:TYR:N	1:D:353:PRO:HD3	2.30	0.47
1:C:352:TYR:N	1:C:353:PRO:HD3	2.29	0.47
1:B:519:VAL:HG13	1:B:524:LEU:HB2	1.96	0.47
1:B:541:ARG:HA	1:B:544:MET:HG2	1.95	0.47
1:C:99:LEU:HB2	1:C:284:LEU:HD23	1.96	0.47
1:D:541:ARG:HA	1:D:544:MET:SD	2.55	0.47
1:A:326:LEU:HD12	1:A:444:TYR:CD2	2.50	0.47
1:D:358:TYR:N	1:D:358:TYR:CD2	2.82	0.47
1:B:543:ILE:HD11	1:B:675:LEU:HD12	1.96	0.47
1:B:677:PHE:CZ	1:B:681:MET:HG3	2.50	0.47
1:C:113:VAL:O	1:C:117:VAL:HG23	2.15	0.47
1:C:442:ARG:NH1	1:C:458:PRO:HB2	2.30	0.47
1:C:385:THR:O	1:C:389:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PRO:HB2	1:A:673:ARG:HB3	1.96	0.47
1:A:211:GLY:O	1:A:214:VAL:HG12	2.15	0.47
1:C:265:TYR:CE1	1:C:474:THR:HG21	2.50	0.47
1:A:543:ILE:HD11	1:A:675:LEU:HD12	1.96	0.47
1:C:451:VAL:HG23	1:C:452:PHE:CD2	2.48	0.47
1:D:449:ARG:HD3	1:D:458:PRO:HG3	1.97	0.47
1:D:344:ILE:HG22	1:D:348:ARG:HH12	1.80	0.47
1:D:534:ARG:HD2	1:D:703:ASP:O	2.15	0.46
1:D:342:ARG:HH12	1:D:520:LEU:HD13	1.80	0.46
1:B:335:ALA:O	1:B:511:ASN:ND2	2.48	0.46
1:A:519:VAL:HG11	1:A:526:TYR:CB	2.45	0.46
1:C:207:VAL:CG1	1:C:427:ALA:HA	2.44	0.46
1:C:558:GLU:HB3	1:C:559:PRO:HD2	1.98	0.46
1:C:588:ILE:CG1	1:C:589:SER:N	2.70	0.46
1:A:165:SER:HB3	1:A:168:PRO:HD2	1.97	0.46
1:A:691:GLU:HB3	1:A:696:VAL:CG2	2.45	0.46
1:A:407:ILE:HG23	1:A:443:LEU:HD11	1.97	0.46
1:D:550:GLU:HG3	1:D:551:PRO:HD2	1.98	0.46
1:D:280:TRP:HZ3	1:D:284:LEU:HD22	1.80	0.46
1:C:557:SER:HB2	1:C:561:HIS:CG	2.51	0.46
1:C:94:ARG:HD2	1:C:229:VAL:HB	1.96	0.46
1:C:185:LEU:HA	1:C:219:ILE:HG12	1.98	0.46
1:D:230:PHE:O	1:D:233:LEU:HB2	2.15	0.46
1:B:544:MET:HE1	1:B:696:VAL:HG12	1.98	0.46
1:C:344:ILE:HG22	1:C:348:ARG:HH12	1.79	0.46
1:D:515:TYR:O	1:D:519:VAL:HG23	2.16	0.46
1:C:210:GLU:HG2	1:C:430:PHE:CB	2.46	0.46
1:D:520:LEU:HA	1:D:706:TYR:CE2	2.51	0.45
1:D:544:MET:HE1	1:D:696:VAL:HG12	1.98	0.45
1:B:527:MET:HE1	1:B:701:ARG:HG3	1.98	0.45
1:C:520:LEU:HA	1:C:706:TYR:CE2	2.52	0.45
1:D:170:MET:SD	1:D:173:ILE:HD12	2.57	0.45
1:D:687:ILE:HB	1:D:699:VAL:CG1	2.47	0.45
1:C:279:PHE:O	1:C:283:VAL:HG23	2.16	0.45
1:A:583:TYR:CE2	1:D:583:TYR:CE2	3.05	0.45
1:D:482:ILE:O	1:D:486:VAL:HG22	2.17	0.45
1:D:543:ILE:HD11	1:D:675:LEU:HD12	1.98	0.45
1:C:149:LEU:HD22	1:C:358:TYR:HB3	1.99	0.45
1:B:185:LEU:HA	1:B:219:ILE:HG12	1.99	0.45
1:C:683:MET:N	1:C:684:PRO:HD3	2.32	0.45
1:D:210:GLU:HG2	1:D:430:PHE:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLU:OE1	1:D:183:SER:HB2	2.16	0.45
1:C:352:TYR:N	1:C:353:PRO:CD	2.80	0.45
1:D:519:VAL:HG11	1:D:526:TYR:CB	2.46	0.45
1:B:211:GLY:O	1:B:212:PRO:C	2.55	0.45
1:C:518:LEU:HD22	2:C:801:CL:CL	2.54	0.45
1:A:520:LEU:HA	1:A:706:TYR:CE2	2.51	0.45
1:B:583:TYR:CE2	1:C:583:TYR:CE2	3.05	0.45
1:A:679:PHE:HA	1:A:684:PRO:HD2	1.98	0.44
1:B:541:ARG:HA	1:B:544:MET:SD	2.57	0.44
1:C:547:ILE:HD12	1:C:695:LEU:HB3	1.99	0.44
1:C:512:ARG:HD3	1:C:516:GLU:HB3	1.98	0.44
1:D:691:GLU:HB3	1:D:696:VAL:CG2	2.46	0.44
1:A:550:GLU:OE2	1:A:550:GLU:HA	2.17	0.44
1:A:496:VAL:O	1:A:500:VAL:HG23	2.17	0.44
1:C:210:GLU:HG2	1:C:430:PHE:H	1.83	0.44
1:C:207:VAL:HG13	1:C:427:ALA:HA	1.99	0.44
1:B:497:LEU:HD23	1:C:287:LEU:HD21	1.99	0.44
1:A:337:PHE:O	1:A:341:VAL:HG23	2.17	0.44
1:A:588:ILE:CG1	1:A:589:SER:N	2.76	0.44
1:C:493:LEU:H	1:C:493:LEU:HD12	1.82	0.44
1:A:515:TYR:O	1:A:519:VAL:HG23	2.17	0.44
1:C:420:SER:HA	1:C:423:LEU:HD13	1.99	0.44
1:B:238:ALA:O	1:B:242:GLN:HG3	2.17	0.44
1:A:671:LEU:HD11	1:A:673:ARG:HG2	1.91	0.44
1:B:691:GLU:HB3	1:B:696:VAL:CG2	2.47	0.44
1:B:519:VAL:HG11	1:B:526:TYR:CB	2.47	0.44
1:A:94:ARG:HD2	1:A:229:VAL:HB	2.00	0.44
1:C:691:GLU:HB3	1:C:696:VAL:CG2	2.47	0.44
1:C:452:PHE:HB2	1:C:456:ILE:HD12	1.99	0.44
1:C:173:ILE:HG12	1:C:181:MET:HB2	1.99	0.44
1:B:519:VAL:HG11	1:B:526:TYR:HB2	1.99	0.44
1:A:687:ILE:HB	1:A:699:VAL:CG1	2.48	0.44
1:D:526:TYR:CD2	1:D:528:PRO:HD2	2.53	0.44
1:B:145:VAL:O	1:B:149:LEU:HG	2.18	0.44
1:D:433:SER:HB2	1:D:470:THR:HG22	2.00	0.43
1:C:469:PHE:O	1:C:473:VAL:HG12	2.18	0.43
1:A:185:LEU:HA	1:A:219:ILE:HG12	1.99	0.43
1:A:177:PHE:CE2	1:A:701:ARG:HD2	2.53	0.43
1:A:683:MET:N	1:A:684:PRO:HD3	2.32	0.43
1:B:106:ALA:O	1:B:110:ILE:HG12	2.18	0.43
1:A:280:TRP:HZ3	1:A:284:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:MET:N	1:C:684:PRO:CD	2.81	0.43
1:A:352:TYR:N	1:A:353:PRO:HD3	2.32	0.43
1:B:520:LEU:HA	1:B:706:TYR:CE2	2.54	0.43
1:C:211:GLY:O	1:C:214:VAL:CG1	2.66	0.43
1:D:420:SER:HA	1:D:423:LEU:HD13	2.00	0.43
1:A:291:ILE:O	1:A:295:LEU:HD13	2.19	0.43
1:D:557:SER:HB2	1:D:561:HIS:CG	2.54	0.43
1:A:701:ARG:HB3	1:A:701:ARG:HE	1.49	0.43
1:B:683:MET:N	1:B:684:PRO:HD3	2.33	0.43
1:D:106:ALA:O	1:D:110:ILE:HG12	2.18	0.43
1:A:557:SER:HB2	1:A:561:HIS:CG	2.53	0.43
1:D:431:VAL:N	1:D:432:PRO:CD	2.82	0.43
1:C:173:ILE:HG23	1:C:178:TYR:HA	2.01	0.43
1:C:558:GLU:HB3	1:C:559:PRO:CD	2.48	0.43
1:B:547:ILE:HD12	1:B:695:LEU:HB3	2.01	0.43
1:C:423:LEU:HA	1:C:424:PRO:HD3	1.91	0.43
1:A:253:ALA:HA	1:A:262:GLY:HA3	2.01	0.43
1:D:541:ARG:HA	1:D:544:MET:HG2	2.01	0.42
1:A:420:SER:HA	1:A:423:LEU:HD13	2.01	0.42
1:B:263:VAL:O	1:B:266:SER:HB3	2.19	0.42
1:B:597:LEU:C	1:B:599:HIS:H	2.23	0.42
1:C:167:LEU:HB3	1:C:168:PRO:CD	2.47	0.42
1:C:326:LEU:O	1:C:330:MET:HB2	2.19	0.42
1:A:547:ILE:HB	1:A:697:GLY:H	1.84	0.42
1:D:404:THR:O	1:D:406:LEU:N	2.52	0.42
1:C:457:VAL:HA	1:C:458:PRO:HD3	1.91	0.42
1:D:457:VAL:HA	1:D:458:PRO:HD3	1.92	0.42
1:B:352:TYR:N	1:B:353:PRO:CD	2.82	0.42
1:B:390:PHE:CD2	1:B:463:VAL:HG22	2.55	0.42
1:C:280:TRP:HZ3	1:C:284:LEU:HD22	1.85	0.42
1:C:384:ALA:O	1:C:387:ASN:ND2	2.52	0.42
1:B:167:LEU:HD12	1:B:214:VAL:HG11	2.01	0.42
1:A:517:THR:HA	1:A:520:LEU:HD12	2.01	0.42
1:C:174:LEU:HD22	1:C:270:ILE:CG2	2.50	0.42
1:A:273:PHE:HE2	1:A:681:MET:HA	1.84	0.42
1:D:584:LEU:O	1:D:585:LEU:HG	2.19	0.42
1:D:185:LEU:HA	1:D:219:ILE:HG12	2.01	0.42
1:A:481:VAL:HG21	1:D:260:LEU:HD21	2.00	0.42
1:C:664:ILE:O	1:C:687:ILE:HG23	2.19	0.42
1:C:544:MET:CE	1:C:696:VAL:HG12	2.50	0.42
1:D:390:PHE:CE2	1:D:483:ILE:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ALA:HB2	1:C:189:VAL:HG13	2.01	0.42
1:A:451:VAL:HG23	1:A:452:PHE:CD2	2.45	0.42
1:A:545:HIS:HA	1:A:546:PRO:HD3	1.89	0.42
1:C:688:TYR:CD2	1:C:688:TYR:N	2.88	0.42
1:C:404:THR:C	1:C:406:LEU:H	2.23	0.42
1:A:518:LEU:HD22	2:A:801:CL:CL	2.57	0.42
1:A:558:GLU:HB3	1:A:559:PRO:CD	2.50	0.42
1:D:150:LEU:HD23	1:D:199:CYS:SG	2.60	0.42
1:A:563:LYS:HA	1:A:563:LYS:HD2	1.83	0.42
1:C:338:ILE:HB	1:C:511:ASN:HD22	1.77	0.42
1:B:211:GLY:O	1:B:214:VAL:HG12	2.19	0.42
1:D:438:ALA:HB2	1:D:466:ALA:HB2	2.01	0.42
1:C:588:ILE:CD1	1:C:591:LYS:HB2	2.50	0.41
1:D:110:ILE:HG13	1:D:213:ASN:OD1	2.20	0.41
1:B:210:GLU:HG2	1:B:430:PHE:CB	2.46	0.41
1:D:246:ALA:O	1:D:250:VAL:HG12	2.19	0.41
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.91	0.41
1:B:588:ILE:HD13	1:B:591:LYS:HB2	2.03	0.41
1:D:167:LEU:HB3	1:D:168:PRO:CD	2.50	0.41
1:B:170:MET:SD	1:B:173:ILE:HD12	2.60	0.41
1:C:187:LEU:HD12	1:C:223:GLN:NE2	2.35	0.41
1:D:265:TYR:CE1	1:D:474:THR:HG21	2.55	0.41
1:C:588:ILE:HD13	1:C:591:LYS:HB2	2.01	0.41
1:D:207:VAL:HG13	1:D:427:ALA:HA	2.02	0.41
1:B:294:GLU:O	1:B:295:LEU:HD12	2.19	0.41
1:D:558:GLU:HB3	1:D:559:PRO:HD2	2.01	0.41
1:D:384:ALA:O	1:D:387:ASN:ND2	2.53	0.41
1:A:683:MET:N	1:A:684:PRO:CD	2.83	0.41
1:B:352:TYR:N	1:B:353:PRO:HD3	2.34	0.41
1:C:584:LEU:HD13	1:C:665:VAL:HG11	2.01	0.41
1:C:545:HIS:HA	1:C:546:PRO:HD3	1.90	0.41
1:A:238:ALA:O	1:A:242:GLN:HG3	2.19	0.41
1:A:352:TYR:N	1:A:353:PRO:CD	2.83	0.41
1:D:352:TYR:N	1:D:353:PRO:CD	2.83	0.41
1:A:541:ARG:HA	1:A:544:MET:HG2	2.02	0.41
1:C:150:LEU:HD23	1:C:199:CYS:SG	2.60	0.41
1:A:553:LEU:HD11	1:A:562:ILE:HG22	2.02	0.41
1:B:557:SER:HB2	1:B:561:HIS:CG	2.55	0.41
1:A:207:VAL:HG13	1:A:427:ALA:HA	2.03	0.41
1:B:687:ILE:HB	1:B:699:VAL:CG1	2.50	0.41
1:C:553:LEU:HD11	1:C:562:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:671:LEU:HD11	1:D:673:ARG:HG2	1.98	0.41
1:D:688:TYR:N	1:D:688:TYR:CD2	2.88	0.41
1:B:171:LYS:HE3	1:B:269:THR:O	2.20	0.41
1:A:210:GLU:HG2	1:A:430:PHE:CB	2.50	0.41
1:A:706:TYR:CG	1:A:706:TYR:O	2.73	0.41
1:C:519:VAL:HG11	1:C:526:TYR:CB	2.50	0.41
1:B:178:TYR:OH	1:B:222:HIS:HE1	2.03	0.41
1:D:478:SER:O	1:D:481:VAL:N	2.54	0.41
1:A:279:PHE:O	1:A:283:VAL:HG23	2.21	0.41
1:C:438:ALA:HB2	1:C:466:ALA:HB2	2.02	0.41
1:D:253:ALA:HB2	1:D:262:GLY:HA3	2.03	0.41
1:D:679:PHE:HA	1:D:684:PRO:HD2	2.03	0.41
1:C:688:TYR:HD2	1:C:688:TYR:N	2.19	0.41
1:C:165:SER:HB3	1:C:168:PRO:HD2	2.03	0.41
1:B:550:GLU:HG2	1:B:698:ILE:HG13	2.03	0.41
1:D:253:ALA:HB1	1:D:259:PRO:HA	2.03	0.41
1:C:701:ARG:HE	1:C:701:ARG:HB3	1.58	0.41
1:D:113:VAL:O	1:D:117:VAL:HG23	2.21	0.41
1:D:701:ARG:HE	1:D:701:ARG:HB3	1.56	0.41
1:D:519:VAL:HG13	1:D:524:LEU:HB2	2.03	0.41
1:C:431:VAL:N	1:C:432:PRO:CD	2.83	0.41
1:A:664:ILE:HD11	1:A:684:PRO:CG	2.26	0.40
1:A:672:VAL:C	1:A:674:GLN:N	2.75	0.40
1:C:541:ARG:HA	1:C:544:MET:HG2	2.03	0.40
1:B:706:TYR:CG	1:B:706:TYR:O	2.74	0.40
1:D:452:PHE:HB2	1:D:456:ILE:HD12	2.03	0.40
1:A:558:GLU:HB3	1:A:559:PRO:HD2	2.04	0.40
1:D:683:MET:N	1:D:684:PRO:HD3	2.36	0.40
1:A:541:ARG:HA	1:A:544:MET:SD	2.62	0.40
1:D:520:LEU:HD23	1:D:706:TYR:CE2	2.56	0.40
1:B:360:LEU:O	1:B:364:VAL:HG23	2.21	0.40
1:A:360:LEU:O	1:A:364:VAL:HG23	2.22	0.40
1:A:477:LEU:HD13	1:D:283:VAL:HG21	2.03	0.40
1:C:479:CYS:HA	1:C:482:ILE:HD12	2.02	0.40
1:D:664:ILE:CD1	1:D:687:ILE:HG12	2.52	0.40
1:C:674:GLN:HE21	1:C:674:GLN:HB3	1.62	0.40
1:C:420:SER:O	1:C:423:LEU:HB2	2.21	0.40
1:D:563:LYS:HD2	1:D:563:LYS:HA	1.90	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	524/632 (83%)	484 (92%)	36 (7%)	4 (1%)	24	70
1	B	524/632 (83%)	483 (92%)	38 (7%)	3 (1%)	30	75
1	C	524/632 (83%)	481 (92%)	37 (7%)	6 (1%)	17	63
1	D	524/632 (83%)	484 (92%)	36 (7%)	4 (1%)	24	70
All	All	2096/2528 (83%)	1932 (92%)	147 (7%)	17 (1%)	24	70

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	VAL
1	B	405	GLU
1	D	405	GLU
1	B	598	GLN
1	D	319	GLN
1	C	182	ARG
1	C	486	VAL
1	C	709	SER
1	D	486	VAL
1	A	405	GLU
1	A	598	GLN
1	B	486	VAL
1	C	405	GLU
1	C	598	GLN
1	C	706	TYR
1	D	598	GLN
1	A	386	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar



resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/522 (82%)	402 (94%)	24 (6%)	26	66
1	B	426/522 (82%)	404 (95%)	22 (5%)	29	68
1	C	426/522 (82%)	401 (94%)	25 (6%)	24	65
1	D	426/522 (82%)	400 (94%)	26 (6%)	23	64
All	All	1704/2088 (82%)	1607 (94%)	97 (6%)	25	66

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	CYS
1	A	127	ILE
1	A	130	LEU
1	A	134	PHE
1	A	157	VAL
1	A	183	SER
1	A	209	TRP
1	A	229	VAL
1	A	264	LEU
1	A	267	ILE
1	A	269	THR
1	A	388	ASP
1	A	425	LEU
1	A	434	PHE
1	A	442	ARG
1	A	443	LEU
1	A	492	HIS
1	A	514	LEU
1	A	534	ARG
1	A	574	VAL
1	A	657	VAL
1	A	671	LEU
1	A	685	SER
1	A	695	LEU
1	B	97	CYS
1	B	127	ILE
1	B	130	LEU
1	B	134	PHE

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Mol	Chain	Res	Type
1	B	183	SER
1	B	187	LEU
1	B	209	TRP
1	B	229	VAL
1	B	264	LEU
1	B	267	ILE
1	B	269	THR
1	B	366	LEU
1	B	425	LEU
1	B	429	VAL
1	B	434	PHE
1	B	442	ARG
1	B	492	HIS
1	B	514	LEU
1	B	534	ARG
1	B	657	VAL
1	B	671	LEU
1	B	673	ARG
1	C	97	CYS
1	C	127	ILE
1	C	130	LEU
1	C	134	PHE
1	C	180	LYS
1	C	183	SER
1	C	209	TRP
1	C	229	VAL
1	C	264	LEU
1	C	267	ILE
1	C	269	THR
1	C	285	SER
1	C	366	LEU
1	C	388	ASP
1	C	425	LEU
1	C	429	VAL
1	C	434	PHE
1	C	442	ARG
1	C	492	HIS
1	C	514	LEU
1	C	534	ARG
1	C	574	VAL
1	C	657	VAL
1	C	671	LEU

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Mol	Chain	Res	Type
1	C	685	SER
1	D	97	CYS
1	D	127	ILE
1	D	130	LEU
1	D	134	PHE
1	D	183	SER
1	D	209	TRP
1	D	213	ASN
1	D	229	VAL
1	D	241	LEU
1	D	264	LEU
1	D	267	ILE
1	D	269	THR
1	D	366	LEU
1	D	388	ASP
1	D	425	LEU
1	D	429	VAL
1	D	434	PHE
1	D	442	ARG
1	D	492	HIS
1	D	514	LEU
1	D	534	ARG
1	D	574	VAL
1	D	657	VAL
1	D	671	LEU
1	D	673	ARG
1	D	683	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	222	HIS
1	A	223	GLN
1	A	319	GLN
1	A	387	ASN
1	B	215	HIS
1	B	222	HIS
1	B	319	GLN
1	B	511	ASN
1	C	215	HIS
1	C	222	HIS

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Mol	Chain	Res	Type
1	C	223	GLN
1	C	319	GLN
1	C	387	ASN
1	C	545	HIS
1	D	215	HIS
1	D	222	HIS
1	D	223	GLN
1	D	319	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	534/632 (84%)	0.12	7 (1%) 79 70	79, 118, 182, 225	1 (0%)
1	B	534/632 (84%)	0.12	9 (1%) 73 64	81, 117, 178, 221	1 (0%)
1	C	534/632 (84%)	0.10	8 (1%) 76 67	81, 117, 178, 221	1 (0%)
1	D	534/632 (84%)	0.12	7 (1%) 79 70	80, 117, 178, 220	1 (0%)
All	All	2136/2528 (84%)	0.12	31 (1%) 76 67	79, 117, 179, 225	4 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	577	VAL	4.0
1	A	553	LEU	3.4
1	D	577	VAL	3.4
1	A	350	ARG	3.2
1	A	562	ILE	3.1
1	B	585	LEU	3.1
1	C	577	VAL	2.8
1	B	553	LEU	2.7
1	D	553	LEU	2.7
1	D	206	PRO	2.7
1	D	350	ARG	2.7
1	B	464	VAL	2.7
1	B	584	LEU	2.6
1	D	360	LEU	2.5
1	A	121	GLU	2.5
1	C	120	LEU	2.5
1	C	560	GLN	2.5
1	B	577	VAL	2.5
1	C	464	VAL	2.4
1	D	562	ILE	2.3
1	C	584	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	374	PRO	2.3
1	B	560	GLN	2.3
1	D	600	VAL	2.3
1	B	562	ILE	2.2
1	C	562	ILE	2.1
1	A	464	VAL	2.1
1	C	553	LEU	2.1
1	B	127	ILE	2.1
1	A	463	VAL	2.1
1	B	390	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	802	1/1	0.98	0.43	1.41	101,101,101,101	0
2	CL	C	802	1/1	0.94	0.38	0.35	95,95,95,95	0
2	CL	A	801	1/1	0.92	0.20	-0.07	99,99,99,99	0
2	CL	D	802	1/1	0.98	0.29	-0.25	97,97,97,97	0
2	CL	B	801	1/1	0.79	0.13	-1.34	102,102,102,102	0
2	CL	C	801	1/1	0.67	0.12	-1.48	102,102,102,102	0
2	CL	D	801	1/1	0.74	0.15	-1.50	97,97,97,97	0
2	CL	B	802	1/1	0.89	0.17	-1.78	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.