



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:54 AM UTC

PDB ID : 3ORG / pdb_00003org
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

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

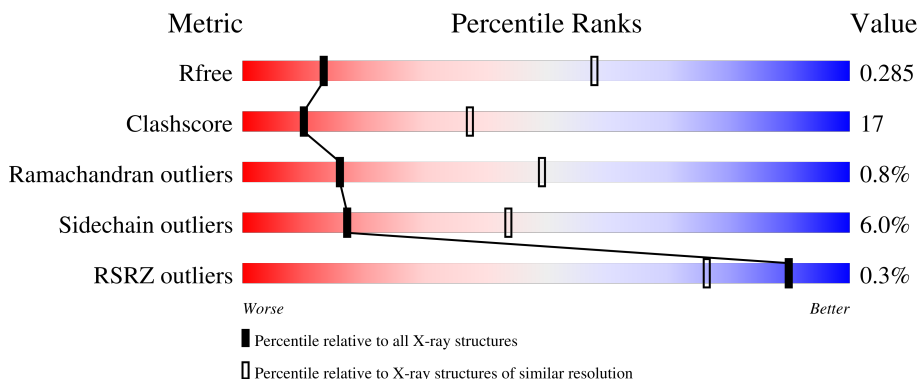
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	632	
1	B	632	
1	C	632	
1	D	632	

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
			Total	C	N	O	S			
1	A	534	4057	2669	675	688	25	0	0	0
1	B	534	4057	2669	675	688	25	0	0	0
1	C	534	4057	2669	675	688	25	0	0	0
1	D	534	4057	2669	675	688	25	0	0	0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.63Å 178.27Å 145.13Å 90.00° 129.21° 90.00°	Depositor
Resolution (Å)	29.66 – 3.50 29.66 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.66-3.50) 97.1 (29.66-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.259 , 0.284 0.258 , 0.285	Depositor DCC
R_{free} test set	2774 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 147.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.429 for -k+1,-h-1,-l 0.418 for k+1,h+1,-l 0.428 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16236	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.56	0/4142	0.95	4/5626 (0.1%)
1	B	0.56	0/4142	0.95	3/5626 (0.1%)
1	C	0.56	0/4142	0.94	3/5626 (0.1%)
1	D	0.56	0/4142	0.94	2/5626 (0.0%)
All	All	0.56	0/16568	0.94	12/22504 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	584	LEU	N-CA-C	6.75	120.08	109.96
1	D	584	LEU	N-CA-C	6.71	120.10	110.10
1	C	584	LEU	N-CA-C	6.65	119.94	109.96
1	B	584	LEU	N-CA-C	6.36	119.50	109.96
1	B	427	ALA	N-CA-C	6.32	117.78	107.23
1	B	356	ASN	N-CA-C	6.29	118.78	108.52
1	C	356	ASN	N-CA-C	6.14	118.53	108.52
1	D	356	ASN	N-CA-C	6.07	118.41	108.52
1	A	356	ASN	N-CA-C	6.01	118.31	108.52
1	C	427	ALA	N-CA-C	5.90	117.08	107.23
1	A	427	ALA	N-CA-C	5.76	116.84	107.23
1	A	582	GLY	N-CA-C	5.24	125.61	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4057	0	4215	153	0
1	B	4057	0	4215	139	0
1	C	4057	0	4215	152	0
1	D	4057	0	4215	152	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	573	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 (573) 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:664:ILE:HD11	1:A:684:PRO:HG3	1.35	1.08
1:B:664:ILE:HD11	1:B:684:PRO:HG3	1.29	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:527:MET:HE1	1:D:701:ARG:HG3	1.38	1.05
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:527:MET:HE3	1:C:705:ALA:HB2	1.42	1.01
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:D:527:MET:HE3	1:D:705:ALA:HB2	1.49	0.95
1:B:504:VAL:O	1:B:508:ASN:HB2	1.66	0.95
1:A:527:MET:HE3	1:A:705:ALA:HB2	1.50	0.93
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:527:MET:HE1	1:B:701:ARG:HG3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:527:MET:HE3	1:B:705:ALA:HB2	1.56	0.87
1:C:317:ARG:HD3	1:C:318:THR:N	1.88	0.86
1:C:544:MET:HE1	1:C:696:VAL:HG12	1.58	0.84
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:A:527:MET:HE1	1:A:701:ARG:HG3	1.59	0.83
1:D:544:MET:HE1	1:D:696:VAL:HG12	1.61	0.81
1:D:671:LEU:CD1	1:D:673:ARG:HG2	2.11	0.81
1:A:338:ILE:HB	1:A:511:ASN:ND2	1.96	0.81
1:B:541:ARG:HG3	1:B:668:SER:HB2	1.63	0.81
1:A:349:MET:O	1:A:353:PRO:HB3	1.82	0.80
1:A:544:MET:HE1	1:A:696:VAL:HG12	1.63	0.80
1:C:588:ILE:HG12	1:C:589:SER:N	1.95	0.79
1:D:338:ILE:HB	1:D:511:ASN:ND2	1.97	0.78
1:B:544:MET:HE1	1:B:696:VAL:HG12	1.66	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:588:ILE:HG12	1:A:589:SER:N	1.98	0.77
1:C:527:MET:HE1	1:C:701:ARG:HG3	1.68	0.76
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: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:C:527:MET:CE	1:C:705:ALA:HB2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:SER:O	1:C:593:ILE:HB	1.91	0.71
1:A:657:VAL:HG22	1:A:658:PRO:HA	1.72	0.71
1:D:484:PHE:HB3	1:D:490:ILE:HG13	1.71	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:B:525:PRO:HA	1:B:707:GLY:HA2	1.72	0.70
1:D:588:ILE:HG12	1:D:589:SER:N	2.06	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:527:MET:HE1	1:D:701:ARG:CG	2.20	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
1:A:449:ARG:NH1	1:A:454:ASN:HA	2.08	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:A:484:PHE:HB3	1:A:490:ILE:HG13	1.74	0.67
1:D:525:PRO:HA	1:D:707:GLY:HA2	1.77	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:B:527:MET:HE1	1:B:701:ARG:CG	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:PRO:HB2	1:B:417:VAL:HG22	1.79	0.65
1:D:588:ILE:CG2	1:D:592:GLU:HB2	2.26	0.65
1:D:589:SER:O	1:D:593:ILE:HB	1.96	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: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:665:VAL:HG12	1:D:688:TYR:HB2	1.78	0.65
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: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
1:B:264:LEU:HD11	1:C:264:LEU:HD21	1.80	0.63
1:C:167:LEU:HB3	1:C:168:PRO:HD3	1.81	0.62
1:C:434:PHE:HZ	1:C:483:ILE:HD13	1.63	0.62
1:A:103:GLY:HA2	1:A:250:VAL:HG21	1.81	0.62
1:B:589:SER:O	1:B:593:ILE:HB	1.99	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:527:MET:HE3	1:D:705:ALA:CB	2.29	0.60
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:D:210:GLU:HG2	1:D:430:PHE:HB2	1.84	0.60
1:B:665:VAL:CG2	1:C:665:VAL:HG23	2.32	0.59
1:C:588:ILE:CG2	1:C:592:GLU:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:VAL:O	1:B:500:VAL:HG23	2.02	0.59
1:B:706:TYR:O	1:B:706:TYR:CD2	2.55	0.59
1:C:676:HIS:O	1:C:680:VAL:HG23	2.03	0.59
1:D:338:ILE:HB	1:D:511:ASN:HD22	1.65	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:A:586:GLY:O	1:A:659:CYS:HB3	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:B:92:LEU:O	1:B:96:VAL:HG23	2.02	0.58
1:B:171:LYS:HE2	1:B:526:TYR:OH	2.04	0.58
1:A:434:PHE:HZ	1:A:483:ILE:HD13	1.67	0.58
1:B:170:MET:HE3	1:B:215:HIS:HA	1.84	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:527:MET:HE3	1:C:705:ALA:CB	2.28	0.57
1:C:531:ARG:HB2	1:C:534:ARG:HG3	1.86	0.57
1:A:206:PRO:HB2	1:A:417:VAL:HG22	1.85	0.57
1:A:497:LEU:HD23	1:D:287:LEU:HD21	1.86	0.57
1:B:469:PHE:O	1:B:473:VAL:HG12	2.05	0.57
1:A:671:LEU:O	1:A:674:GLN:HG2	2.04	0.57
1:B:390:PHE:HE2	1:B:483:ILE:HD11	1.69	0.57
1:C:664:ILE:CD1	1:C:684:PRO:HG3	2.25	0.57
1:D:206:PRO:HB2	1:D:417:VAL:HG22	1.86	0.57
1:A:210:GLU:HG2	1:A:430:PHE:HB2	1.87	0.57
1:A:531:ARG:HB2	1:A:534:ARG:HG3	1.86	0.57
1:B:664:ILE:HG21	1:B:682:LEU:HD13	1.86	0.57
1:A:706:TYR:O	1:A:706:TYR:CD2	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:O	1:D:706:TYR:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:326:LEU:HD22	1:A:464:VAL:HG12	1.88	0.55
1:B:527:MET:CE	1:B:705:ALA:HB2	2.31	0.55
1:D:451:VAL:HG23	1:D:452:PHE:HD2	1.72	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:B:320:THR:HA	1:B:323:TYR:HD2	1.73	0.54
1:B:486:VAL:HG23	1:B:487:THR:H	1.71	0.54
1:C:664:ILE:HG21	1:C:682:LEU:HD13	1.88	0.54
1:D:155:CYS:SG	1:D:426:PRO:HD3	2.46	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:A:222:HIS:HA	1:A:225:TYR:CD1	2.42	0.54
1:C:222:HIS:O	1:C:225:TYR:HB2	2.06	0.54
1:C:321:LEU:O	1:C:325:ILE:HG12	2.07	0.54
1:A:321:LEU:O	1:A:325:ILE:HG12	2.08	0.54
1:B:578:ILE:HD12	1:B:582:GLY:HA3	1.89	0.54
1:C:326:LEU:HD22	1:C:464:VAL:HG12	1.90	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:527:MET:CE	1:D:705:ALA:HB2	2.28	0.54
1:A:691:GLU:HB3	1:A:696:VAL:HG21	1.89	0.54
1:D:671:LEU:O	1:D:674:GLN:HG2	2.07	0.54
1:A:449:ARG:HD3	1:A:458:PRO:HG3	1.89	0.54
1:A:364:VAL:HG21	1:A:423:LEU:HD11	1.91	0.53
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:174:LEU:HD22	1:A:270:ILE:HG22	1.89	0.53
1:A:214:VAL:HG23	1:A:248:CYS:HA	1.90	0.53
1:D:484:PHE:CZ	1:D:493:LEU:HA	2.43	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: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:480:ALA:HB2	1:B:500:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LEU:HD22	2:B:801:CL:CL	2.46	0.53
1:B:664:ILE:O	1:B:687:ILE:HG23	2.08	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:D:404:THR:C	1:D:406:LEU:H	2.17	0.53
1:C:174:LEU:HD22	1:C:270:ILE:HG22	1.91	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:691:GLU:HB3	1:C:696:VAL:HG21	1.90	0.53
1:A:484:PHE:CZ	1:A:493:LEU:HA	2.44	0.53
1:B:481:VAL:CG2	1:C:260:LEU:HD21	2.39	0.53
1:C:364:VAL:HG21	1:C:423:LEU:HD11	1.90	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
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:664:ILE:HG21	1:D:682:LEU:HD13	1.91	0.52
1:D:326:LEU:O	1:D:330:MET:HB2	2.10	0.52
1:A:385:THR:O	1:A:389:LEU:HD12	2.10	0.52
1:B:338:ILE:HB	1:B:511:ASN:HD22	1.74	0.52
1:B:534:ARG:HD2	1:B:703:ASP:O	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:526:TYR:CD2	1:C:528:PRO:HD2	2.46	0.51
1:C:534:ARG:HD2	1:C:703:ASP:O	2.11	0.51
1:A:335:ALA:O	1:A:511:ASN:ND2	2.44	0.51
1:B:434:PHE:HZ	1:B:483:ILE:HD13	1.76	0.51
1:D:588:ILE:CG1	1:D:589:SER:N	2.72	0.51
1:D:691:GLU:HB3	1:D:696:VAL:HG21	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ILE:HG12	1:B:589:SER:H	1.76	0.51
1:A:527:MET:HE1	1:A:701:ARG:CG	2.36	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:A:512:ARG:HD3	1:A:516:GLU:HB3	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:C:358:TYR:CD2	1:C:358:TYR:N	2.77	0.50
1:B:167:LEU:HB3	1:B:168:PRO:HD3	1.93	0.50
1:B:409:MET:HB3	1:B:410:PRO:HD3	1.93	0.50
1:D:588:ILE:HD13	1:D:591:LYS:HB2	1.94	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:A:534:ARG:HD2	1:A:703:ASP:O	2.12	0.50
1:A:677:PHE:CZ	1:A:681:MET:HG3	2.47	0.50
1:B:407:ILE:HG23	1:B:443:LEU:HD11	1.94	0.50
1:B:452:PHE:HB2	1:B:456:ILE:HD12	1.94	0.50
1:A:174:LEU:HD22	1:A:270:ILE:CG2	2.41	0.50
1:A:470:THR:O	1:A:474:THR:HB	2.11	0.50
1:A:493:LEU:H	1:A:493:LEU:HD12	1.77	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:D:496:VAL:O	1:D:500:VAL:HG23	2.12	0.50
1:A:155:CYS:SG	1:A:426:PRO:HD3	2.52	0.50
1:A:578:ILE:HD12	1:A:582:GLY:HA3	1.94	0.50
1:B:484:PHE:CZ	1:B:493:LEU:HA	2.47	0.50
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:D:442:ARG:NH1	1:D:458:PRO:HB2	2.27	0.49
1:B:358:TYR:CD2	1:B:358:TYR:N	2.77	0.49
1:B:558:GLU:HB3	1:B:559:PRO:CD	2.42	0.49
1:B:211:GLY:O	1:B:212:PRO:C	2.55	0.49
1:B:279:PHE:O	1:B:283:VAL:HG23	2.13	0.49
1:C:706:TYR:O	1:C:706:TYR:CD2	2.66	0.49
1:A:326:LEU:O	1:A:330:MET:HB2	2.13	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:A:519:VAL:HG11	1:A:526:TYR:HB2	1.94	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:252:LEU:HD13	1:C:265:TYR:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:170:MET:HE3	1:A:215:HIS:HA	1.95	0.49
1:B:120:LEU:HD23	1:B:202:GLY:HA3	1.95	0.49
1:B:526:TYR:CD2	1:B:528:PRO:HD2	2.47	0.48
1:B:665:VAL:HG23	1:C:665:VAL:HG23	1.95	0.48
1:B:701:ARG:HE	1:B:701:ARG:HB3	1.48	0.48
1:B:326:LEU:O	1:B:330:MET:HB2	2.13	0.48
1:D:214:VAL:HG23	1:D:248:CYS:HA	1.94	0.48
1:D:517:THR:O	1:D:521:MET:HB2	2.13	0.48
1:A:260:LEU:HD21	1:D:481:VAL:CG2	2.43	0.48
1:A:320:THR:HA	1:A:323:TYR:HD2	1.78	0.48
1:C:679:PHE:HA	1:C:684:PRO:HD2	1.96	0.48
1:B:449:ARG:HD3	1:B:458:PRO:HG3	1.95	0.48
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:A:584:LEU:HD21	1:A:695:LEU:HG	1.95	0.48
1:B:280:TRP:HZ3	1:B:284:LEU:HD22	1.78	0.48
1:A:384:ALA:O	1:A:387:ASN:ND2	2.47	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:D:519:VAL:HG11	1:D:526:TYR:HB2	1.95	0.48
1:A:526:TYR:CD2	1:A:528:PRO:HD2	2.49	0.48
1:A:550:GLU:HG2	1:A:698:ILE:HG13	1.96	0.48
1:B:553:LEU:HD11	1:B:562:ILE:HG22	1.96	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:D:335:ALA:O	1:D:511:ASN:ND2	2.47	0.48
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:222:HIS:HA	1:B:225:TYR:CD1	2.49	0.47
1:B:470:THR:O	1:B:474:THR:HB	2.14	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:D:170:MET:HE3	1:D:215:HIS:HA	1.96	0.47
1:A:452:PHE:HB2	1:A:456:ILE:HD12	1.95	0.47
1:B:691:GLU:HB3	1:B:696:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:519:VAL:HG13	1:B:524:LEU:HB2	1.96	0.47
1:B:597:LEU:C	1:B:599:HIS:H	2.23	0.47
1:C:352:TYR:N	1:C:353:PRO:HD3	2.29	0.47
1:D:352:TYR:N	1:D:353:PRO:HD3	2.30	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: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:385:THR:O	1:C:389:LEU:HD12	2.15	0.47
1:C:442:ARG:NH1	1:C:458:PRO:HB2	2.30	0.47
1:D:358:TYR:CD2	1:D:358:TYR:N	2.82	0.47
1:A:211:GLY:O	1:A:214:VAL:HG12	2.15	0.47
1:A:536:PRO:HB2	1:A:673:ARG:HB3	1.96	0.47
1:A:543:ILE:HD11	1:A:675:LEU:HD12	1.96	0.47
1:C:265:TYR:CE1	1:C:474:THR:HG21	2.50	0.47
1:C:451:VAL:HG23	1:C:452:PHE:CD2	2.48	0.47
1:D:344:ILE:HG22	1:D:348:ARG:HH12	1.80	0.47
1:D:449:ARG:HD3	1:D:458:PRO:HG3	1.97	0.47
1:C:404:THR:C	1:C:406:LEU:H	2.23	0.46
1:D:342:ARG:HH12	1:D:520:LEU:HD13	1.80	0.46
1:D:534:ARG:HD2	1:D:703:ASP:O	2.15	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:A:165:SER:HB3	1:A:168:PRO:HD2	1.97	0.46
1:A:407:ILE:HG23	1:A:443:LEU:HD11	1.97	0.46
1:A:691:GLU:HB3	1:A:696:VAL:CG2	2.45	0.46
1:C:557:SER:HB2	1:C:561:HIS:CG	2.51	0.46
1:C:588:ILE:CG1	1:C:589:SER:N	2.70	0.46
1:D:280:TRP:HZ3	1:D:284:LEU:HD22	1.80	0.46
1:D:550:GLU:HG3	1:D:551:PRO:HD2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ILE:HG22	1:C:348:ARG:HH12	1.79	0.46
1:C:210:GLU:HG2	1:C:430:PHE:CB	2.46	0.46
1:D:515:TYR:O	1:D:519:VAL:HG23	2.16	0.46
1:D:520:LEU:HA	1:D:706:TYR:CE2	2.51	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:A:672:VAL:C	1:A:674:GLN:N	2.75	0.45
1:A:583:TYR:CE2	1:D:583:TYR:CE2	3.05	0.45
1:C:279:PHE:O	1:C:283:VAL:HG23	2.16	0.45
1:D:687:ILE:HB	1:D:699:VAL:CG1	2.47	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:B:185:LEU:HA	1:B:219:ILE:HG12	1.99	0.45
1:C:149:LEU:HD22	1:C:358:TYR:HB3	1.99	0.45
1:C:683:MET:N	1:C:684:PRO:HD3	2.32	0.45
1:D:161:GLU:OE1	1:D:183:SER:HB2	2.16	0.45
1:D:210:GLU:HG2	1:D:430:PHE:CB	2.45	0.45
1:C:352:TYR:N	1:C:353:PRO:CD	2.80	0.45
1:C:518:LEU:HD22	2:C:801:CL:CL	2.54	0.45
1:D:519:VAL:HG11	1:D:526:TYR:CB	2.46	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:512:ARG:HD3	1:C:516:GLU:HB3	1.98	0.44
1:C:547:ILE:HD12	1:C:695:LEU:HB3	1.99	0.44
1:A:496:VAL:O	1:A:500:VAL:HG23	2.17	0.44
1:A:550:GLU:HA	1:A:550:GLU:OE2	2.17	0.44
1:D:691:GLU:HB3	1:D:696:VAL:CG2	2.46	0.44
1:A:337:PHE:O	1:A:341:VAL:HG23	2.17	0.44
1:B:497:LEU:HD23	1:C:287:LEU:HD21	1.99	0.44
1:C:207:VAL:HG13	1:C:427:ALA:HA	1.99	0.44
1:C:210:GLU:HG2	1:C:430:PHE:H	1.83	0.44
1:A:515:TYR:O	1:A:519:VAL:HG23	2.17	0.44
1:A:588:ILE:CG1	1:A:589:SER:N	2.76	0.44
1:B:238:ALA:O	1:B:242:GLN:HG3	2.17	0.44
1:C:420:SER:HA	1:C:423:LEU:HD13	1.99	0.44
1:C:493:LEU:H	1:C:493:LEU:HD12	1.82	0.44
1:A:94:ARG:HD2	1:A:229:VAL:HB	2.00	0.44
1:A:671:LEU:HD11	1:A:673:ARG:HG2	1.91	0.44
1:B:519:VAL:HG11	1:B:526:TYR:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:GLU:HB3	1:B:696:VAL:CG2	2.47	0.44
1:C:173:ILE:HG12	1:C:181:MET:HB2	1.99	0.44
1:C:452:PHE:HB2	1:C:456:ILE:HD12	1.99	0.44
1:C:691:GLU:HB3	1:C:696:VAL:CG2	2.47	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:B:145:VAL:O	1:B:149:LEU:HG	2.18	0.44
1:B:404:THR:C	1:B:406:LEU:H	2.26	0.44
1:D:526:TYR:CD2	1:D:528:PRO:HD2	2.53	0.44
1:C:469:PHE:O	1:C:473:VAL:HG12	2.18	0.43
1:D:433:SER:HB2	1:D:470:THR:HG22	2.00	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:280:TRP:HZ3	1:A:284:LEU:HD22	1.83	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:352:TYR:N	1:A:353:PRO:HD3	2.32	0.43
1:C:683:MET:N	1:C:684:PRO:CD	2.81	0.43
1:A:291:ILE:O	1:A:295:LEU:HD13	2.19	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:D:557:SER:HB2	1:D:561:HIS:CG	2.54	0.43
1:A:701:ARG:HE	1:A:701:ARG:HB3	1.49	0.43
1:A:557:SER:HB2	1:A:561:HIS:CG	2.53	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:D:431:VAL:N	1:D:432:PRO:CD	2.82	0.43
1:B:547:ILE:HD12	1:B:695:LEU:HB3	2.01	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:A:253:ALA:HA	1:A:262:GLY:HA3	2.01	0.43
1:C:423:LEU:HA	1:C:424:PRO:HD3	1.91	0.43
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:D:318:THR:C	1:D:320:THR:H	2.27	0.42
1:D:541:ARG:HA	1:D:544:MET:HG2	2.01	0.42
1:A:547:ILE:HB	1:A:697:GLY:H	1.84	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:C:457:VAL:HA	1:C:458:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:THR:O	1:D:406:LEU:N	2.52	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:A:273:PHE:HE2	1:A:681:MET:HA	1.84	0.42
1:A:481:VAL:HG21	1:D:260:LEU:HD21	2.00	0.42
1:A:517:THR:HA	1:A:520:LEU:HD12	2.01	0.42
1:B:167:LEU:HD12	1:B:214:VAL:HG11	2.01	0.42
1:C:174:LEU:HD22	1:C:270:ILE:CG2	2.50	0.42
1:D:185:LEU:HA	1:D:219:ILE:HG12	2.01	0.42
1:D:527:MET:CE	1:D:701:ARG:HG3	2.28	0.42
1:D:584:LEU:O	1:D:585:LEU:HG	2.19	0.42
1:C:664:ILE:O	1:C:687:ILE:HG23	2.19	0.42
1:C:162:ALA:HB2	1:C:189:VAL:HG13	2.01	0.42
1:D:390:PHE:CE2	1:D:483:ILE:HD11	2.48	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: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:A:563:LYS:HD2	1:A:563:LYS:HA	1.83	0.42
1:C:688:TYR:CD2	1:C:688:TYR:N	2.88	0.42
1:D:150:LEU:HD23	1:D:199:CYS:SG	2.60	0.42
1:B:211:GLY:O	1:B:214:VAL:HG12	2.19	0.42
1:C:338:ILE:HB	1:C:511:ASN:HD22	1.77	0.42
1:D:438:ALA:HB2	1:D:466:ALA:HB2	2.01	0.42
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.91	0.41
1:B:210:GLU:HG2	1:B:430:PHE:CB	2.46	0.41
1:B:550:GLU:CD	1:B:551:PRO:HD2	2.45	0.41
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:D:246:ALA:O	1:D:250:VAL:HG12	2.19	0.41
1:B:170:MET:SD	1:B:173:ILE:HD12	2.60	0.41
1:B:588:ILE:HD13	1:B:591:LYS:HB2	2.03	0.41
1:C:187:LEU:HD12	1:C:223:GLN:NE2	2.35	0.41
1:D:167:LEU:HB3	1:D:168:PRO:CD	2.50	0.41
1:D:265:TYR:CE1	1:D:474:THR:HG21	2.55	0.41
1:D:318:THR:C	1:D:320:THR:N	2.78	0.41
1:A:597:LEU:C	1:A:599:HIS:H	2.29	0.41
1:A:672:VAL:C	1:A:674:GLN:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLU:CD	1:B:211:GLY:N	2.78	0.41
1:B:294:GLU:O	1:B:295:LEU:HD12	2.19	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:D:384:ALA:O	1:D:387:ASN:ND2	2.53	0.41
1:D:558:GLU:HB3	1:D:559:PRO:HD2	2.01	0.41
1:A:238:ALA:O	1:A:242:GLN:HG3	2.19	0.41
1:A:527:MET:HE3	1:A:705:ALA:CB	2.35	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:545:HIS:HA	1:C:546:PRO:HD3	1.90	0.41
1:C:584:LEU:HD13	1:C:665:VAL:HG11	2.01	0.41
1:A:207:VAL:HG13	1:A:427:ALA:HA	2.03	0.41
1:A:352:TYR:N	1:A:353:PRO:CD	2.83	0.41
1:A:541:ARG:HA	1:A:544:MET:HG2	2.02	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:C:150:LEU:HD23	1:C:199:CYS:SG	2.60	0.41
1:D:352:TYR:N	1:D:353:PRO:CD	2.83	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
1:A:210:GLU:HG2	1:A:430:PHE:CB	2.50	0.41
1:A:706:TYR:O	1:A:706:TYR:CG	2.73	0.41
1:B:171:LYS:HE3	1:B:269:THR:O	2.20	0.41
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:A:279:PHE:O	1:A:283:VAL:HG23	2.21	0.41
1:A:444:TYR:CZ	1:A:448:MET:HE3	2.56	0.41
1:B:178:TYR:OH	1:B:222:HIS:HE1	2.03	0.41
1:C:438:ALA:HB2	1:C:466:ALA:HB2	2.02	0.41
1:C:519:VAL:HG11	1:C:526:TYR:CB	2.50	0.41
1:D:253:ALA:HB2	1:D:262:GLY:HA3	2.03	0.41
1:D:478:SER:O	1:D:481:VAL:N	2.54	0.41
1:B:550:GLU:HG2	1:B:698:ILE:HG13	2.03	0.41
1:C:165:SER:HB3	1:C:168:PRO:HD2	2.03	0.41
1:C:597:LEU:C	1:C:599:HIS:H	2.29	0.41
1:C:688:TYR:N	1:C:688:TYR:HD2	2.19	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:253:ALA:HB1	1:D:259:PRO:HA	2.03	0.41
1:D:679:PHE:HA	1:D:684:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:VAL:N	1:C:432:PRO:CD	2.83	0.41
1:D:519:VAL:HG13	1:D:524:LEU:HB2	2.03	0.41
1:D:701:ARG:HE	1:D:701:ARG:HB3	1.56	0.41
1:A:558:GLU:HB3	1:A:559:PRO:HD2	2.04	0.40
1:A:664:ILE:HD11	1:A:684:PRO:CG	2.26	0.40
1:B:706:TYR:O	1:B:706:TYR:CG	2.74	0.40
1:C:541:ARG:HA	1:C:544:MET:HG2	2.03	0.40
1:D:452:PHE:HB2	1:D:456:ILE:HD12	2.03	0.40
1:A:360:LEU:O	1:A:364:VAL:HG23	2.22	0.40
1:A:541:ARG:HA	1:A:544:MET:SD	2.62	0.40
1:B:360:LEU:O	1:B:364:VAL:HG23	2.21	0.40
1:D:520:LEU:HD23	1:D:706:TYR:CE2	2.56	0.40
1:D:597:LEU:C	1:D:599:HIS:H	2.30	0.40
1:D:683:MET:N	1:D:684:PRO:HD3	2.36	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:A:404:THR:C	1:A:406:LEU:H	2.29	0.40
1:C:674:GLN:HE21	1:C:674:GLN:HB3	1.62	0.40
1:D:664:ILE:CD1	1:D:687:ILE:HG12	2.52	0.40
1:C:420:SER:O	1:C:423:LEU:HB2	2.21	0.40
1:D:563:LYS:HA	1:D:563:LYS:HD2	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%)	16 49
1	B	524/632 (83%)	483 (92%)	38 (7%)	3 (1%)	21 54
1	C	524/632 (83%)	481 (92%)	37 (7%)	6 (1%)	11 43
1	D	524/632 (83%)	484 (92%)	36 (7%)	4 (1%)	16 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2096/2528 (83%)	1932 (92%)	147 (7%)	17 (1%)	16	49

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%)	399 (94%)	27 (6%)	16	42
1	B	426/522 (82%)	402 (94%)	24 (6%)	19	46
1	C	426/522 (82%)	399 (94%)	27 (6%)	16	42
1	D	426/522 (82%)	401 (94%)	25 (6%)	18	44
All	All	1704/2088 (82%)	1601 (94%)	103 (6%)	17	44

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	CYS
1	A	108	LEU
1	A	127	ILE
1	A	130	LEU
1	A	157	VAL
1	A	167	LEU
1	A	183	SER
1	A	187	LEU
1	A	190	LEU
1	A	193	LYS
1	A	223	GLN
1	A	229	VAL
1	A	241	LEU
1	A	264	LEU
1	A	267	ILE
1	A	269	THR
1	A	366	LEU
1	A	443	LEU
1	A	492	HIS
1	A	496	VAL
1	A	514	LEU
1	A	534	ARG
1	A	553	LEU
1	A	574	VAL
1	A	657	VAL
1	A	671	LEU
1	A	695	LEU
1	B	97	CYS
1	B	108	LEU
1	B	127	ILE
1	B	130	LEU
1	B	183	SER
1	B	187	LEU
1	B	190	LEU
1	B	193	LYS
1	B	229	VAL
1	B	263	VAL
1	B	264	LEU
1	B	267	ILE
1	B	269	THR
1	B	366	LEU
1	B	429	VAL
1	B	473	VAL

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Mol	Chain	Res	Type
1	B	492	HIS
1	B	496	VAL
1	B	514	LEU
1	B	534	ARG
1	B	553	LEU
1	B	574	VAL
1	B	657	VAL
1	B	671	LEU
1	C	97	CYS
1	C	102	LEU
1	C	127	ILE
1	C	130	LEU
1	C	180	LYS
1	C	183	SER
1	C	190	LEU
1	C	213	ASN
1	C	223	GLN
1	C	229	VAL
1	C	241	LEU
1	C	264	LEU
1	C	267	ILE
1	C	269	THR
1	C	285	SER
1	C	366	LEU
1	C	425	LEU
1	C	429	VAL
1	C	492	HIS
1	C	496	VAL
1	C	514	LEU
1	C	534	ARG
1	C	553	LEU
1	C	574	VAL
1	C	657	VAL
1	C	671	LEU
1	C	674	GLN
1	D	97	CYS
1	D	108	LEU
1	D	127	ILE
1	D	130	LEU
1	D	180	LYS
1	D	183	SER
1	D	190	LEU

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Mol	Chain	Res	Type
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	429	VAL
1	D	443	LEU
1	D	492	HIS
1	D	496	VAL
1	D	514	LEU
1	D	534	ARG
1	D	553	LEU
1	D	574	VAL
1	D	600	VAL
1	D	657	VAL
1	D	671	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	222	HIS
1	A	223	GLN
1	A	242	GLN
1	A	277	GLN
1	A	319	GLN
1	A	356	ASN
1	A	387	ASN
1	A	552	HIS
1	A	560	GLN
1	B	215	HIS
1	B	222	HIS
1	B	319	GLN
1	B	356	ASN
1	B	387	ASN
1	B	511	ASN
1	B	560	GLN
1	C	169	GLN
1	C	215	HIS
1	C	222	HIS

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Mol	Chain	Res	Type
1	C	223	GLN
1	C	387	ASN
1	C	545	HIS
1	C	560	GLN
1	D	169	GLN
1	D	215	HIS
1	D	222	HIS
1	D	223	GLN
1	D	356	ASN
1	D	387	ASN
1	D	560	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	534/632 (84%)	-0.66	3 (0%) 85 65	79, 118, 182, 225	1 (0%)
1	B	534/632 (84%)	-0.62	2 (0%) 88 72	81, 117, 178, 221	1 (0%)
1	C	534/632 (84%)	-0.65	0 100 100	81, 117, 178, 221	1 (0%)
1	D	534/632 (84%)	-0.64	1 (0%) 91 82	80, 117, 178, 220	1 (0%)
All	All	2136/2528 (84%)	-0.64	6 (0%) 90 76	79, 117, 179, 225	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	GLN	2.6
1	B	560	GLN	2.4
1	D	388	ASP	2.4
1	A	656	VAL	2.3
1	B	183	SER	2.1
1	A	450	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	D	801	1/1	0.96	0.17	97,97,97,97	0
2	CL	B	801	1/1	0.97	0.08	102,102,102,102	0
2	CL	C	802	1/1	0.98	0.07	95,95,95,95	0
2	CL	D	802	1/1	0.98	0.08	97,97,97,97	0
2	CL	C	801	1/1	0.99	0.11	102,102,102,102	0
2	CL	A	802	1/1	0.99	0.05	101,101,101,101	0
2	CL	A	801	1/1	0.99	0.10	99,99,99,99	0
2	CL	B	802	1/1	0.99	0.06	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.