



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:17 AM UTC

PDB ID : 4I1P / pdb_00004i1p
Title : Human MALT1 (caspase-IG3) in complex with activity based-probe
Authors : Schlauderer, F.; Lammens, K.; Hopfner, K.P.
Deposited on : 2012-11-21
Resolution : 2.40 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

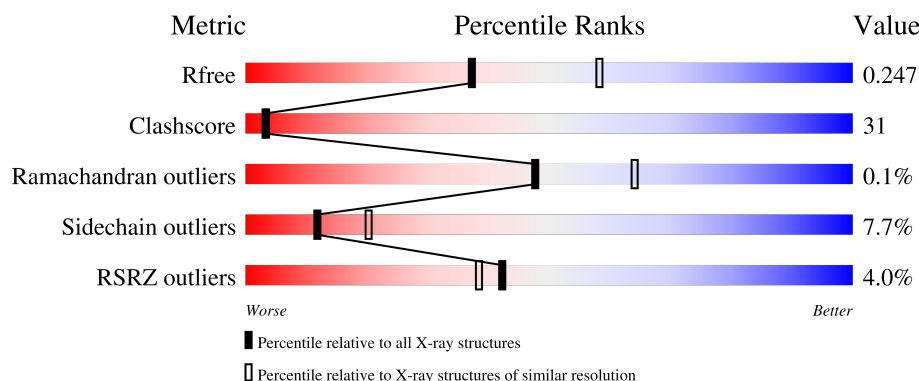
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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	388	
1	C	388	
2	B	5	
2	D	5	

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
3	ACT	A	801	-	-	X	-
3	ACT	A	803	-	-	X	-
3	ACT	A	804	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6256 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 Mucosa-associated lymphoid tissue lymphoma translocation protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	124	0	0
			3007	1925	487	574	21			
1	C	380	Total	C	N	O	S	113	0	0
			3015	1930	488	575	22			

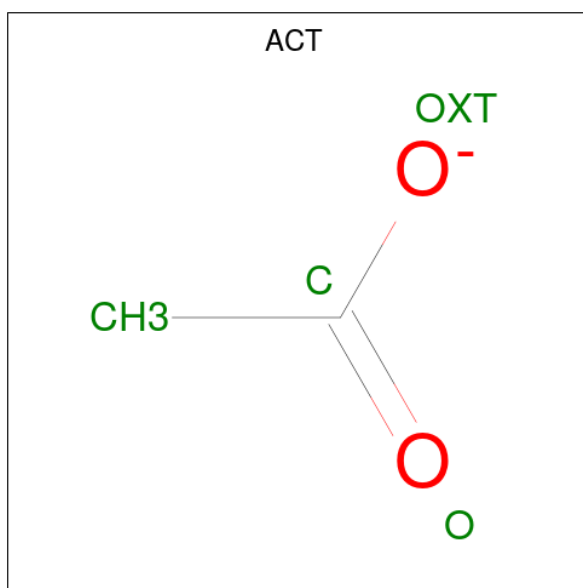
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	338	MET	-	initiating methionine	UNP Q9UDY8
A	720	HIS	-	expression tag	UNP Q9UDY8
A	721	HIS	-	expression tag	UNP Q9UDY8
A	722	HIS	-	expression tag	UNP Q9UDY8
A	723	HIS	-	expression tag	UNP Q9UDY8
A	724	HIS	-	expression tag	UNP Q9UDY8
A	725	HIS	-	expression tag	UNP Q9UDY8
C	338	MET	-	expression tag	UNP Q9UDY8
C	720	HIS	-	expression tag	UNP Q9UDY8
C	721	HIS	-	expression tag	UNP Q9UDY8
C	722	HIS	-	expression tag	UNP Q9UDY8
C	723	HIS	-	expression tag	UNP Q9UDY8
C	724	HIS	-	expression tag	UNP Q9UDY8
C	725	HIS	-	expression tag	UNP Q9UDY8

- Molecule 2 is a protein called tetrapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	1
			39	23	10	6			
2	D	5	Total	C	N	O	0	0	1
			39	23	10	6			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	58	Total O 58 58	0	0

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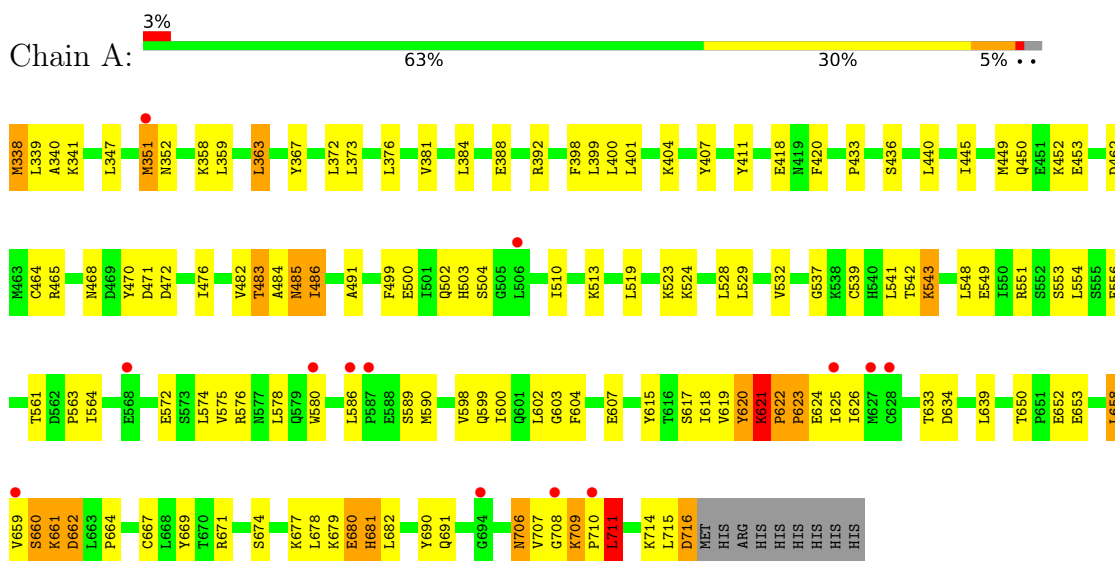
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	O 2	0	0
4	C	55	Total 55	O 55	0	0
4	D	1	Total 1	O 1	0	0

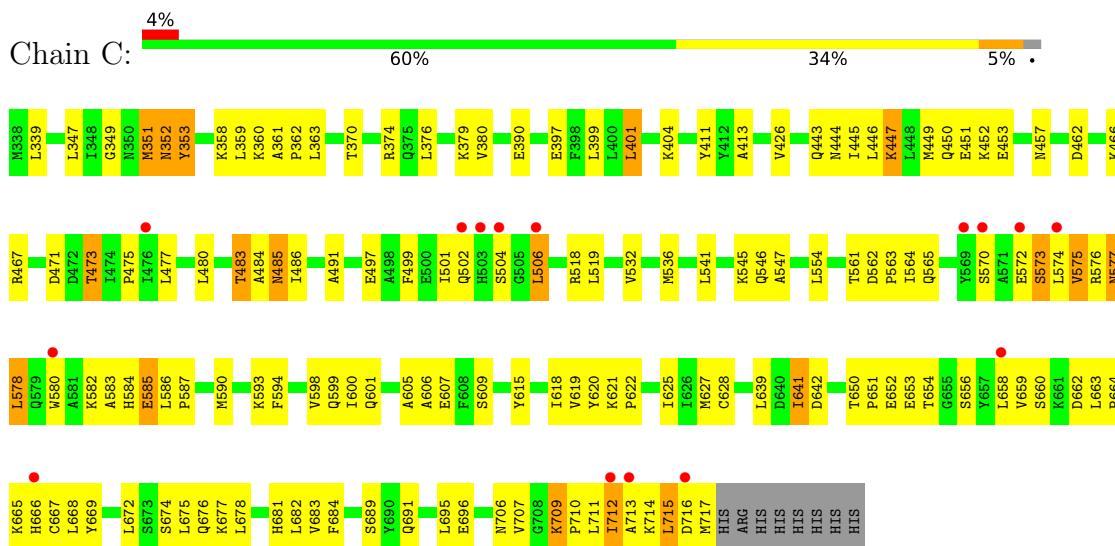
3 Residue-property plots [i](#)

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: Mucosa-associated lymphoid tissue lymphoma translocation protein 1



- Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1



- Molecule 2: tetrapeptide





● Molecule 2: tetrapeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.24Å 53.48Å 78.74Å 90.00° 103.80° 90.00°	Depositor
Resolution (Å)	43.94 – 2.40 43.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.94-2.40) 96.3 (43.94-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.198 , 0.245 0.199 , 0.247	Depositor DCC
R_{free} test set	1370 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6256	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: ACT, 4AR

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	0.73	4/3062 (0.1%)	1.00	8/4141 (0.2%)
1	C	0.68	0/3070	0.95	8/4151 (0.2%)
2	B	0.17	0/26	0.52	0/32
2	D	0.33	0/26	0.66	0/32
All	All	0.70	4/6184 (0.1%)	0.97	16/8356 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	LYS	C-N	6.48	1.41	1.33
1	A	623	PRO	N-CD	5.29	1.55	1.47
1	A	622	PRO	N-CD	5.23	1.55	1.47
1	A	681	HIS	CA-C	-5.13	1.46	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	LYS	N-CA-C	-11.05	100.45	113.38
1	C	715	LEU	N-CA-C	10.82	122.64	111.07
1	C	352	ASN	CA-C-N	-10.24	107.75	122.19
1	C	352	ASN	C-N-CA	-10.24	107.75	122.19
1	A	662	ASP	N-CA-C	-7.92	102.69	113.30
1	A	626	ILE	N-CA-C	7.70	118.50	110.72
1	A	621	LYS	CA-C-N	-7.57	112.59	120.38
1	A	621	LYS	C-N-CA	-7.57	112.59	120.38
1	C	716	ASP	N-CA-C	7.49	120.45	109.07
1	C	564	ILE	N-CA-C	6.56	117.74	108.36
1	A	620	TYR	N-CA-C	6.44	120.00	109.06
1	C	642	ASP	CA-C-N	5.93	125.80	119.28
1	C	642	ASP	C-N-CA	5.93	125.80	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	LEU	CB-CA-C	-5.70	109.99	116.54
1	A	681	HIS	N-CA-C	-5.42	103.19	110.24
1	C	590	MET	N-CA-C	5.28	118.06	109.24

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	3007	0	3029	160	0
1	C	3015	0	3037	193	0
2	B	39	0	38	8	0
2	D	39	0	38	18	0
3	A	20	0	15	12	0
3	C	20	0	15	2	0
4	A	58	0	0	8	0
4	B	2	0	0	0	0
4	C	55	0	0	3	0
4	D	1	0	0	0	0
All	All	6256	0	6172	359	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 (359) 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)
2:D:4:4AR:C7	2:D:4:4AR:C	1.92	1.45
1:A:483:THR:HB	1:A:485:ASN:ND2	1.40	1.35
1:C:473:THR:CG2	1:C:475:PRO:HD3	1.61	1.29
1:A:464:CYS:CB	2:B:4:4AR:C7	2.17	1.22
1:C:572:GLU:O	1:C:576:ARG:HG3	1.38	1.21
1:C:627:MET:HE2	1:C:691:GLN:CD	1.68	1.18
1:A:551:ARG:CD	3:A:801:ACT:H1	1.73	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:LEU:CD2	1:C:658:LEU:HD11	1.75	1.14
1:C:607:GLU:HG3	1:C:659:VAL:HG23	1.18	1.09
1:C:363:LEU:CD2	1:C:658:LEU:CD1	2.31	1.09
1:A:483:THR:CB	1:A:485:ASN:HD21	1.66	1.08
1:C:473:THR:HG23	1:C:475:PRO:HD3	1.18	1.07
1:A:551:ARG:HD3	3:A:801:ACT:CH3	1.84	1.07
1:C:578:LEU:CD1	1:C:582:LYS:NZ	2.20	1.05
1:C:363:LEU:HD23	1:C:658:LEU:HD11	1.08	1.05
1:A:401:LEU:HD21	1:A:580:TRP:CE3	1.91	1.03
1:A:551:ARG:HD3	3:A:801:ACT:H1	1.06	1.03
2:D:4:4AR:C7	2:D:4:4AR:CA	2.37	1.02
1:A:401:LEU:CD2	1:A:580:TRP:CE3	2.44	1.00
1:C:541:LEU:HG	2:D:1:LEU:HD11	1.42	1.00
1:C:363:LEU:HD23	1:C:658:LEU:CD1	1.92	0.99
1:A:551:ARG:CD	3:A:801:ACT:CH3	2.39	0.98
1:A:483:THR:CB	1:A:485:ASN:ND2	2.24	0.97
1:C:587:PRO:HB3	1:C:707:VAL:CG1	1.93	0.97
1:C:587:PRO:CG	1:C:707:VAL:HG11	1.95	0.97
4:C:930:HOH:O	2:D:2:ARG:HD2	1.65	0.96
1:C:363:LEU:HD21	1:C:658:LEU:CD1	1.93	0.95
1:A:483:THR:HB	1:A:485:ASN:HD21	1.14	0.95
1:A:401:LEU:HD21	1:A:580:TRP:HE3	1.25	0.94
1:C:483:THR:HB	1:C:485:ASN:ND2	1.83	0.94
1:C:352:ASN:HB2	1:C:358:LYS:HE3	1.50	0.93
1:C:484:ALA:O	1:C:554:LEU:HA	1.69	0.93
1:C:351:MET:HG2	1:C:359:LEU:O	1.70	0.92
1:A:681:HIS:HB3	1:A:708:GLY:HA2	1.48	0.92
1:C:578:LEU:HD12	1:C:582:LYS:NZ	1.83	0.92
1:C:615:TYR:CE2	1:C:664:PRO:HG2	2.05	0.91
1:C:627:MET:HE2	1:C:691:GLN:NE2	1.87	0.90
1:C:676:GLN:HB2	3:C:803:ACT:H2	1.53	0.89
1:C:587:PRO:HB3	1:C:707:VAL:HG13	1.52	0.89
1:C:374:ARG:CZ	1:C:584:HIS:HE1	1.84	0.89
1:C:615:TYR:HE2	1:C:664:PRO:HG2	1.35	0.88
1:A:572:GLU:O	1:A:575:VAL:HG12	1.74	0.88
1:C:353:TYR:HE2	1:C:426:VAL:O	1.55	0.88
1:C:541:LEU:CG	2:D:1:LEU:HD11	2.03	0.88
1:C:587:PRO:HG3	1:C:707:VAL:HG11	1.53	0.87
1:C:473:THR:HG22	1:C:475:PRO:HD3	1.54	0.87
1:C:586:LEU:HD11	1:C:606:ALA:N	1.91	0.86
1:C:578:LEU:HD12	1:C:582:LYS:HZ3	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:LEU:CD1	1:C:582:LYS:HZ2	1.84	0.86
1:C:587:PRO:CB	1:C:707:VAL:HG11	2.04	0.86
1:C:578:LEU:CD1	1:C:582:LYS:HZ3	1.86	0.85
2:D:4:4AR:C7	2:D:4:4AR:N	2.40	0.85
1:A:352:ASN:HB2	4:A:915:HOH:O	1.76	0.85
1:A:586:LEU:HD13	1:A:604:PHE:HB2	1.57	0.85
1:A:464:CYS:HG	2:B:4:4AR:C7	0.89	0.84
1:C:627:MET:CE	1:C:691:GLN:NE2	2.40	0.84
1:C:583:ALA:O	1:C:711:LEU:HA	1.76	0.84
1:A:667:CYS:O	1:A:669:TYR:CE2	2.30	0.84
1:C:353:TYR:CE2	1:C:426:VAL:O	2.30	0.83
1:C:587:PRO:CB	1:C:707:VAL:CG1	2.56	0.83
1:A:603:GLY:HA3	1:A:615:TYR:CE1	2.14	0.83
1:A:352:ASN:OD1	1:A:358:LYS:HD3	1.79	0.82
1:A:660:SER:C	1:A:662:ASP:H	1.83	0.82
1:C:572:GLU:O	1:C:576:ARG:CG	2.26	0.82
1:A:483:THR:HB	1:A:485:ASN:CG	2.04	0.82
1:A:468:ASN:HB2	4:A:957:HOH:O	1.81	0.81
1:C:541:LEU:CD2	2:D:1:LEU:HD11	2.10	0.81
1:A:401:LEU:CD2	1:A:580:TRP:CZ3	2.63	0.80
1:C:483:THR:HB	1:C:485:ASN:CG	2.05	0.80
1:A:381:VAL:HG23	1:A:580:TRP:CZ2	2.16	0.80
1:C:707:VAL:HG12	1:C:707:VAL:O	1.80	0.80
1:A:367:TYR:CB	1:A:658:LEU:HD21	2.12	0.78
1:C:607:GLU:HG3	1:C:659:VAL:CG2	2.08	0.77
1:A:401:LEU:HD23	1:A:580:TRP:CZ3	2.19	0.76
1:C:586:LEU:HD23	1:C:711:LEU:CD1	2.15	0.76
1:C:678:LEU:HD12	1:C:678:LEU:O	1.84	0.76
1:A:598:VAL:HG13	1:A:620:TYR:O	1.86	0.75
2:D:4:4AR:C7	2:D:4:4AR:O	2.35	0.75
1:C:374:ARG:CZ	1:C:584:HIS:CE1	2.70	0.74
1:C:473:THR:HG23	1:C:475:PRO:CD	2.10	0.74
1:A:551:ARG:HD2	3:A:801:ACT:CH3	2.17	0.74
1:A:401:LEU:HG	1:A:580:TRP:CZ3	2.23	0.73
1:A:660:SER:C	1:A:662:ASP:N	2.43	0.73
1:A:450:GLN:NE2	1:A:483:THR:OG1	2.20	0.73
1:A:681:HIS:CD2	1:A:708:GLY:HA3	2.23	0.73
1:C:447:LYS:HE2	1:C:480:LEU:HD23	1.71	0.73
1:A:681:HIS:CD2	1:A:708:GLY:CA	2.72	0.72
1:A:681:HIS:CB	1:A:708:GLY:HA2	2.20	0.72
1:C:627:MET:HE2	1:C:691:GLN:CG	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:THR:CG2	1:A:485:ASN:OD1	2.37	0.71
1:A:420:PHE:CE2	4:A:949:HOH:O	2.43	0.71
1:C:363:LEU:HD21	1:C:658:LEU:HD12	1.72	0.71
1:C:578:LEU:HD11	1:C:582:LYS:NZ	2.06	0.71
1:C:609:SER:O	1:C:712:ILE:HG22	1.91	0.70
1:C:483:THR:HB	1:C:485:ASN:HD21	1.55	0.70
1:C:473:THR:CG2	1:C:475:PRO:CD	2.56	0.70
1:C:483:THR:CB	1:C:485:ASN:HD21	2.04	0.69
1:A:617:SER:HB3	1:A:667:CYS:SG	2.33	0.68
1:C:397:GLU:HG2	1:C:715:LEU:HD13	1.74	0.68
1:C:593:LYS:HG3	1:C:599:GLN:HG2	1.73	0.68
1:A:404:LYS:HA	1:A:453:GLU:O	1.93	0.68
1:A:551:ARG:NH2	4:A:923:HOH:O	2.23	0.67
1:C:600:ILE:HG22	1:C:618:ILE:HA	1.76	0.67
1:C:615:TYR:CE2	1:C:664:PRO:CG	2.77	0.67
1:C:501:ILE:HG22	1:C:504:SER:HB3	1.77	0.67
1:C:712:ILE:C	1:C:712:ILE:HD13	2.19	0.67
1:C:674:SER:HB3	1:C:677:LYS:HG3	1.75	0.67
1:C:401:LEU:HD13	1:C:580:TRP:CE3	2.30	0.66
1:C:682:LEU:HD23	1:C:684:PHE:HD1	1.60	0.66
1:A:551:ARG:HD2	3:A:801:ACT:H1	1.73	0.66
1:A:711:LEU:O	1:A:714:LYS:HG3	1.95	0.66
1:C:712:ILE:HD13	1:C:712:ILE:O	1.96	0.66
1:C:586:LEU:HD23	1:C:711:LEU:HD13	1.76	0.65
1:C:483:THR:CB	1:C:485:ASN:ND2	2.58	0.65
1:A:621:LYS:HD3	1:A:625:ILE:O	1.96	0.65
1:A:420:PHE:HE2	4:A:949:HOH:O	1.79	0.65
1:C:675:LEU:O	1:C:678:LEU:HG	1.97	0.65
1:C:586:LEU:HD23	1:C:711:LEU:HD11	1.78	0.64
1:C:363:LEU:HD21	1:C:658:LEU:CG	2.26	0.64
1:C:615:TYR:CE2	1:C:664:PRO:HD2	2.32	0.64
1:C:659:VAL:HG12	1:C:659:VAL:O	1.95	0.64
1:C:682:LEU:CD2	1:C:684:PHE:CD1	2.81	0.64
1:A:401:LEU:HD23	1:A:580:TRP:HZ3	1.63	0.64
1:A:338:MET:HE3	1:A:338:MET:HA	1.80	0.64
1:A:681:HIS:HD2	1:A:708:GLY:CA	2.10	0.64
1:C:598:VAL:HG13	1:C:620:TYR:O	1.98	0.64
1:C:374:ARG:NH2	1:C:584:HIS:HE1	1.95	0.64
1:A:681:HIS:HD2	1:A:708:GLY:HA3	1.63	0.63
1:C:536:MET:HE1	1:C:546:GLN:HG2	1.80	0.63
1:A:551:ARG:CD	3:A:801:ACT:H2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:666:HIS:O	1:C:667:CYS:SG	2.54	0.63
1:A:398:PHE:HE2	1:A:449:MET:HE2	1.64	0.63
1:C:682:LEU:HD23	1:C:684:PHE:CD1	2.34	0.63
1:A:339:LEU:CD2	1:A:563:PRO:HB2	2.29	0.63
1:A:706:ASN:O	1:A:706:ASN:ND2	2.32	0.63
1:C:352:ASN:HB3	4:C:907:HOH:O	1.99	0.62
1:A:445:ILE:HG22	1:A:449:MET:HE3	1.80	0.62
1:A:351:MET:HB3	1:A:359:LEU:O	1.99	0.62
1:C:605:ALA:CB	1:C:663:LEU:HD11	2.30	0.62
1:A:483:THR:HG22	1:A:485:ASN:OD1	1.98	0.62
1:C:363:LEU:CD2	1:C:658:LEU:CG	2.78	0.62
1:C:628:CYS:HA	1:C:689:SER:O	1.99	0.62
1:C:361:ALA:N	1:C:362:PRO:CD	2.63	0.61
1:A:715:LEU:O	1:A:716:ASP:CB	2.47	0.61
1:C:594:PHE:CE1	1:C:600:ILE:HD11	2.34	0.61
1:C:363:LEU:HD21	1:C:658:LEU:HG	1.81	0.61
1:C:586:LEU:HD11	1:C:606:ALA:HB2	1.83	0.61
1:A:392:ARG:NH1	3:A:803:ACT:OXT	2.29	0.61
1:A:600:ILE:CD1	1:A:618:ILE:HD13	2.31	0.61
1:C:615:TYR:CE2	1:C:664:PRO:CD	2.84	0.61
1:A:572:GLU:O	1:A:575:VAL:CG1	2.49	0.61
1:A:401:LEU:CG	1:A:580:TRP:CZ3	2.84	0.60
1:C:379:LYS:HE2	1:C:577:ASN:ND2	2.16	0.60
1:C:709:LYS:O	1:C:714:LYS:HE3	2.01	0.60
1:C:501:ILE:CG2	1:C:504:SER:HB3	2.31	0.60
1:C:541:LEU:HG	2:D:1:LEU:CD1	2.25	0.60
1:C:586:LEU:HD11	1:C:606:ALA:CB	2.31	0.60
1:A:682:LEU:HD23	1:A:707:VAL:HG22	1.83	0.60
1:A:621:LYS:CD	1:A:625:ILE:O	2.50	0.60
1:C:586:LEU:CD2	1:C:711:LEU:HD11	2.32	0.60
1:A:715:LEU:O	1:A:716:ASP:HB3	2.01	0.59
1:C:466:LYS:HE3	1:C:497:GLU:HG3	1.84	0.59
1:A:418:GLU:OE1	1:A:465:ARG:HD2	2.01	0.59
1:A:483:THR:O	1:A:484:ALA:HB3	2.00	0.59
1:A:532:VAL:HG12	1:A:548:LEU:HD12	1.84	0.59
1:C:659:VAL:HG12	1:C:663:LEU:CD1	2.33	0.59
1:A:664:PRO:O	1:A:669:TYR:OH	2.21	0.59
1:C:641:ILE:HD11	1:C:672:LEU:HD22	1.85	0.59
1:C:707:VAL:CG1	1:C:707:VAL:O	2.50	0.59
1:C:601:GLN:HB2	1:C:619:VAL:CG2	2.34	0.58
1:C:483:THR:O	1:C:484:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:LEU:HD21	1:C:678:LEU:HD23	1.86	0.58
1:A:603:GLY:HA3	1:A:615:TYR:CZ	2.38	0.58
1:C:450:GLN:NE2	1:C:483:THR:OG1	2.34	0.58
1:C:715:LEU:O	3:C:805:ACT:H1	2.04	0.58
1:A:347:LEU:HG	1:A:411:TYR:HB3	1.86	0.57
1:A:464:CYS:HB2	2:B:4:4AR:C7	2.29	0.57
1:A:682:LEU:HD23	1:A:707:VAL:CG2	2.35	0.57
1:C:627:MET:CE	1:C:691:GLN:CD	2.59	0.56
1:A:681:HIS:HD2	1:A:709:LYS:N	2.03	0.56
1:C:536:MET:CE	1:C:546:GLN:HG2	2.36	0.56
1:A:503:HIS:CE1	1:A:504:SER:O	2.58	0.56
1:C:682:LEU:CD2	1:C:684:PHE:CE1	2.89	0.56
1:C:607:GLU:CG	1:C:659:VAL:HG23	2.13	0.56
1:C:374:ARG:NH2	1:C:584:HIS:CE1	2.73	0.56
1:A:367:TYR:HB3	1:A:658:LEU:HD21	1.88	0.55
1:A:600:ILE:HD12	1:A:618:ILE:HD13	1.87	0.55
1:A:367:TYR:CG	1:A:658:LEU:CD2	2.89	0.55
1:C:578:LEU:HD11	1:C:582:LYS:HZ3	1.67	0.55
1:A:599:GLN:O	1:A:619:VAL:HG12	2.05	0.55
1:C:363:LEU:CD2	1:C:658:LEU:HG	2.37	0.55
1:A:543:LYS:HE3	4:A:932:HOH:O	2.07	0.54
1:C:678:LEU:HD12	1:C:678:LEU:C	2.31	0.54
1:A:484:ALA:O	1:A:554:LEU:HA	2.07	0.54
1:C:541:LEU:HD21	2:D:1:LEU:HD11	1.89	0.54
1:C:621:LYS:HE3	1:C:625:ILE:O	2.08	0.54
1:C:483:THR:HB	1:C:485:ASN:OD1	2.07	0.54
1:C:627:MET:HE1	1:C:691:GLN:NE2	2.22	0.54
1:C:351:MET:CG	1:C:359:LEU:O	2.50	0.54
1:C:499:PHE:CG	2:D:1:LEU:HD23	2.43	0.54
1:A:551:ARG:HD2	3:A:801:ACT:H2	1.90	0.53
1:A:367:TYR:HB2	1:A:658:LEU:HD21	1.88	0.53
1:A:476:ILE:HG22	1:A:476:ILE:O	2.09	0.53
1:C:347:LEU:HG	1:C:411:TYR:HB3	1.90	0.53
1:C:473:THR:HG22	1:C:475:PRO:CD	2.32	0.53
1:C:656:SER:O	1:C:660:SER:OG	2.26	0.53
1:C:599:GLN:NE2	4:C:917:HOH:O	2.41	0.53
1:A:485:ASN:ND2	1:A:485:ASN:H	2.06	0.53
1:A:680:GLU:O	1:A:681:HIS:C	2.51	0.53
1:C:659:VAL:HG12	1:C:663:LEU:HD13	1.91	0.53
1:A:482:VAL:HG12	1:A:482:VAL:O	2.08	0.52
1:A:537:GLY:O	1:A:543:LYS:NZ	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:HIS:HD2	1:A:709:LYS:H	1.58	0.52
1:A:660:SER:O	1:A:662:ASP:N	2.42	0.52
1:C:570:SER:OG	1:C:573:SER:HB2	2.09	0.52
1:C:682:LEU:HD13	1:C:710:PRO:HG3	1.90	0.52
1:A:500:GLU:CG	2:B:2:ARG:HB3	2.40	0.52
1:A:639:LEU:HD21	1:A:678:LEU:HG	1.91	0.52
1:A:367:TYR:CB	1:A:658:LEU:CD2	2.86	0.52
1:C:573:SER:HA	1:C:576:ARG:HD2	1.92	0.52
1:C:578:LEU:HD12	1:C:582:LYS:CE	2.39	0.52
1:C:401:LEU:HD22	1:C:580:TRP:CD2	2.45	0.52
1:A:667:CYS:O	1:A:669:TYR:CD2	2.62	0.52
1:A:589:SER:HB2	1:A:602:LEU:O	2.09	0.52
1:C:578:LEU:HD13	1:C:582:LYS:HZ2	1.72	0.52
2:D:4:4AR:C7	2:D:4:4AR:C3	2.88	0.51
1:A:622:PRO:HB2	1:A:624:GLU:CD	2.35	0.51
1:A:445:ILE:O	1:A:449:MET:HG3	2.11	0.51
1:C:363:LEU:CD2	1:C:658:LEU:HD12	2.34	0.51
1:C:390:GLU:OE2	1:C:677:LYS:HE3	2.11	0.51
1:C:518:ARG:HG3	1:C:532:VAL:HG22	1.92	0.51
1:A:659:VAL:HG13	1:A:662:ASP:HB3	1.93	0.50
1:C:445:ILE:O	1:C:449:MET:HG3	2.11	0.50
1:A:388:GLU:O	1:A:392:ARG:HG3	2.12	0.50
1:C:353:TYR:N	1:C:353:TYR:CD1	2.79	0.50
1:A:401:LEU:CG	1:A:580:TRP:CE3	2.95	0.50
1:C:585:GLU:O	1:C:711:LEU:HD12	2.11	0.50
1:A:399:LEU:O	1:A:452:LYS:NZ	2.39	0.50
1:A:674:SER:HB3	1:A:677:LYS:HD2	1.94	0.50
1:A:500:GLU:HG3	2:B:2:ARG:HB3	1.94	0.50
1:C:541:LEU:HD21	2:D:1:LEU:CD1	2.42	0.50
1:C:652:GLU:OE2	1:C:660:SER:HB3	2.11	0.50
1:C:682:LEU:HD21	1:C:684:PHE:CD1	2.47	0.49
1:A:618:ILE:HG22	1:A:618:ILE:O	2.11	0.49
1:A:625:ILE:HG21	1:A:690:TYR:HB2	1.94	0.49
1:C:502:GLN:HG3	2:D:2:ARG:NH1	2.27	0.49
1:A:485:ASN:HD22	1:A:486:ILE:HG13	1.78	0.49
1:A:662:ASP:OD1	1:A:662:ASP:O	2.30	0.49
1:C:352:ASN:HB3	1:C:358:LYS:HD3	1.95	0.49
1:C:609:SER:HB3	1:C:712:ILE:HB	1.95	0.49
1:C:536:MET:HE2	1:C:547:ALA:HA	1.93	0.48
1:A:499:PHE:HA	2:B:2:ARG:O	2.13	0.48
1:C:374:ARG:NE	1:C:584:HIS:CE1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LYS:HE3	1:A:556:GLU:O	2.14	0.48
1:C:471:ASP:OD1	1:C:473:THR:HB	2.14	0.48
1:A:625:ILE:HG23	1:A:691:GLN:O	2.14	0.48
1:A:376:LEU:HD22	1:A:561:THR:HG22	1.96	0.48
1:A:590:MET:HE1	1:A:707:VAL:HG12	1.95	0.48
1:A:339:LEU:HD22	1:A:563:PRO:HB2	1.95	0.48
1:A:367:TYR:CG	1:A:658:LEU:HD21	2.48	0.48
1:A:650:THR:OG1	1:A:653:GLU:HG3	2.13	0.48
1:C:586:LEU:CD1	1:C:606:ALA:N	2.72	0.47
1:A:367:TYR:HB2	1:A:658:LEU:CD2	2.45	0.47
1:C:361:ALA:HB3	2:D:4:4AR:HH11	1.79	0.47
1:C:578:LEU:O	1:C:582:LYS:HD3	2.15	0.47
1:A:392:ARG:HB3	3:A:803:ACT:H1	1.96	0.47
1:C:659:VAL:O	1:C:659:VAL:CG1	2.61	0.47
1:A:338:MET:HA	1:A:338:MET:CE	2.43	0.47
1:C:370:THR:HG23	1:C:380:VAL:HG11	1.97	0.47
1:A:623:PRO:O	1:A:624:GLU:C	2.58	0.47
1:A:392:ARG:HH12	3:A:804:ACT:C	2.28	0.46
1:A:510:ILE:O	1:A:513:LYS:HB3	2.14	0.46
1:C:502:GLN:HG3	2:D:2:ARG:HH12	1.80	0.46
1:A:706:ASN:ND2	1:A:706:ASN:C	2.73	0.46
1:C:574:LEU:O	1:C:578:LEU:HB2	2.16	0.46
1:A:574:LEU:O	1:A:578:LEU:HD23	2.16	0.46
1:A:513:LYS:HG2	4:A:950:HOH:O	2.14	0.46
1:C:627:MET:HE2	1:C:691:GLN:HG3	1.96	0.46
1:C:651:PRO:O	1:C:654:THR:OG1	2.30	0.46
1:A:529:LEU:O	1:A:532:VAL:HB	2.16	0.45
1:C:379:LYS:HE2	1:C:577:ASN:HD21	1.80	0.45
1:C:681:HIS:CE1	1:C:709:LYS:HD2	2.52	0.45
1:C:404:LYS:HA	1:C:453:GLU:O	2.17	0.45
1:A:660:SER:O	1:A:661:LYS:HB2	2.16	0.45
1:C:609:SER:O	1:C:712:ILE:CG2	2.61	0.45
1:A:502:GLN:H	2:B:0:ALA:C	2.25	0.45
1:C:572:GLU:HA	1:C:575:VAL:HG12	1.99	0.45
1:C:359:LEU:HD23	2:D:2:ARG:HD3	1.99	0.45
1:C:587:PRO:CB	1:C:707:VAL:HG13	2.29	0.45
1:A:607:GLU:OE2	1:A:671:ARG:NH2	2.46	0.45
1:A:433:PRO:HG2	1:A:470:TYR:CE1	2.52	0.44
1:A:575:VAL:HG13	1:A:576:ARG:N	2.31	0.44
1:A:681:HIS:CG	1:A:708:GLY:HA2	2.52	0.44
1:A:572:GLU:C	1:A:575:VAL:HG12	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:THR:OG1	1:C:653:GLU:HG3	2.17	0.44
1:C:717:MET:HE2	1:C:717:MET:HB3	1.87	0.44
1:A:381:VAL:HG23	1:A:580:TRP:CE2	2.52	0.44
1:A:483:THR:O	1:A:484:ALA:CB	2.66	0.44
1:C:572:GLU:O	1:C:575:VAL:HG13	2.16	0.44
1:C:506:LEU:H	1:C:506:LEU:HG	1.54	0.44
1:A:401:LEU:HG	1:A:580:TRP:CE3	2.52	0.44
1:A:465:ARG:HH22	1:A:549:GLU:CD	2.26	0.44
1:C:601:GLN:HB2	1:C:619:VAL:HG23	1.98	0.44
1:A:528:LEU:O	1:A:532:VAL:HG23	2.18	0.44
1:C:353:TYR:N	1:C:353:TYR:HD1	2.15	0.44
1:C:594:PHE:HE1	1:C:600:ILE:HD11	1.77	0.44
1:C:462:ASP:HA	1:C:491:ALA:HB2	2.00	0.44
1:C:586:LEU:HD11	1:C:606:ALA:CA	2.48	0.44
1:A:483:THR:CB	1:A:485:ASN:CG	2.83	0.43
1:A:652:GLU:OE1	1:A:652:GLU:N	2.42	0.43
1:C:519:LEU:O	1:C:519:LEU:HG	2.19	0.43
1:C:598:VAL:HG22	1:C:622:PRO:HD2	2.00	0.43
1:C:682:LEU:HD21	1:C:684:PHE:CE1	2.53	0.43
1:C:352:ASN:CB	1:C:358:LYS:HE3	2.35	0.43
1:A:539:CYS:HB3	1:A:542:THR:OG1	2.18	0.43
1:C:443:GLN:HB3	1:C:477:LEU:HD22	2.00	0.43
1:C:683:VAL:HG22	1:C:706:ASN:OD1	2.19	0.43
1:C:583:ALA:HB1	1:C:712:ILE:HA	2.01	0.43
1:A:372:LEU:HB3	1:A:519:LEU:HD23	2.01	0.43
1:A:659:VAL:C	1:A:660:SER:OG	2.62	0.43
1:A:363:LEU:HD12	1:A:384:LEU:HD11	2.00	0.42
1:C:712:ILE:O	1:C:713:ALA:C	2.62	0.42
1:A:340:ALA:HB2	1:A:407:TYR:CE1	2.54	0.42
1:A:340:ALA:HB2	1:A:407:TYR:CZ	2.54	0.42
1:C:483:THR:O	1:C:484:ALA:CB	2.68	0.42
1:C:586:LEU:CD2	1:C:711:LEU:CD1	2.90	0.42
1:A:440:LEU:HA	3:A:804:ACT:O	2.20	0.42
1:A:633:THR:OG1	1:A:634:ASP:N	2.52	0.42
1:C:376:LEU:HD22	1:C:561:THR:HG22	2.01	0.42
1:C:562:ASP:HA	1:C:563:PRO:HD3	1.83	0.42
1:C:586:LEU:HD11	1:C:606:ALA:H	1.77	0.42
1:A:401:LEU:CD2	1:A:580:TRP:HE3	1.98	0.42
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.81	0.42
1:A:599:GLN:O	1:A:619:VAL:CG1	2.68	0.42
1:C:499:PHE:CB	2:D:1:LEU:HD23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ASN:ND2	1:C:485:ASN:ND2	2.67	0.42
1:C:627:MET:CE	1:C:691:GLN:HG3	2.50	0.42
1:A:715:LEU:O	1:A:716:ASP:OD1	2.37	0.41
1:C:651:PRO:HD3	1:C:669:TYR:CE2	2.55	0.41
1:C:583:ALA:HA	1:C:711:LEU:O	2.20	0.41
1:A:658:LEU:HD12	1:A:658:LEU:HA	1.81	0.41
1:A:681:HIS:CD2	1:A:708:GLY:HA2	2.55	0.41
1:C:349:GLY:HA2	1:C:413:ALA:O	2.19	0.41
1:A:621:LYS:HD2	1:A:625:ILE:O	2.19	0.41
1:A:436:SER:HB3	1:A:471:ASP:OD2	2.21	0.41
1:A:602:LEU:HA	1:A:602:LEU:HD12	1.74	0.41
1:C:379:LYS:HB3	1:C:580:TRP:CD1	2.56	0.41
1:C:615:TYR:CZ	1:C:664:PRO:CD	3.03	0.41
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.86	0.41
1:C:681:HIS:HE1	1:C:709:LYS:HD2	1.86	0.41
1:A:500:GLU:OE2	2:B:2:ARG:HD2	2.21	0.41
1:A:549:GLU:OE2	4:A:942:HOH:O	2.22	0.41
1:C:399:LEU:O	1:C:452:LYS:NZ	2.52	0.41
1:C:712:ILE:HG23	1:C:713:ALA:N	2.36	0.41
1:C:444:ASN:OD1	1:C:477:LEU:HD21	2.21	0.40
1:A:483:THR:HG1	1:A:485:ASN:HD21	1.68	0.40
1:A:462:ASP:HA	1:A:491:ALA:HB2	2.02	0.40
1:A:483:THR:HG21	1:A:485:ASN:OD1	2.17	0.40
1:C:712:ILE:C	1:C:712:ILE:CD1	2.88	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	377/388 (97%)	366 (97%)	10 (3%)	1 (0%)	36 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	378/388 (97%)	366 (97%)	12 (3%)	0	100	100
2	B	3/5 (60%)	3 (100%)	0	0	100	100
2	D	3/5 (60%)	3 (100%)	0	0	100	100
All	All	761/786 (97%)	738 (97%)	22 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	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	336/345 (97%)	314 (94%)	22 (6%)	15	27
1	C	337/345 (98%)	308 (91%)	29 (9%)	10	16
2	B	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	679/696 (98%)	627 (92%)	52 (8%)	12	20

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	MET
1	A	341	LYS
1	A	351	MET
1	A	363	LEU
1	A	472	ASP
1	A	483	THR
1	A	485	ASN
1	A	486	ILE
1	A	523	LYS
1	A	541	LEU

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Mol	Chain	Res	Type
1	A	543	LYS
1	A	553	SER
1	A	564	ILE
1	A	621	LYS
1	A	658	LEU
1	A	660	SER
1	A	679	LYS
1	A	680	GLU
1	A	706	ASN
1	A	709	LYS
1	A	711	LEU
1	A	716	ASP
2	B	1	LEU
1	C	339	LEU
1	C	351	MET
1	C	353	TYR
1	C	360	LYS
1	C	401	LEU
1	C	446	LEU
1	C	447	LYS
1	C	451	GLU
1	C	467	ARG
1	C	473	THR
1	C	483	THR
1	C	485	ASN
1	C	486	ILE
1	C	506	LEU
1	C	545	LYS
1	C	565	GLN
1	C	573	SER
1	C	575	VAL
1	C	577	ASN
1	C	578	LEU
1	C	585	GLU
1	C	641	ILE
1	C	662	ASP
1	C	665	LYS
1	C	668	LEU
1	C	695	LEU
1	C	696	GLU
1	C	709	LYS
1	C	712	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	485	ASN
1	A	565	GLN
1	A	599	GLN
1	A	681	HIS
1	C	485	ASN
1	C	577	ASN
1	C	584	HIS
1	C	599	GLN
1	C	601	GLN
1	C	681	HIS
1	C	691	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	4AR	B	4	1,2	10,11,23	1.84	1 (10%)	8,13,30	6.67	1 (12%)
2	4AR	D	4	1,2	10,11,23	5.54	1 (10%)	8,13,30	5.46	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4AR	B	4	1,2	-	2/10/11/20	-
2	4AR	D	4	1,2	-	0/10/11/20	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	4AR	C7-C	17.50	1.92	1.49
2	B	4	4AR	C7-C	5.73	1.63	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	4AR	O-C-C7	-18.83	87.94	121.17
2	D	4	4AR	O-C-C7	-15.36	94.07	121.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	4AR	O-C-CA-N
2	B	4	4AR	C4-C3-CA-C

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	4AR	3	0
2	D	4	4AR	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	A	804	-	3,3,3	0.94	0	3,3,3	1.12	0
3	ACT	C	801	-	3,3,3	0.82	0	3,3,3	0.71	0
3	ACT	C	803	-	3,3,3	0.82	0	3,3,3	0.75	0
3	ACT	C	805	-	3,3,3	0.82	0	3,3,3	0.74	0
3	ACT	A	801	-	3,3,3	0.93	0	3,3,3	0.44	0
3	ACT	C	802	-	3,3,3	0.94	0	3,3,3	0.64	0
3	ACT	C	804	-	3,3,3	0.93	0	3,3,3	0.67	0
3	ACT	A	805	-	3,3,3	0.92	0	3,3,3	0.57	0
3	ACT	A	802	-	3,3,3	0.83	0	3,3,3	0.75	0
3	ACT	A	803	-	3,3,3	0.94	0	3,3,3	0.76	0

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.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	ACT	2	0
3	C	803	ACT	1	0
3	C	805	ACT	1	0
3	A	801	ACT	8	0
3	A	803	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	379/388 (97%)	0.20	13 (3%)	48 44	28, 63, 117, 155	29 (7%)
1	C	379/388 (97%)	0.20	15 (3%)	42 38	27, 64, 115, 150	27 (7%)
2	B	4/5 (80%)	1.21	1 (25%)	2 1	61, 69, 75, 84	0
2	D	4/5 (80%)	1.24	2 (50%)	0 0	64, 78, 84, 87	0
All	All	766/786 (97%)	0.21	31 (4%)	42 38	27, 63, 117, 155	56 (7%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	PRO	4.2
1	A	506	LEU	3.2
1	C	503	HIS	3.1
1	A	586	LEU	3.0
1	C	712	ILE	2.9
1	C	580	TRP	2.9
1	A	580	TRP	2.9
1	C	504	SER	2.8
1	A	659	VAL	2.8
1	C	666	HIS	2.7
1	C	569	TYR	2.6
1	C	570	SER	2.6
1	A	625	ILE	2.5
2	B	0	ALA	2.5
1	C	574	LEU	2.4
1	C	502	GLN	2.4
1	C	658	LEU	2.4
1	C	506	LEU	2.4
1	C	572	GLU	2.4
1	A	627	MET	2.3
1	A	708	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	716	ASP	2.3
1	A	694	GLY	2.3
1	A	628	CYS	2.3
1	A	351	MET	2.2
1	C	476	ILE	2.2
2	D	0	ALA	2.2
1	C	713	ALA	2.1
2	D	1	LEU	2.1
1	A	568	GLU	2.1
1	A	587	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	4AR	B	4	12/23	0.95	0.08	48,51,59,124	0
2	4AR	D	4	12/23	0.95	0.08	49,53,56,98	0

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
3	ACT	C	805	4/4	0.36	0.21	122,125,126,126	0
3	ACT	A	805	4/4	0.72	0.21	109,110,111,112	0
3	ACT	A	804	4/4	0.74	0.23	81,82,83,86	0
3	ACT	C	804	4/4	0.78	0.12	97,97,98,98	0
3	ACT	A	802	4/4	0.79	0.14	106,107,108,109	0
3	ACT	C	803	4/4	0.79	0.21	98,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	A	803	4/4	0.83	0.21	82,83,84,86	0
3	ACT	C	801	4/4	0.85	0.18	88,89,90,92	0
3	ACT	A	801	4/4	0.86	0.17	77,80,80,82	0
3	ACT	C	802	4/4	0.87	0.15	94,95,95,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.