



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:31 PM UTC

PDB ID : 4HZK / pdb_00004hzk
Title : Crystal structure of free CRM1 (crystal form 2)
Authors : Monecke, T.; Neumann, P.; Dickmanns, A.; Ficner, R.
Deposited on : 2012-11-15
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

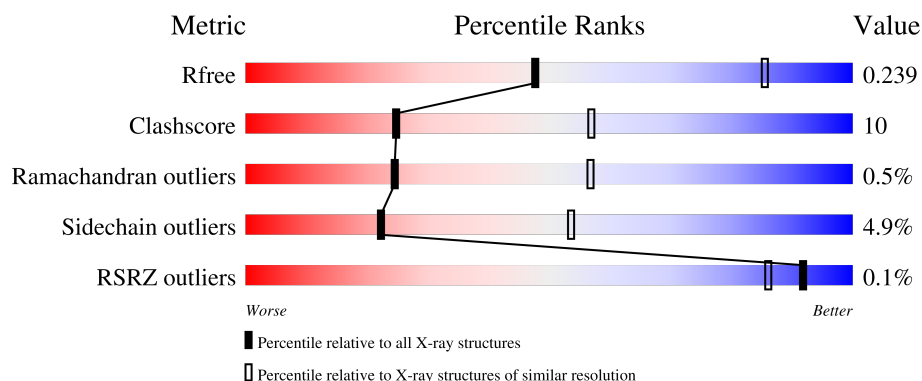
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1086	 69% 24% • 5%
1	B	1086	 67% 26% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16642 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 CRM1 Nuclear transport receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1033	Total	C	N	O	S	0	0	0
			8326	5316	1404	1543	63			
1	B	1031	Total	C	N	O	S	0	0	0
			8316	5313	1403	1537	63			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP G0RZB7
A	-7	ALA	-	expression tag	UNP G0RZB7
A	-6	ALA	-	expression tag	UNP G0RZB7
A	-5	ALA	-	expression tag	UNP G0RZB7
A	-4	SER	-	expression tag	UNP G0RZB7
A	-3	GLY	-	expression tag	UNP G0RZB7
A	-2	SER	-	expression tag	UNP G0RZB7
A	-1	GLU	-	expression tag	UNP G0RZB7
A	0	PHE	-	expression tag	UNP G0RZB7
A	22	GLN	-	SEE REMARK 999	UNP G0RZB7
A	23	GLN	-	SEE REMARK 999	UNP G0RZB7
A	24	LYS	-	SEE REMARK 999	UNP G0RZB7
A	25	ALA	-	SEE REMARK 999	UNP G0RZB7
A	26	ALA	-	SEE REMARK 999	UNP G0RZB7
A	27	GLN	-	SEE REMARK 999	UNP G0RZB7
A	28	ALA	-	SEE REMARK 999	UNP G0RZB7
A	29	ALA	-	SEE REMARK 999	UNP G0RZB7
A	30	LEU	-	SEE REMARK 999	UNP G0RZB7
A	31	ASN	-	SEE REMARK 999	UNP G0RZB7
A	57	PHE	-	SEE REMARK 999	UNP G0RZB7
A	58	LEU	-	SEE REMARK 999	UNP G0RZB7
A	59	ALA	-	SEE REMARK 999	UNP G0RZB7
A	60	LEU	-	SEE REMARK 999	UNP G0RZB7
A	61	GLN	-	SEE REMARK 999	UNP G0RZB7
A	62	VAL	-	SEE REMARK 999	UNP G0RZB7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	63	LEU	-	SEE REMARK 999	UNP G0RZB7
A	64	ASP	-	SEE REMARK 999	UNP G0RZB7
A	65	ASN	-	SEE REMARK 999	UNP G0RZB7
A	66	VAL	-	SEE REMARK 999	UNP G0RZB7
A	67	ILE	-	SEE REMARK 999	UNP G0RZB7
A	68	MET	-	SEE REMARK 999	UNP G0RZB7
A	69	THR	-	SEE REMARK 999	UNP G0RZB7
A	70	ARG	-	SEE REMARK 999	UNP G0RZB7
A	71	TRP	-	SEE REMARK 999	UNP G0RZB7
A	72	LYS	-	SEE REMARK 999	UNP G0RZB7
A	73	VAL	-	SEE REMARK 999	UNP G0RZB7
A	74	LEU	-	SEE REMARK 999	UNP G0RZB7
A	75	PRO	-	SEE REMARK 999	UNP G0RZB7
A	76	ARG	-	SEE REMARK 999	UNP G0RZB7
A	77	GLU	-	SEE REMARK 999	UNP G0RZB7
A	78	GLN	-	SEE REMARK 999	UNP G0RZB7
A	80	GLN	-	SEE REMARK 999	UNP G0RZB7
A	81	GLY	-	SEE REMARK 999	UNP G0RZB7
B	-8	GLY	-	expression tag	UNP G0RZB7
B	-7	ALA	-	expression tag	UNP G0RZB7
B	-6	ALA	-	expression tag	UNP G0RZB7
B	-5	ALA	-	expression tag	UNP G0RZB7
B	-4	SER	-	expression tag	UNP G0RZB7
B	-3	GLY	-	expression tag	UNP G0RZB7
B	-2	SER	-	expression tag	UNP G0RZB7
B	-1	GLU	-	expression tag	UNP G0RZB7
B	0	PHE	-	expression tag	UNP G0RZB7
B	22	GLN	-	SEE REMARK 999	UNP G0RZB7
B	23	GLN	-	SEE REMARK 999	UNP G0RZB7
B	24	LYS	-	SEE REMARK 999	UNP G0RZB7
B	25	ALA	-	SEE REMARK 999	UNP G0RZB7
B	26	ALA	-	SEE REMARK 999	UNP G0RZB7
B	27	GLN	-	SEE REMARK 999	UNP G0RZB7
B	28	ALA	-	SEE REMARK 999	UNP G0RZB7
B	29	ALA	-	SEE REMARK 999	UNP G0RZB7
B	30	LEU	-	SEE REMARK 999	UNP G0RZB7
B	31	ASN	-	SEE REMARK 999	UNP G0RZB7
B	57	PHE	-	SEE REMARK 999	UNP G0RZB7
B	58	LEU	-	SEE REMARK 999	UNP G0RZB7
B	59	ALA	-	SEE REMARK 999	UNP G0RZB7
B	60	LEU	-	SEE REMARK 999	UNP G0RZB7
B	61	GLN	-	SEE REMARK 999	UNP G0RZB7

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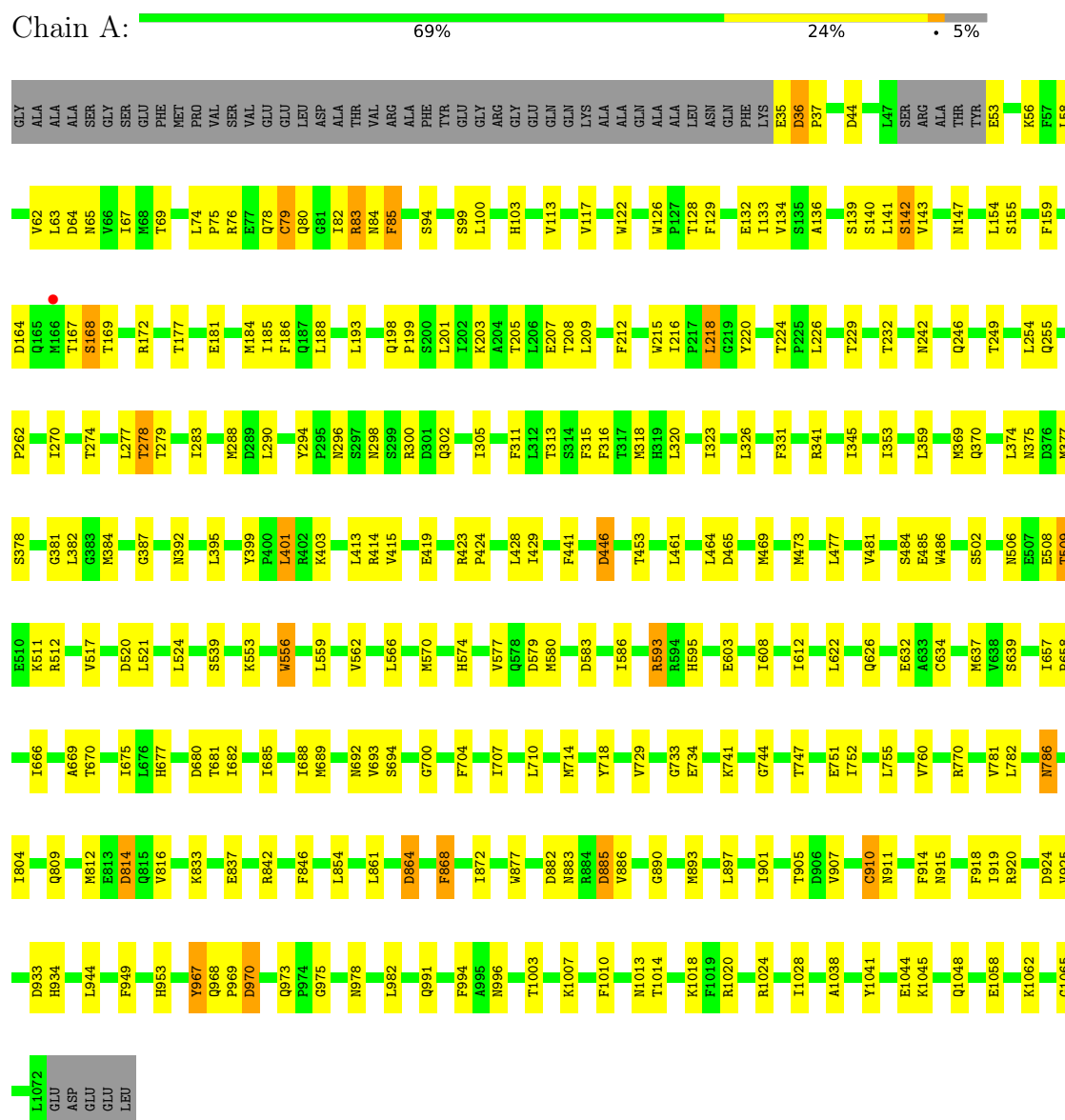
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Chain	Residue	Modelled	Actual	Comment	Reference
B	62	VAL	-	SEE REMARK 999	UNP G0RZB7
B	63	LEU	-	SEE REMARK 999	UNP G0RZB7
B	64	ASP	-	SEE REMARK 999	UNP G0RZB7
B	65	ASN	-	SEE REMARK 999	UNP G0RZB7
B	66	VAL	-	SEE REMARK 999	UNP G0RZB7
B	67	ILE	-	SEE REMARK 999	UNP G0RZB7
B	68	MET	-	SEE REMARK 999	UNP G0RZB7
B	69	THR	-	SEE REMARK 999	UNP G0RZB7
B	70	ARG	-	SEE REMARK 999	UNP G0RZB7
B	71	TRP	-	SEE REMARK 999	UNP G0RZB7
B	72	LYS	-	SEE REMARK 999	UNP G0RZB7
B	73	VAL	-	SEE REMARK 999	UNP G0RZB7
B	74	LEU	-	SEE REMARK 999	UNP G0RZB7
B	75	PRO	-	SEE REMARK 999	UNP G0RZB7
B	76	ARG	-	SEE REMARK 999	UNP G0RZB7
B	77	GLU	-	SEE REMARK 999	UNP G0RZB7
B	78	GLN	-	SEE REMARK 999	UNP G0RZB7
B	80	GLN	-	SEE REMARK 999	UNP G0RZB7
B	81	GLY	-	SEE REMARK 999	UNP G0RZB7

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: CRM1 Nuclear transport receptor



- Molecule 1: CRM1 Nuclear transport receptor

Chain B:  67% 26% 5%

GLY	ALA	ALA	ALA	SER	GLY	SER	GLU	PHE	PRO	VAL	SER	VAL	GLU	GLU	LEU	ASP	ALA	THR	VAL	ARG	ALA	PHE	TYR	GLU	GLY	ARG	GLY	GLY	GLN	GLN	LYS	ALA	ALA	GLN	ALA	ALA	LEU	ASN	GLN	F33	K34	A39	V43	ASP	GLU	ILE	LEU	SER	ARG	ALA	THR	E53	K56	F57																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	89.82Å 89.82Å 316.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.07 – 3.10 49.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.07-3.10) 97.1 (49.07-3.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.216 , 0.236 0.215 , 0.239	Depositor DCC
R_{free} test set	1997 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	105.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 85.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.094 for -h,-k,l 0.407 for h,-h-k,-l 0.097 for -k,-h,-l	Xtriage
Reported twinning fraction	0.460 for h,-h-k,-l	Depositor
Outliers	0 of 50204 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16642	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

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	0.33	0/8491	0.85	9/11493 (0.1%)
1	B	0.34	0/8482	0.87	17/11479 (0.1%)
All	All	0.33	0/16973	0.86	26/22972 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LEU	CA-C-N	6.77	126.53	119.76
1	A	74	LEU	C-N-CA	6.77	126.53	119.76
1	B	169	THR	N-CA-C	-6.59	105.36	113.41
1	A	381	GLY	N-CA-C	-6.24	106.01	115.00
1	B	198	GLN	CA-C-N	6.16	125.37	118.97
1	B	198	GLN	C-N-CA	6.16	125.37	118.97
1	B	774	ILE	N-CA-C	6.13	119.70	112.35
1	A	700	GLY	CA-C-N	6.09	126.54	119.47
1	A	700	GLY	C-N-CA	6.09	126.54	119.47
1	B	959	ALA	CA-C-N	6.07	127.43	119.84
1	B	959	ALA	C-N-CA	6.07	127.43	119.84
1	B	955	ALA	N-CA-C	-6.02	105.86	112.72
1	A	36	ASP	CA-C-N	-6.00	112.31	118.85
1	A	36	ASP	C-N-CA	-6.00	112.31	118.85
1	A	485	GLU	N-CA-C	-5.80	106.25	113.15
1	B	700	GLY	CA-C-N	5.74	126.12	119.47
1	B	700	GLY	C-N-CA	5.74	126.12	119.47
1	B	159	PHE	N-CA-C	5.26	117.01	111.28
1	B	441	PHE	N-CA-C	5.23	116.83	111.03
1	A	782	LEU	N-CA-C	5.19	116.80	111.03
1	B	74	LEU	CA-C-N	-5.12	112.94	120.46
1	B	74	LEU	C-N-CA	-5.12	112.94	120.46
1	B	739	MET	CA-C-N	5.07	124.68	119.05
1	B	739	MET	C-N-CA	5.07	124.68	119.05
1	B	485	GLU	N-CA-C	-5.02	107.18	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	956	ASP	CB-CA-C	-5.00	109.17	116.53

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	8326	0	8346	161	0
1	B	8316	0	8345	166	0
All	All	16642	0	16691	326	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 10.

All (326) 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:298:ASN:HD21	1:A:300:ARG:HE	1.24	0.85
1:B:915:ASN:ND2	1:B:967:TYR:O	2.16	0.78
1:B:462:THR:HG22	1:B:469:MET:HG2	1.66	0.77
1:B:94:SER:HB3	1:B:143:VAL:HG22	1.65	0.76
1:B:100:LEU:HD22	1:B:142:SER:HB3	1.69	0.75
1:B:288:MET:O	1:B:341:ARG:NH2	2.23	0.72
1:A:99:SER:O	1:A:103:HIS:ND1	2.22	0.72
1:A:682:ILE:HD13	1:A:744:GLY:HA3	1.71	0.72
1:B:659:ASN:OD1	1:B:706:GLN:NE2	2.23	0.71
1:B:372:LEU:O	1:B:375:ASN:ND2	2.23	0.71
1:B:837:GLU:O	1:B:842:ARG:NH1	2.25	0.69
1:A:970:ASP:OD1	1:A:970:ASP:N	2.17	0.69
1:A:167:THR:O	1:A:172:ARG:NH1	2.25	0.68
1:B:526:GLU:OE2	1:B:565:LYS:NZ	2.21	0.68
1:B:487:SER:OG	1:B:490:ASN:OD1	2.12	0.68
1:A:80:GLN:HA	1:A:83:ARG:HD3	1.74	0.68
1:B:869:LYS:HD3	1:B:917:PHE:HE2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:HA	1:A:100:LEU:HD21	1.76	0.66
1:B:970:ASP:OD2	1:B:970:ASP:N	2.28	0.66
1:B:324:GLU:OE2	1:B:406:TYR:OH	2.14	0.66
1:A:414:ARG:HH12	1:A:465:ASP:HB3	1.59	0.66
1:A:1020:ARG:NH2	1:A:1044:GLU:OE2	2.28	0.66
1:B:689:MET:HE3	1:B:752:ILE:HG12	1.76	0.66
1:B:283:ILE:HG23	1:B:284:ILE:HG13	1.78	0.66
1:B:746:ARG:NH1	1:B:794:ASP:OD1	2.25	0.66
1:A:288:MET:O	1:A:341:ARG:NH1	2.29	0.66
1:B:1045:LYS:O	1:B:1048:GLN:HG2	1.96	0.65
1:A:53:GLU:HB2	1:A:56:LYS:HE2	1.79	0.65
1:A:915:ASN:ND2	1:A:967:TYR:O	2.30	0.64
1:B:688:ILE:O	1:B:692:ASN:ND2	2.30	0.64
1:A:553:LYS:O	1:A:595:HIS:NE2	2.30	0.64
1:A:688:ILE:O	1:A:692:ASN:ND2	2.28	0.64
1:A:82:ILE:HG13	1:A:85:PHE:HE1	1.63	0.63
1:A:714:MET:HE2	1:A:752:ILE:HG23	1.80	0.63
1:B:883:ASN:HB3	1:B:886:VAL:HG22	1.81	0.63
1:B:313:THR:HG21	1:B:353:ILE:HG22	1.81	0.62
1:B:315:PHE:HE1	1:B:323:ILE:HD11	1.64	0.62
1:B:770:ARG:NH2	1:B:814:ASP:OD2	2.33	0.62
1:B:376:ASP:N	1:B:376:ASP:OD1	2.26	0.62
1:A:218:LEU:HD23	1:A:218:LEU:H	1.64	0.61
1:A:392:ASN:HB3	1:A:395:LEU:HD13	1.81	0.61
1:B:646:GLN:OE1	1:B:649:ARG:NH2	2.32	0.61
1:B:432:ASN:OD1	1:B:436:GLU:N	2.32	0.61
1:B:99:SER:O	1:B:103:HIS:ND1	2.30	0.61
1:A:428:LEU:H	1:A:580:MET:HE2	1.66	0.61
1:A:374:LEU:HD12	1:A:377:MET:HE3	1.83	0.60
1:A:579:ASP:OD1	1:A:626:GLN:NE2	2.28	0.60
1:A:814:ASP:N	1:A:814:ASP:OD1	2.32	0.60
1:B:536:VAL:O	1:B:540:ASN:ND2	2.28	0.60
1:A:885:ASP:N	1:A:885:ASP:OD1	2.34	0.60
1:B:843:VAL:O	1:B:847:ASN:ND2	2.33	0.60
1:B:553:LYS:O	1:B:595:HIS:NE2	2.32	0.60
1:A:134:VAL:HG22	1:A:188:LEU:HD11	1.83	0.59
1:A:481:VAL:HA	1:A:524:LEU:HD21	1.84	0.59
1:B:270:ILE:HD13	1:B:326:LEU:HD21	1.85	0.59
1:B:816:VAL:HA	1:B:819:ILE:HD12	1.85	0.59
1:A:399:TYR:HB3	1:A:401:LEU:HD13	1.85	0.59
1:B:834:ASP:HB3	1:B:837:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:SER:OG	1:A:169:THR:N	2.32	0.58
1:A:864:ASP:OD1	1:A:864:ASP:N	2.37	0.58
1:B:888:THR:O	1:B:892:ASN:ND2	2.32	0.57
1:B:182:PHE:CE1	1:B:215:TRP:HB3	2.40	0.57
1:B:579:ASP:OD2	1:B:626:GLN:NE2	2.30	0.57
1:A:925:VAL:HG21	1:A:944:LEU:HD22	1.85	0.57
1:B:907:VAL:O	1:B:911:ASN:ND2	2.33	0.57
1:A:126:TRP:CD1	1:A:128:THR:HG1	2.23	0.56
1:A:481:VAL:HG21	1:A:520:ASP:HB3	1.88	0.56
1:A:973:GLN:HG3	1:A:975:GLY:H	1.69	0.56
1:A:79:CYS:SG	1:A:80:GLN:N	2.79	0.56
1:B:814:ASP:OD1	1:B:814:ASP:N	2.38	0.56
1:B:33:PHE:HD1	1:B:34:LYS:HG2	1.70	0.56
1:B:901:ILE:O	1:B:905:THR:OG1	2.22	0.56
1:A:134:VAL:HG13	1:A:188:LEU:HD21	1.88	0.56
1:A:255:GLN:NE2	1:A:318:MET:SD	2.79	0.56
1:A:920:ARG:NH1	1:A:924:ASP:OD2	2.38	0.56
1:B:806:THR:O	1:B:809:GLN:NE2	2.30	0.55
1:A:277:LEU:HD23	1:A:331:PHE:HD1	1.71	0.55
1:A:991:GLN:OE1	1:B:866:ARG:NH2	2.39	0.55
1:B:1056:ASP:O	1:B:1060:ARG:HG2	2.07	0.55
1:B:56:LYS:HD2	1:B:106:LEU:HD13	1.89	0.55
1:B:714:MET:HE2	1:B:752:ILE:HG23	1.88	0.55
1:B:680:ASP:OD2	1:B:680:ASP:N	2.38	0.54
1:A:82:ILE:HA	1:A:85:PHE:HD1	1.71	0.54
1:A:35:GLU:C	1:A:37:PRO:HD3	2.32	0.54
1:A:846:PHE:CZ	1:A:890:GLY:HA2	2.43	0.54
1:B:711:TYR:OH	1:B:773:MET:O	2.25	0.54
1:B:319:HIS:HB3	1:B:322:LEU:HD13	1.90	0.54
1:B:935:LYS:O	1:B:938:PHE:HB3	2.08	0.54
1:B:230:LEU:HA	1:B:234:PHE:HD2	1.73	0.54
1:A:100:LEU:HD11	1:A:142:SER:HB3	1.90	0.53
1:A:205:THR:O	1:A:208:THR:OG1	2.26	0.53
1:B:920:ARG:NH1	1:B:924:ASP:OD1	2.41	0.53
1:B:268:GLN:OE1	1:B:268:GLN:N	2.38	0.53
1:A:270:ILE:HD13	1:A:326:LEU:HD21	1.90	0.53
1:B:230:LEU:HA	1:B:234:PHE:CD2	2.43	0.53
1:A:666:ILE:O	1:A:670:THR:OG1	2.22	0.53
1:A:910:CYS:SG	1:A:911:ASN:N	2.82	0.53
1:A:140:SER:HB3	1:A:143:VAL:HG23	1.90	0.52
1:B:895:LEU:O	1:B:899:ASN:ND2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:O	1:A:159:PHE:HB3	2.10	0.52
1:A:704:PHE:HA	1:A:707:ILE:HG22	1.92	0.52
1:A:370:GLN:O	1:A:375:ASN:ND2	2.42	0.52
1:A:933:ASP:OD1	1:A:934:HIS:N	2.37	0.52
1:A:446:ASP:N	1:A:446:ASP:OD1	2.42	0.52
1:A:677:HIS:O	1:A:677:HIS:ND1	2.43	0.52
1:A:1058:GLU:O	1:A:1062:LYS:HG3	2.10	0.52
1:B:480:GLN:HE22	1:B:490:ASN:HB2	1.74	0.52
1:A:1020:ARG:HH22	1:A:1044:GLU:HG2	1.74	0.51
1:B:740:PRO:HA	1:B:743:ARG:HE	1.75	0.51
1:B:1024:ARG:O	1:B:1028:ILE:HG13	2.11	0.51
1:A:570:MET:HG3	1:A:622:LEU:HD21	1.92	0.51
1:B:155:SER:HB2	1:B:212:PHE:CZ	2.46	0.51
1:A:136:ALA:O	1:A:139:SER:OG	2.25	0.51
1:B:181:GLU:O	1:B:185:ILE:HG13	2.11	0.51
1:A:122:TRP:CD1	1:A:126:TRP:HB3	2.45	0.51
1:B:910:CYS:SG	1:B:911:ASN:N	2.83	0.51
1:B:492:ASN:HA	1:B:540:ASN:OD1	2.12	0.50
1:A:953:HIS:O	1:A:1013:ASN:ND2	2.45	0.50
1:A:126:TRP:CD1	1:A:129:PHE:H	2.30	0.50
1:A:1045:LYS:O	1:A:1048:GLN:HG2	2.12	0.49
1:B:318:MET:HG3	1:B:319:HIS:CE1	2.47	0.49
1:B:510:GLU:OE2	1:B:550:ARG:NH2	2.33	0.49
1:A:897:LEU:O	1:A:901:ILE:HG12	2.12	0.49
1:A:718:TYR:CZ	1:A:781:VAL:HG12	2.47	0.49
1:B:831:ILE:HG23	1:B:842:ARG:HG2	1.94	0.49
1:A:1003:THR:O	1:A:1007:LYS:HG2	2.12	0.49
1:B:374:LEU:HD21	1:B:399:TYR:OH	2.12	0.49
1:B:911:ASN:HB3	1:B:966:ILE:HB	1.93	0.49
1:B:144:CYS:O	1:B:148:MET:HG2	2.13	0.49
1:A:883:ASN:HB3	1:A:886:VAL:HG22	1.94	0.49
1:B:57:PHE:HE1	1:B:106:LEU:HA	1.76	0.49
1:B:220:TYR:O	1:B:224:THR:OG1	2.19	0.49
1:A:556:TRP:O	1:A:559:LEU:HB3	2.12	0.49
1:B:659:ASN:CG	1:B:706:GLN:HE22	2.20	0.49
1:A:181:GLU:O	1:A:185:ILE:HG13	2.12	0.49
1:B:33:PHE:CD1	1:B:34:LYS:HG2	2.47	0.49
1:B:111:ASN:ND2	1:B:146:ASN:OD1	2.46	0.49
1:B:110:LEU:O	1:B:113:VAL:HG12	2.13	0.49
1:B:94:SER:O	1:B:142:SER:OG	2.19	0.48
1:B:863:LEU:HG	1:B:867:GLN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:GLU:O	1:B:761:GLU:HG3	2.13	0.48
1:A:315:PHE:HE2	1:A:323:ILE:HD11	1.78	0.48
1:A:378:SER:HA	1:A:382:LEU:O	2.14	0.48
1:A:949:PHE:CE1	1:A:982:LEU:HD21	2.49	0.48
1:B:887:GLU:OE2	1:B:937:GLY:N	2.46	0.48
1:A:1010:PHE:O	1:A:1013:ASN:ND2	2.47	0.48
1:A:414:ARG:NH1	1:A:465:ASP:HB3	2.27	0.48
1:A:63:LEU:HD11	1:A:82:ILE:HD11	1.96	0.48
1:A:129:PHE:O	1:A:133:ILE:HG12	2.13	0.48
1:B:939:LYS:NZ	1:B:1046:GLU:OE1	2.47	0.48
1:B:968:GLN:HG2	1:B:969:PRO:HD2	1.95	0.48
1:A:359:LEU:HD22	1:A:453:THR:HG23	1.96	0.47
1:B:421:MET:SD	1:B:422:VAL:N	2.85	0.47
1:B:148:MET:HE2	1:B:205:THR:HA	1.96	0.47
1:A:583:ASP:HA	1:A:586:ILE:HG22	1.97	0.47
1:A:689:MET:O	1:A:693:VAL:HG23	2.15	0.47
1:B:481:VAL:HG12	1:B:524:LEU:HD13	1.97	0.47
1:A:770:ARG:NH2	1:A:814:ASP:OD2	2.48	0.47
1:B:221:ILE:HG22	1:B:227:ILE:HD11	1.97	0.47
1:A:574:HIS:O	1:A:577:VAL:HG12	2.15	0.47
1:A:249:THR:HG23	1:A:311:PHE:HA	1.97	0.47
1:A:632:GLU:HB2	1:A:694:SER:HB3	1.97	0.46
1:B:141:LEU:HD23	1:B:201:LEU:HD13	1.96	0.46
1:B:812:MET:O	1:B:816:VAL:HG23	2.14	0.46
1:A:968:GLN:HB2	1:A:969:PRO:HD2	1.96	0.46
1:B:74:LEU:HD21	1:B:124:HIS:HE1	1.80	0.46
1:B:218:LEU:H	1:B:218:LEU:HD12	1.81	0.46
1:A:133:ILE:HG23	1:A:147:ASN:HB3	1.97	0.46
1:B:166:MET:O	1:B:167:THR:OG1	2.28	0.46
1:B:753:LEU:O	1:B:757:GLU:HG3	2.15	0.46
1:A:593:ARG:NH1	1:A:639:SER:OG	2.49	0.46
1:A:155:SER:HB2	1:A:212:PHE:CZ	2.50	0.46
1:B:154:LEU:O	1:B:158:VAL:HG12	2.15	0.46
1:B:456:GLU:HG2	1:B:1066:LEU:HD22	1.98	0.46
1:B:146:ASN:O	1:B:150:ILE:HG13	2.16	0.46
1:B:159:PHE:HB2	1:B:215:TRP:HE1	1.78	0.46
1:B:529:ARG:O	1:B:533:ASN:ND2	2.46	0.46
1:A:278:THR:H	1:A:278:THR:HG1	1.44	0.45
1:A:882:ASP:OD1	1:A:882:ASP:N	2.49	0.45
1:B:100:LEU:HD21	1:B:101:ARG:HE	1.80	0.45
1:A:242:ASN:O	1:A:246:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:PHE:HB3	1:A:996:ASN:OD1	2.16	0.45
1:B:718:TYR:CZ	1:B:781:VAL:HG12	2.51	0.45
1:A:729:VAL:O	1:A:733:GLY:N	2.49	0.45
1:B:590:LYS:HE2	1:B:636:TYR:CZ	2.51	0.45
1:B:459:VAL:O	1:B:462:THR:OG1	2.28	0.45
1:B:951:PHE:HD1	1:B:963:GLN:HG3	1.80	0.45
1:A:67:ILE:HG21	1:A:117:VAL:HG22	1.99	0.45
1:A:83:ARG:HG2	1:A:84:ASN:N	2.31	0.45
1:B:121:GLU:O	1:B:124:HIS:HB3	2.16	0.45
1:B:682:ILE:HD13	1:B:744:GLY:HA3	1.98	0.45
1:A:274:THR:O	1:A:278:THR:OG1	2.35	0.45
1:A:477:LEU:HD22	1:A:517:VAL:HG22	1.99	0.45
1:B:1013:ASN:OD1	1:B:1013:ASN:N	2.50	0.45
1:A:714:MET:HE1	1:A:755:LEU:HD23	1.99	0.45
1:B:857:PHE:N	1:B:858:PRO:HD2	2.32	0.45
1:A:429:ILE:HD11	1:A:539:SER:HB3	1.99	0.45
1:A:786:ASN:C	1:A:786:ASN:HD22	2.25	0.45
1:B:677:HIS:O	1:B:677:HIS:ND1	2.49	0.45
1:B:994:PHE:CZ	1:B:1030:LEU:HD13	2.52	0.45
1:A:53:GLU:O	1:A:56:LYS:HG2	2.17	0.45
1:A:634:CYS:HA	1:A:637:MET:HE2	1.99	0.45
1:B:979:ARG:HG3	1:B:1010:PHE:CE1	2.51	0.45
1:B:369:MET:HE3	1:B:396:LEU:HD13	1.98	0.44
1:B:479:ARG:HA	1:B:479:ARG:HD3	1.65	0.44
1:B:514:LEU:HD21	1:B:548:TYR:CD1	2.52	0.44
1:A:423:ARG:HA	1:A:424:PRO:HD3	1.79	0.44
1:A:44:ASP:OD2	1:A:44:ASP:N	2.50	0.44
1:A:1024:ARG:O	1:A:1028:ILE:HG13	2.17	0.44
1:B:224:THR:C	1:B:226:LEU:H	2.25	0.44
1:A:469:MET:HG3	1:A:473:MET:HE2	1.98	0.44
1:B:323:ILE:HG22	1:B:332:LEU:HB2	1.98	0.44
1:B:1018:LYS:O	1:B:1022:VAL:HG12	2.18	0.44
1:A:313:THR:HG21	1:A:353:ILE:HG22	2.00	0.44
1:B:1059:ARG:NH2	1:B:1060:ARG:HE	2.16	0.44
1:A:669:ALA:HB2	1:A:675:ILE:HD11	2.00	0.44
1:A:1018:LYS:H	1:A:1018:LYS:HG2	1.61	0.44
1:A:65:ASN:O	1:A:69:THR:OG1	2.23	0.44
1:A:316:PHE:O	1:A:320:LEU:HB2	2.18	0.44
1:A:415:VAL:O	1:A:419:GLU:HG3	2.18	0.44
1:A:608:ILE:O	1:A:612:ILE:HG12	2.18	0.44
1:B:71:TRP:CE2	1:B:120:GLN:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ILE:HA	1:B:283:ILE:HG22	2.00	0.44
1:B:392:ASN:HB3	1:B:395:LEU:HG	1.99	0.44
1:B:662:TRP:O	1:B:666:ILE:HG12	2.17	0.44
1:A:128:THR:O	1:A:132:GLU:HG3	2.17	0.44
1:B:56:LYS:HB2	1:B:56:LYS:HE3	1.77	0.44
1:A:58:LEU:O	1:A:62:VAL:HG23	2.18	0.43
1:B:284:ILE:HA	1:B:285:PRO:HD3	1.86	0.43
1:B:876:MET:HE2	1:B:924:ASP:HB3	2.00	0.43
1:A:122:TRP:HD1	1:A:126:TRP:HB3	1.84	0.43
1:A:203:LYS:O	1:A:207:GLU:HG2	2.18	0.43
1:B:151:LEU:O	1:B:154:LEU:HG	2.18	0.43
1:A:186:PHE:CE2	1:A:224:THR:HG21	2.52	0.43
1:A:403:LYS:HD2	1:A:464:LEU:HB3	1.98	0.43
1:A:868:PHE:O	1:A:872:ILE:HG12	2.19	0.43
1:B:509:THR:HG23	1:B:512:ARG:HH21	1.82	0.43
1:A:747:THR:O	1:A:751:GLU:HG2	2.18	0.43
1:A:812:MET:O	1:A:816:VAL:HG23	2.17	0.43
1:B:469:MET:HG3	1:B:473:MET:HE2	2.01	0.43
1:B:746:ARG:HD2	1:B:794:ASP:OD1	2.17	0.43
1:A:274:THR:HG23	1:A:331:PHE:CE1	2.53	0.43
1:B:1030:LEU:HD12	1:B:1033:PHE:CD1	2.53	0.43
1:B:729:VAL:O	1:B:733:GLY:N	2.49	0.43
1:A:212:PHE:O	1:A:216:ILE:HG13	2.18	0.43
1:A:681:THR:O	1:A:685:ILE:HG13	2.19	0.43
1:A:842:ARG:HD3	1:A:877:TRP:CZ3	2.54	0.43
1:B:704:PHE:CG	1:B:705:PRO:HD3	2.54	0.43
1:A:134:VAL:HG21	1:A:184:MET:SD	2.58	0.43
1:A:159:PHE:HD1	1:A:215:TRP:HZ2	1.66	0.43
1:B:824:PHE:HZ	1:B:870:PHE:HB2	1.83	0.43
1:B:959:ALA:O	1:B:961:LYS:N	2.52	0.43
1:A:760:VAL:HG11	1:A:804:ILE:HG22	2.00	0.43
1:B:511:LYS:O	1:B:515:VAL:HG23	2.19	0.43
1:B:867:GLN:O	1:B:871:VAL:HG23	2.19	0.43
1:B:415:VAL:O	1:B:419:GLU:HG3	2.19	0.43
1:A:75:PRO:HG2	1:A:78:GLN:HB3	2.00	0.42
1:A:914:PHE:HB3	1:A:918:PHE:HB2	2.01	0.42
1:B:423:ARG:HA	1:B:424:PRO:HD3	1.87	0.42
1:B:838:TYR:O	1:B:842:ARG:HG3	2.19	0.42
1:A:296:ASN:OD1	1:A:296:ASN:N	2.52	0.42
1:A:484:SER:C	1:A:486:TRP:H	2.26	0.42
1:B:506:ASN:ND2	1:B:508:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:SER:O	1:A:1065:GLY:HA2	2.19	0.42
1:B:112:LEU:O	1:B:115:VAL:HG12	2.19	0.42
1:B:155:SER:HB2	1:B:212:PHE:CE2	2.55	0.42
1:B:198:GLN:HA	1:B:199:PRO:HD3	1.84	0.42
1:A:996:ASN:OD1	1:A:996:ASN:N	2.48	0.42
1:B:953:HIS:O	1:B:1013:ASN:ND2	2.52	0.42
1:A:520:ASP:O	1:A:524:LEU:HG	2.20	0.42
1:B:1003:THR:O	1:B:1007:LYS:HG2	2.20	0.42
1:A:294:TYR:CE1	1:A:302:GLN:HG2	2.54	0.42
1:A:315:PHE:CE2	1:A:323:ILE:HD11	2.55	0.42
1:A:414:ARG:HH22	1:A:465:ASP:HB3	1.83	0.42
1:B:455:ARG:NH1	1:B:1068:LYS:HG2	2.34	0.42
1:B:666:ILE:O	1:B:670:THR:OG1	2.22	0.42
1:A:198:GLN:HA	1:A:199:PRO:HD3	1.93	0.42
1:A:413:LEU:HD23	1:A:461:LEU:HD21	2.00	0.42
1:A:521:LEU:HD23	1:A:524:LEU:HD12	2.01	0.42
1:B:811:LEU:HD23	1:B:811:LEU:HA	1.86	0.42
1:B:1057:LEU:O	1:B:1061:SER:N	2.49	0.42
1:A:198:GLN:HB3	1:A:201:LEU:HG	2.02	0.41
1:A:556:TRP:CZ2	1:A:603:GLU:HG2	2.55	0.41
1:A:1038:ALA:HB1	1:A:1041:TYR:CD2	2.55	0.41
1:B:39:ALA:HB1	1:B:63:LEU:HD12	2.02	0.41
1:B:109:LYS:O	1:B:112:LEU:HG	2.20	0.41
1:B:940:THR:O	1:B:944:LEU:N	2.45	0.41
1:A:562:VAL:O	1:A:566:LEU:HG	2.20	0.41
1:A:506:ASN:OD1	1:A:509:THR:OG1	2.34	0.41
1:B:518:ILE:O	1:B:522:LEU:HG	2.20	0.41
1:B:984:ASN:O	1:B:988:THR:HG23	2.20	0.41
1:A:279:THR:O	1:A:283:ILE:HG13	2.21	0.41
1:A:657:ILE:HB	1:A:658:PRO:HD3	2.02	0.41
1:B:580:MET:HE2	1:B:580:MET:HB3	1.93	0.41
1:A:226:LEU:O	1:A:229:THR:OG1	2.28	0.41
1:A:294:TYR:HD1	1:A:305:ILE:HD12	1.86	0.41
1:A:477:LEU:HD21	1:A:517:VAL:HA	2.03	0.41
1:A:833:LYS:HE3	1:A:833:LYS:HB3	1.93	0.41
1:A:369:MET:HE2	1:A:384:MET:HE1	2.02	0.41
1:A:374:LEU:HA	1:A:377:MET:HE2	2.03	0.41
1:A:508:GLU:O	1:A:511:LYS:HB3	2.21	0.41
1:B:80:GLN:HA	1:B:83:ARG:HD3	2.02	0.41
1:B:723:GLN:O	1:B:727:GLU:HG3	2.20	0.41
1:A:64:ASP:HB2	1:A:113:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LEU:O	1:B:462:THR:HG23	2.20	0.41
1:A:270:ILE:HG23	1:A:326:LEU:HD11	2.03	0.40
1:A:316:PHE:HE1	1:A:323:ILE:HD12	1.85	0.40
1:A:509:THR:HG22	1:A:512:ARG:NH2	2.36	0.40
1:B:148:MET:HE2	1:B:205:THR:HG23	2.02	0.40
1:B:607:PHE:O	1:B:611:ILE:HG13	2.21	0.40
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.92	0.40
1:A:837:GLU:O	1:A:842:ARG:NH2	2.54	0.40
1:B:103:HIS:O	1:B:107:LEU:HG	2.21	0.40
1:B:846:PHE:CE1	1:B:890:GLY:HA2	2.55	0.40
1:B:927:PHE:HD1	1:B:927:PHE:HA	1.77	0.40
1:B:1058:GLU:O	1:B:1062:LYS:HG2	2.21	0.40
1:A:710:LEU:O	1:A:714:MET:HG3	2.21	0.40
1:B:414:ARG:O	1:B:418:ILE:HG13	2.22	0.40
1:B:417:MET:HE2	1:B:457:CYS:SG	2.62	0.40
1:B:678:GLU:HA	1:B:679:PRO:HD3	1.91	0.40
1:B:77:GLU:H	1:B:77:GLU:HG3	1.66	0.40
1:B:747:THR:O	1:B:751:GLU:HG2	2.21	0.40
1:B:1015:GLN:HG3	1:B:1018:LYS:HD2	2.03	0.40
1:A:290:LEU:HD23	1:A:345:ILE:HD11	2.03	0.40
1:B:604:ASN:OD1	1:B:605:GLU:N	2.55	0.40
1:B:999:PRO:O	1:B:1003:THR:OG1	2.37	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	1029/1086 (95%)	996 (97%)	30 (3%)	3 (0%)	36 67
1	B	1027/1086 (95%)	991 (96%)	29 (3%)	7 (1%)	18 49
All	All	2056/2172 (95%)	1987 (97%)	59 (3%)	10 (0%)	24 57

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	PRO
1	B	960	PRO
1	A	168	SER
1	A	387	GLY
1	B	376	ASP
1	B	435	GLY
1	B	260	GLY
1	B	124	HIS
1	B	125	ASN
1	B	262	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	930/971 (96%)	888 (96%)	42 (4%)	24	56
1	B	929/971 (96%)	880 (95%)	49 (5%)	20	51
All	All	1859/1942 (96%)	1768 (95%)	91 (5%)	22	53

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	76	ARG
1	A	79	CYS
1	A	83	ARG
1	A	85	PHE
1	A	141	LEU
1	A	142	SER
1	A	154	LEU
1	A	164	ASP
1	A	177	THR
1	A	193	LEU
1	A	209	LEU
1	A	218	LEU

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Mol	Chain	Res	Type
1	A	220	TYR
1	A	232	THR
1	A	278	THR
1	A	401	LEU
1	A	441	PHE
1	A	446	ASP
1	A	509	THR
1	A	556	TRP
1	A	593	ARG
1	A	680	ASP
1	A	734	GLU
1	A	741	LYS
1	A	786	ASN
1	A	809	GLN
1	A	814	ASP
1	A	854	LEU
1	A	861	LEU
1	A	864	ASP
1	A	868	PHE
1	A	885	ASP
1	A	893	MET
1	A	905	THR
1	A	907	VAL
1	A	910	CYS
1	A	919	ILE
1	A	967	TYR
1	A	970	ASP
1	A	978	ASN
1	A	1014	THR
1	B	77	GLU
1	B	97	GLU
1	B	100	LEU
1	B	105	THR
1	B	118	LEU
1	B	119	LYS
1	B	122	TRP
1	B	125	ASN
1	B	158	VAL
1	B	169	THR
1	B	197	THR
1	B	201	LEU
1	B	210	LEU

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Mol	Chain	Res	Type
1	B	220	TYR
1	B	226	LEU
1	B	241	ARG
1	B	245	LEU
1	B	296	ASN
1	B	338	TYR
1	B	374	LEU
1	B	376	ASP
1	B	377	MET
1	B	421	MET
1	B	442	VAL
1	B	558	PHE
1	B	574	HIS
1	B	680	ASP
1	B	707	ILE
1	B	772	GLN
1	B	809	GLN
1	B	825	GLU
1	B	910	CYS
1	B	919	ILE
1	B	922	LEU
1	B	926	PHE
1	B	927	PHE
1	B	935	LYS
1	B	938	PHE
1	B	944	LEU
1	B	962	ILE
1	B	970	ASP
1	B	982	LEU
1	B	991	GLN
1	B	994	PHE
1	B	1003	THR
1	B	1013	ASN
1	B	1015	GLN
1	B	1023	LEU
1	B	1063	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	298	ASN

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Mol	Chain	Res	Type
1	A	307	ASN
1	A	328	ASN
1	A	334	HIS
1	A	375	ASN
1	A	449	GLN
1	A	647	GLN
1	A	934	HIS
1	A	992	ASN
1	A	1042	GLN
1	B	65	ASN
1	B	88	GLN
1	B	111	ASN
1	B	124	HIS
1	B	287	GLN
1	B	319	HIS
1	B	328	ASN
1	B	449	GLN
1	B	463	HIS
1	B	480	GLN
1	B	659	ASN
1	B	706	GLN
1	B	788	ASN
1	B	815	GLN
1	B	973	GLN
1	B	984	ASN
1	B	996	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	1033/1086 (95%)	-1.13	1 (0%) 92 86	71, 100, 175, 211	0
1	B	1031/1086 (94%)	-1.11	2 (0%) 91 83	74, 105, 175, 204	0
All	All	2064/2172 (95%)	-1.12	3 (0%) 92 86	71, 102, 175, 211	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	3.7
1	A	166	MET	2.4
1	B	960	PRO	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.