



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 PM UTC

PDB ID : 4A2W / pdb_00004a2w
Title : Structure of full-length duck RIG-I
Authors : Kowalinski, E.; Lunardi, T.; McCarthy, A.A.; Cusack, S.
Deposited on : 2011-09-29
Resolution : 3.70 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

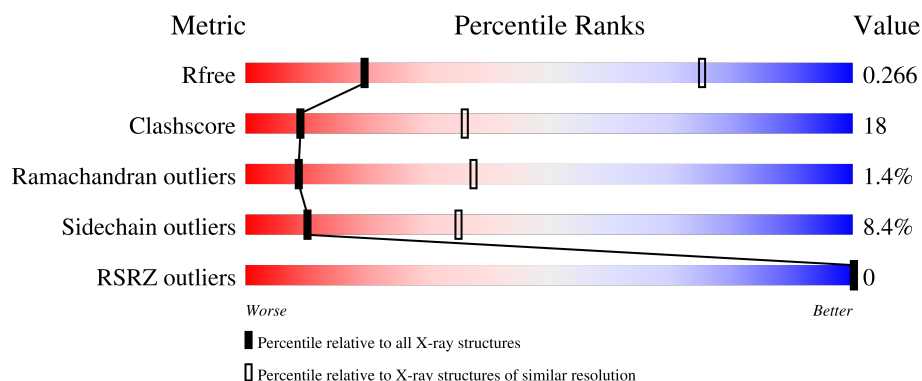
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

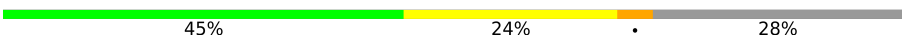
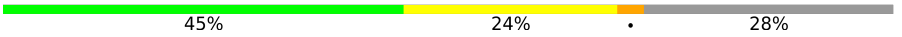
The reported resolution of this entry is 3.70 Å.

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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	936	 45% 24% • 28%
1	B	936	 45% 24% • 28%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10880 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 RETINOIC ACID INDUCIBLE PROTEIN I.

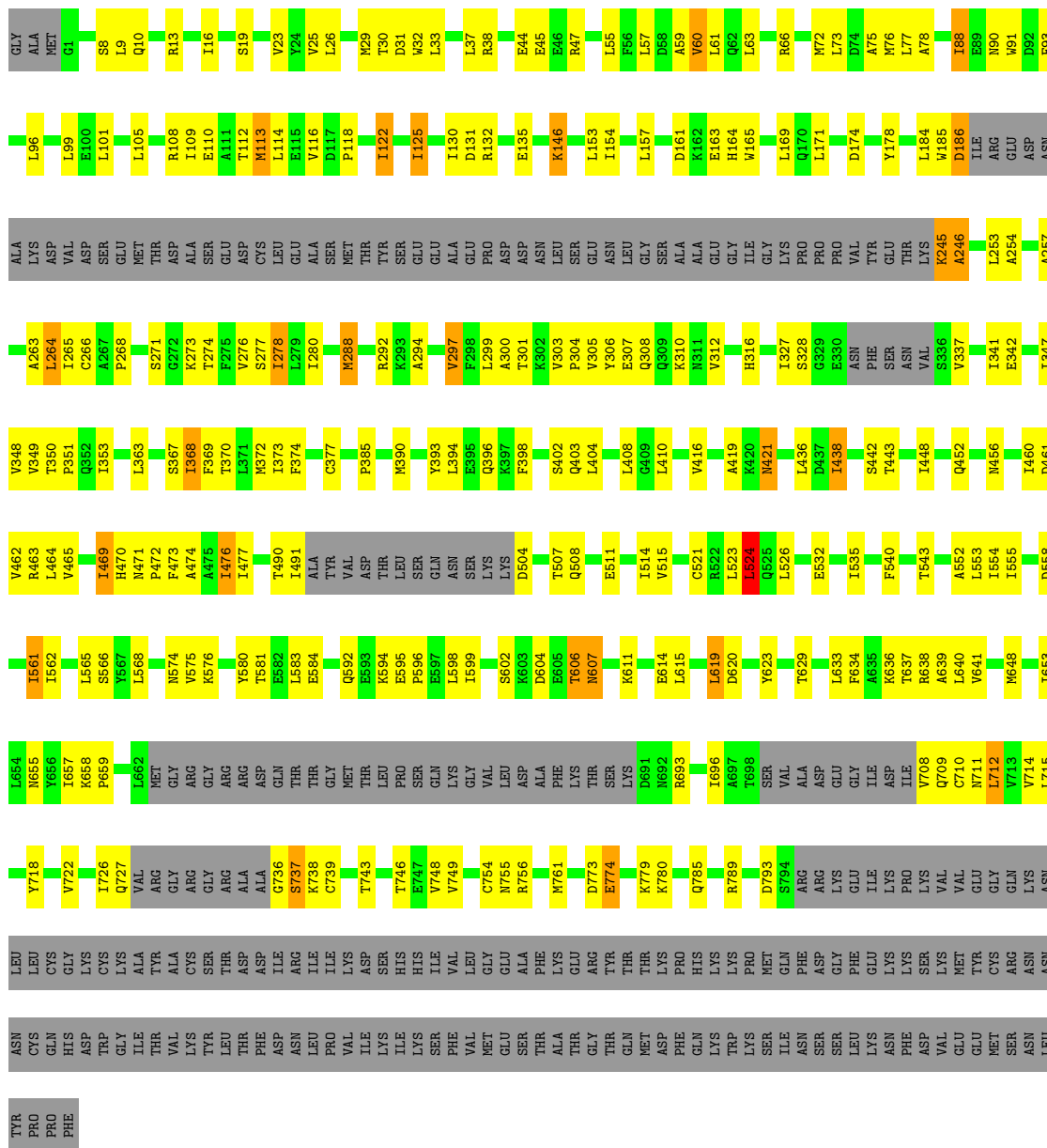
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	678	Total	C	N	O	S	0	0	0
			5454	3446	940	1035	33			
1	B	674	Total	C	N	O	S	0	0	0
			5426	3427	936	1030	33			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D3TI84
A	-1	ALA	-	expression tag	UNP D3TI84
A	0	MET	-	expression tag	UNP D3TI84
A	1	GLY	-	expression tag	UNP D3TI84
B	-2	GLY	-	expression tag	UNP D3TI84
B	-1	ALA	-	expression tag	UNP D3TI84
B	0	MET	-	expression tag	UNP D3TI84
B	1	GLY	-	expression tag	UNP D3TI84

- Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I

Chain B: 45% 24% . 28%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.32Å 163.32Å 152.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.77 – 3.70 42.77 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.77-3.70) 99.8 (42.77-3.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.218 , 0.274 (Not available) , 0.266	Depositor DCC
R_{free} test set	1160 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	135.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 135.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10880	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.45% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/5539	0.85	2/7473 (0.0%)
1	B	0.64	0/5511	0.82	3/7434 (0.0%)
All	All	0.66	0/11050	0.84	5/14907 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ILE	CB-CA-C	-6.72	107.31	113.70
1	A	368	ILE	CB-CA-C	-6.37	103.55	112.14
1	A	739	CYS	N-CA-C	6.32	118.75	108.26
1	B	739	CYS	N-CA-C	5.79	118.09	108.13
1	B	368	ILE	CB-CA-C	-5.50	104.92	111.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	699	SER	Peptide

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	5454	0	5500	207	1
1	B	5426	0	5466	196	1
All	All	10880	0	10966	401	1

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 18.

All (401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:LEU:HD23	1:B:526:LEU:HD12	1.25	1.14
1:A:524:LEU:HD23	1:A:526:LEU:HD12	1.27	1.14
1:B:524:LEU:CD2	1:B:526:LEU:HD12	1.87	1.04
1:A:524:LEU:CD2	1:A:526:LEU:HD12	1.87	1.04
1:A:743:THR:HG21	1:A:748:VAL:HG11	1.45	0.99
1:B:328:SER:HA	1:B:353:ILE:HD11	1.51	0.92
1:A:555:ILE:HD11	1:A:639:ALA:HB1	1.52	0.92
1:A:60:VAL:HG11	1:A:72:MET:HE1	1.52	0.91
1:B:37:LEU:HD21	1:B:59:ALA:CB	2.02	0.89
1:A:328:SER:HA	1:A:353:ILE:HD11	1.55	0.89
1:A:465:VAL:HG21	1:A:742:VAL:HG13	1.56	0.88
1:B:37:LEU:HD21	1:B:59:ALA:HB1	1.56	0.88
1:A:37:LEU:HD21	1:A:59:ALA:HB1	1.57	0.86
1:A:465:VAL:HG21	1:A:742:VAL:CG1	2.06	0.86
1:A:37:LEU:HD21	1:A:59:ALA:CB	2.05	0.86
1:B:465:VAL:HG11	1:B:611:LYS:HA	1.58	0.85
1:B:328:SER:HA	1:B:353:ILE:CD1	2.07	0.85
1:B:60:VAL:HG11	1:B:72:MET:HE1	1.57	0.83
1:B:32:TRP:HB3	1:B:63:LEU:HD21	1.61	0.83
1:B:464:LEU:HB2	1:B:749:VAL:HG21	1.58	0.83
1:A:328:SER:HA	1:A:353:ILE:CD1	2.08	0.82
1:B:465:VAL:HG13	1:B:614:GLU:HG3	1.61	0.82
1:B:743:THR:HG21	1:B:748:VAL:CG1	2.10	0.81
1:A:125:ILE:HD11	1:A:157:LEU:CD1	2.10	0.81
1:A:125:ILE:HD11	1:A:157:LEU:HD13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:GLU:OE2	1:A:744:SER:OG	1.98	0.81
1:B:524:LEU:HD23	1:B:526:LEU:CD1	2.09	0.80
1:A:524:LEU:HD23	1:A:526:LEU:CD1	2.09	0.80
1:A:32:TRP:HB3	1:A:63:LEU:HD21	1.63	0.80
1:B:615:LEU:HD22	1:B:648:MET:HE1	1.65	0.79
1:B:33:LEU:HD22	1:B:37:LEU:HD23	1.64	0.78
1:A:464:LEU:HD13	1:A:749:VAL:HG21	1.66	0.77
1:A:33:LEU:HD22	1:A:37:LEU:HD23	1.67	0.76
1:B:416:VAL:HG13	1:B:419:ALA:HB3	1.68	0.76
1:B:88:ILE:HG22	1:B:93:PHE:CZ	2.23	0.74
1:B:274:THR:O	1:B:278:ILE:HG23	1.88	0.74
1:A:604:ASP:HB3	1:A:606:THR:HB	1.71	0.72
1:A:274:THR:O	1:A:278:ILE:HG23	1.91	0.71
1:A:363:LEU:HD11	1:A:368:ILE:HD11	1.73	0.71
1:B:743:THR:HG21	1:B:748:VAL:HG13	1.72	0.71
1:A:615:LEU:HD12	1:A:716:TYR:CD1	2.25	0.71
1:A:416:VAL:HG13	1:A:419:ALA:HB3	1.73	0.70
1:A:349:VAL:HG12	1:A:350:THR:O	1.93	0.69
1:A:552:ALA:HB2	1:A:568:LEU:HD21	1.74	0.69
1:A:711:ASN:C	1:A:711:ASN:HD22	1.99	0.69
1:B:726:ILE:HG22	1:B:727:GLN:N	2.07	0.68
1:A:16:ILE:HD11	1:A:88:ILE:HG21	1.74	0.68
1:B:363:LEU:HD11	1:B:368:ILE:HD11	1.75	0.68
1:B:349:VAL:HG12	1:B:350:THR:O	1.93	0.68
1:B:374:PHE:CE2	1:B:390:MET:HE3	2.29	0.68
1:B:615:LEU:HD23	1:B:619:LEU:HD22	1.76	0.67
1:A:615:LEU:HD22	1:A:648:MET:HE1	1.76	0.67
1:B:16:ILE:HD11	1:B:88:ILE:HG21	1.76	0.67
1:A:75:ALA:O	1:A:78:ALA:HB3	1.93	0.67
1:A:60:VAL:HG11	1:A:72:MET:CE	2.26	0.66
1:B:615:LEU:CD2	1:B:619:LEU:HD22	2.25	0.66
1:B:327:ILE:HG22	1:B:349:VAL:HG22	1.78	0.66
1:A:288:MET:HG3	1:A:294:ALA:HB2	1.79	0.65
1:B:109:ILE:HG22	1:B:109:ILE:O	1.96	0.65
1:A:558:ASP:HB2	1:A:640:LEU:HD11	1.78	0.65
1:A:327:ILE:HG22	1:A:349:VAL:HG22	1.78	0.65
1:A:299:LEU:HD12	1:A:374:PHE:CE1	2.32	0.64
1:B:88:ILE:HG22	1:B:93:PHE:HZ	1.63	0.64
1:B:288:MET:HG3	1:B:294:ALA:HB2	1.78	0.64
1:A:465:VAL:CG2	1:A:742:VAL:HG13	2.28	0.64
1:A:468:ARG:NH1	1:A:556:SER:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HD13	1:A:316:HIS:CD2	2.34	0.63
1:A:374:PHE:CE2	1:A:390:MET:HE3	2.33	0.63
1:A:615:LEU:HD23	1:A:619:LEU:HD22	1.80	0.63
1:B:328:SER:CA	1:B:353:ILE:HD11	2.25	0.63
1:A:308:GLN:O	1:A:312:VAL:HG23	1.98	0.63
1:A:615:LEU:CD2	1:A:619:LEU:HD22	2.27	0.63
1:B:558:ASP:HB2	1:B:640:LEU:HD11	1.79	0.63
1:B:299:LEU:HD12	1:B:374:PHE:CE1	2.33	0.63
1:B:254:ALA:HB2	1:B:276:VAL:HG13	1.80	0.63
1:A:473:PHE:CE2	1:A:598:LEU:HD22	2.33	0.62
1:A:254:ALA:HB2	1:A:276:VAL:HG13	1.82	0.62
1:B:37:LEU:CD2	1:B:59:ALA:HB1	2.30	0.62
1:B:265:ILE:HD13	1:B:442:SER:HB3	1.82	0.61
1:B:308:GLN:O	1:B:312:VAL:HG23	1.99	0.61
1:B:44:GLU:OE1	1:B:47:ARG:NH1	2.33	0.61
1:B:125:ILE:HD11	1:B:157:LEU:CD2	2.31	0.61
1:B:125:ILE:HD11	1:B:157:LEU:HD13	1.82	0.61
1:B:125:ILE:HD11	1:B:157:LEU:HD22	1.82	0.61
1:B:278:ILE:HD13	1:B:316:HIS:CD2	2.36	0.61
1:A:37:LEU:CD2	1:A:59:ALA:HB1	2.31	0.60
1:B:37:LEU:HD21	1:B:59:ALA:HB3	1.82	0.60
1:B:60:VAL:HG11	1:B:72:MET:CE	2.30	0.60
1:A:328:SER:CA	1:A:353:ILE:HD11	2.30	0.60
1:A:363:LEU:HD11	1:A:368:ILE:CD1	2.32	0.60
1:B:508:GLN:NE2	1:B:636:LYS:O	2.35	0.60
1:B:363:LEU:HD11	1:B:368:ILE:CD1	2.32	0.59
1:B:110:GLU:CD	1:B:154:ILE:HD11	2.27	0.59
1:B:125:ILE:HD11	1:B:157:LEU:CD1	2.33	0.59
1:A:265:ILE:HD13	1:A:442:SER:HB3	1.85	0.59
1:B:25:VAL:HG23	1:B:75:ALA:C	2.27	0.59
1:B:109:ILE:HG22	1:B:112:THR:HB	1.85	0.59
1:A:109:ILE:HG22	1:A:112:THR:HB	1.85	0.59
1:A:462:VAL:CG2	1:A:741:LEU:HD23	2.33	0.59
1:A:710:CYS:SG	1:A:711:ASN:N	2.75	0.59
1:B:268:PRO:O	1:B:271:SER:OG	2.21	0.59
1:A:125:ILE:HD11	1:A:157:LEU:CD2	2.33	0.58
1:A:37:LEU:HD21	1:A:59:ALA:HB3	1.84	0.58
1:B:351:PRO:HB2	1:B:385:PRO:HB2	1.84	0.58
1:B:25:VAL:HG23	1:B:75:ALA:O	2.03	0.58
1:A:351:PRO:HB2	1:A:385:PRO:HB2	1.84	0.58
1:A:707:ILE:O	1:A:707:ILE:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:HD11	1:A:708:VAL:HG21	1.85	0.58
1:B:25:VAL:CG2	1:B:75:ALA:HB1	2.33	0.58
1:A:257:ALA:HB3	1:A:280:ILE:HD12	1.84	0.58
1:A:631:THR:OG1	1:A:712:LEU:HD23	2.03	0.58
1:A:562:ILE:HD11	1:A:607:ASN:HD21	1.68	0.58
1:B:55:LEU:HD12	1:B:55:LEU:O	2.04	0.58
1:B:73:LEU:HG	1:B:88:ILE:HD11	1.86	0.58
1:B:169:LEU:HD23	1:B:185:TRP:CE2	2.39	0.57
1:A:25:VAL:HG23	1:A:75:ALA:C	2.30	0.57
1:A:44:GLU:OE1	1:A:47:ARG:NH1	2.38	0.57
1:A:524:LEU:HD21	1:A:526:LEU:HD12	1.80	0.57
1:B:277:SER:HB2	1:B:373:ILE:HD13	1.86	0.57
1:B:552:ALA:HB2	1:B:568:LEU:HD21	1.87	0.57
1:A:25:VAL:CG2	1:A:75:ALA:HB1	2.35	0.56
1:A:109:ILE:HG22	1:A:109:ILE:O	2.05	0.56
1:B:465:VAL:CG1	1:B:611:LYS:HA	2.33	0.56
1:B:565:LEU:C	1:B:565:LEU:HD23	2.30	0.56
1:A:55:LEU:HD12	1:A:55:LEU:O	2.05	0.56
1:A:615:LEU:HD12	1:A:716:TYR:CE1	2.42	0.55
1:B:561:ILE:HB	1:B:607:ASN:HB2	1.89	0.55
1:A:277:SER:HB2	1:A:373:ILE:HD13	1.89	0.55
1:B:263:ALA:HB3	1:B:408:LEU:HD12	1.89	0.55
1:A:268:PRO:O	1:A:271:SER:OG	2.23	0.55
1:A:23:VAL:HG12	1:A:23:VAL:O	2.07	0.54
1:B:398:PHE:HB2	1:B:789:ARG:NH2	2.22	0.54
1:B:641:VAL:HG13	1:B:696:ILE:HG22	1.88	0.54
1:A:565:LEU:C	1:A:565:LEU:HD23	2.32	0.54
1:B:108:ARG:NH2	1:B:532:GLU:OE2	2.40	0.54
1:B:554:ILE:HD13	1:B:637:THR:HG21	1.89	0.54
1:B:472:PRO:O	1:B:476:ILE:HD12	2.08	0.54
1:A:743:THR:HG21	1:A:748:VAL:CG1	2.29	0.53
1:B:524:LEU:HD21	1:B:526:LEU:HD12	1.82	0.53
1:A:641:VAL:HG13	1:A:696:ILE:HG22	1.91	0.53
1:B:125:ILE:CD1	1:B:157:LEU:HD22	2.38	0.53
1:A:462:VAL:HG22	1:A:741:LEU:HB3	1.91	0.53
1:B:30:THR:HG23	1:B:31:ASP:OD1	2.09	0.53
1:A:73:LEU:HG	1:A:88:ILE:HD11	1.91	0.52
1:B:576:LYS:HA	1:B:580:TYR:CD1	2.44	0.52
1:A:108:ARG:NH2	1:A:532:GLU:OE2	2.43	0.52
1:B:10:GLN:OE1	1:B:61:LEU:HD12	2.10	0.52
1:A:185:TRP:O	1:A:186:ASP:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:PHE:HB2	1:A:715:LEU:HD23	1.91	0.52
1:B:347:ILE:HG22	1:B:349:VAL:CG2	2.40	0.52
1:A:23:VAL:HA	1:A:26:LEU:HD12	1.91	0.52
1:A:277:SER:HB3	1:A:410:LEU:HD11	1.90	0.52
1:A:465:VAL:CG1	1:A:611:LYS:HA	2.40	0.52
1:B:25:VAL:HG22	1:B:75:ALA:HB1	1.92	0.52
1:A:711:ASN:C	1:A:711:ASN:ND2	2.67	0.51
1:A:471:ASN:O	1:A:474:ALA:HB3	2.10	0.51
1:A:723:THR:O	1:A:727:GLN:NE2	2.42	0.51
1:B:288:MET:HE2	1:B:294:ALA:HB2	1.92	0.51
1:B:448:ILE:HG22	1:B:452:GLN:OE1	2.10	0.51
1:A:288:MET:HE1	1:A:292:ARG:HG2	1.93	0.51
1:A:576:LYS:HA	1:A:580:TYR:CD1	2.45	0.51
1:B:113:MET:O	1:B:114:LEU:C	2.52	0.51
1:A:25:VAL:HG22	1:A:25:VAL:O	2.11	0.51
1:A:125:ILE:HD11	1:A:157:LEU:HD22	1.93	0.51
1:B:300:ALA:HB1	1:B:305:VAL:HG12	1.93	0.51
1:A:184:LEU:HD12	1:A:522:ARG:HD3	1.92	0.50
1:B:23:VAL:HG12	1:B:23:VAL:O	2.12	0.50
1:A:257:ALA:HB3	1:A:280:ILE:CD1	2.40	0.50
1:A:561:ILE:HB	1:A:607:ASN:HB2	1.94	0.50
1:A:125:ILE:CD1	1:A:157:LEU:HD22	2.41	0.50
1:B:288:MET:HE1	1:B:292:ARG:HG2	1.92	0.50
1:A:125:ILE:CD1	1:A:157:LEU:HD13	2.38	0.50
1:A:466:LYS:NZ	1:A:614:GLU:OE2	2.34	0.50
1:A:641:VAL:HG13	1:A:696:ILE:CG2	2.41	0.50
1:B:288:MET:HE2	1:B:294:ALA:CA	2.41	0.50
1:B:416:VAL:HG11	1:B:761:MET:HE3	1.93	0.50
1:A:25:VAL:HG23	1:A:75:ALA:O	2.11	0.50
1:B:185:TRP:O	1:B:186:ASP:C	2.54	0.50
1:B:257:ALA:HB3	1:B:280:ILE:HD12	1.93	0.50
1:A:110:GLU:HG3	1:A:154:ILE:HD11	1.93	0.50
1:A:169:LEU:HD23	1:A:185:TRP:CE2	2.47	0.50
1:B:110:GLU:OE2	1:B:154:ILE:HD11	2.12	0.50
1:A:130:ILE:HG22	1:A:131:ASP:N	2.27	0.49
1:A:726:ILE:HD11	1:A:739:CYS:SG	2.52	0.49
1:A:592:GLN:HA	1:A:595:GLU:HB2	1.94	0.49
1:B:72:MET:HG2	1:B:76:MET:HE3	1.94	0.49
1:B:641:VAL:HG13	1:B:696:ILE:CG2	2.42	0.49
1:B:592:GLN:HA	1:B:595:GLU:HB2	1.95	0.49
1:A:25:VAL:HG22	1:A:75:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:CD	1:A:154:ILE:HD11	2.37	0.49
1:B:473:PHE:CE2	1:B:598:LEU:HD22	2.47	0.49
1:B:110:GLU:HG3	1:B:154:ILE:HD11	1.93	0.49
1:A:300:ALA:HB1	1:A:305:VAL:HG12	1.94	0.49
1:A:105:LEU:O	1:A:108:ARG:HB3	2.13	0.48
1:A:722:VAL:O	1:A:723:THR:C	2.56	0.48
1:B:130:ILE:HG22	1:B:131:ASP:N	2.28	0.48
1:A:490:THR:HG22	1:A:491:ILE:HD12	1.94	0.48
1:B:23:VAL:HA	1:B:26:LEU:HD12	1.95	0.48
1:B:25:VAL:HG22	1:B:25:VAL:O	2.13	0.48
1:A:153:LEU:HD23	1:A:153:LEU:C	2.39	0.48
1:A:347:ILE:HG22	1:A:349:VAL:CG2	2.43	0.48
1:A:363:LEU:CD1	1:A:368:ILE:HD11	2.43	0.48
1:B:416:VAL:HG11	1:B:761:MET:CE	2.44	0.48
1:A:26:LEU:HD22	1:A:38:ARG:HG2	1.96	0.48
1:A:398:PHE:HB2	1:A:789:ARG:NH2	2.28	0.48
1:B:153:LEU:C	1:B:153:LEU:HD23	2.39	0.48
1:A:581:THR:OG1	1:A:584:GLU:HG3	2.13	0.48
1:B:75:ALA:O	1:B:78:ALA:HB3	2.13	0.48
1:A:19:SER:OG	1:A:161:ASP:HB3	2.14	0.47
1:B:416:VAL:CG1	1:B:419:ALA:HB3	2.41	0.47
1:A:30:THR:HG23	1:A:31:ASP:OD1	2.14	0.47
1:B:634:PHE:HB2	1:B:715:LEU:HD23	1.96	0.47
1:A:565:LEU:HD12	1:A:598:LEU:HB3	1.94	0.47
1:B:594:LYS:C	1:B:596:PRO:HD2	2.40	0.47
1:A:288:MET:HE2	1:A:294:ALA:HB2	1.96	0.47
1:A:700:VAL:HG11	1:A:728:VAL:HG12	1.95	0.47
1:B:105:LEU:O	1:B:108:ARG:HB3	2.14	0.47
1:A:113:MET:O	1:A:114:LEU:C	2.58	0.47
1:A:288:MET:HE2	1:A:294:ALA:CA	2.44	0.47
1:A:396:GLN:HB3	1:A:404:LEU:HD21	1.97	0.47
1:A:473:PHE:CD2	1:A:598:LEU:CD2	2.97	0.47
1:B:710:CYS:SG	1:B:711:ASN:N	2.82	0.47
1:A:416:VAL:CG1	1:A:419:ALA:HB3	2.45	0.47
1:A:461:ASP:O	1:A:740:ILE:HA	2.14	0.47
1:A:606:THR:O	1:A:606:THR:CG2	2.63	0.47
1:A:615:LEU:HD23	1:A:615:LEU:C	2.40	0.47
1:B:633:LEU:HD12	1:B:714:VAL:CG1	2.45	0.47
1:A:369:PHE:O	1:A:405:PRO:HB3	2.16	0.46
1:A:560:ARG:NH1	1:A:647:CYS:HA	2.29	0.46
1:B:555:ILE:HD11	1:B:639:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ASN:O	1:A:577:ASN:N	2.48	0.46
1:B:297:VAL:HG22	1:B:369:PHE:CD1	2.50	0.46
1:A:416:VAL:HG11	1:A:761:MET:HE3	1.96	0.46
1:A:462:VAL:HG22	1:A:741:LEU:HD23	1.98	0.46
1:A:615:LEU:HD23	1:A:615:LEU:O	2.15	0.46
1:B:110:GLU:CG	1:B:154:ILE:HD11	2.45	0.46
1:B:460:ILE:HD13	1:B:722:VAL:HG11	1.97	0.46
1:B:490:THR:HG22	1:B:491:ILE:HD12	1.98	0.46
1:A:477:ILE:CD1	1:A:598:LEU:HD21	2.46	0.46
1:B:25:VAL:CG2	1:B:75:ALA:CB	2.94	0.46
1:B:736:GLY:O	1:B:737:SER:CB	2.63	0.46
1:A:574:ASN:O	1:A:575:VAL:C	2.59	0.46
1:B:254:ALA:HB1	1:B:280:ILE:CD1	2.46	0.46
1:B:464:LEU:HD23	1:B:464:LEU:O	2.15	0.46
1:A:773:ASP:O	1:A:774:GLU:C	2.59	0.46
1:B:514:ILE:HG23	1:B:543:THR:HB	1.98	0.46
1:B:562:ILE:HD12	1:B:607:ASN:OD1	2.16	0.46
1:A:363:LEU:HD21	1:A:368:ILE:CD1	2.46	0.46
1:B:310:LYS:HA	1:B:348:VAL:HG21	1.98	0.46
1:B:464:LEU:CD1	1:B:746:THR:HG23	2.46	0.46
1:A:288:MET:CE	1:A:370:THR:HG21	2.46	0.45
1:A:394:LEU:HD21	1:A:785:GLN:NE2	2.31	0.45
1:B:13:ARG:HE	1:B:57:LEU:HD23	1.81	0.45
1:B:438:ILE:N	1:B:438:ILE:CD1	2.79	0.45
1:B:363:LEU:CD1	1:B:368:ILE:HD11	2.45	0.45
1:B:474:ALA:HA	1:B:553:LEU:HD23	1.99	0.45
1:A:114:LEU:HD21	1:A:575:VAL:HA	1.99	0.45
1:B:633:LEU:HD12	1:B:714:VAL:HG12	1.98	0.45
1:A:263:ALA:HB3	1:A:408:LEU:HD12	1.98	0.45
1:B:337:VAL:HG12	1:B:341:ILE:CD1	2.47	0.45
1:B:708:VAL:HG13	1:B:709:GLN:O	2.16	0.45
1:A:297:VAL:HG22	1:A:369:PHE:CD1	2.52	0.45
1:A:297:VAL:HG21	1:A:369:PHE:CD2	2.52	0.45
1:A:306:TYR:CZ	1:A:328:SER:HB2	2.52	0.45
1:A:10:GLN:OE1	1:A:61:LEU:HD12	2.16	0.45
1:A:580:TYR:CE2	1:B:599:ILE:HD12	2.52	0.45
1:B:658:LYS:HA	1:B:659:PRO:HD3	1.84	0.45
1:A:101:LEU:O	1:A:101:LEU:HD12	2.17	0.45
1:B:746:THR:O	1:B:746:THR:HG22	2.17	0.45
1:B:254:ALA:HB1	1:B:280:ILE:HD11	1.98	0.44
1:A:552:ALA:HB2	1:A:568:LEU:CD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:CYS:HB3	1:B:443:THR:HG22	1.99	0.44
1:A:473:PHE:CD2	1:A:598:LEU:HD22	2.52	0.44
1:B:26:LEU:HD22	1:B:38:ARG:HG2	1.99	0.44
1:A:29:MET:HE1	1:A:72:MET:HA	2.00	0.44
1:A:33:LEU:HD22	1:A:37:LEU:CD2	2.44	0.44
1:B:416:VAL:CG1	1:B:416:VAL:O	2.65	0.44
1:B:461:ASP:OD2	1:B:463:ARG:NE	2.50	0.44
1:A:25:VAL:CG2	1:A:75:ALA:CB	2.95	0.44
1:A:337:VAL:HG12	1:A:341:ILE:CD1	2.48	0.44
1:A:552:ALA:CB	1:A:568:LEU:HD21	2.46	0.44
1:A:468:ARG:NH2	1:A:607:ASN:O	2.51	0.44
1:A:604:ASP:HB3	1:A:606:THR:H	1.83	0.44
1:B:116:VAL:HG13	1:B:178:TYR:CE2	2.52	0.44
1:B:623:TYR:CE2	1:B:657:ILE:CD1	3.00	0.44
1:A:583:LEU:HD11	1:A:587:LEU:HD11	1.99	0.44
1:B:101:LEU:HD12	1:B:101:LEU:O	2.18	0.44
1:A:594:LYS:C	1:A:596:PRO:HD2	2.42	0.44
1:B:402:SER:OG	1:B:403:GLN:N	2.48	0.44
1:B:604:ASP:CG	1:B:606:THR:HB	2.42	0.44
1:A:327:ILE:CG2	1:A:349:VAL:HG13	2.48	0.44
1:B:132:ARG:HA	1:B:135:GLU:HG2	2.00	0.44
1:B:264:LEU:CD1	1:B:377:CYS:SG	3.06	0.44
1:B:372:MET:HE2	1:B:374:PHE:CZ	2.53	0.44
1:A:514:ILE:HG23	1:A:543:THR:HB	2.00	0.43
1:B:726:ILE:O	1:B:727:GLN:C	2.61	0.43
1:A:13:ARG:HE	1:A:57:LEU:HD23	1.83	0.43
1:B:169:LEU:HD23	1:B:185:TRP:CZ2	2.53	0.43
1:B:245:LYS:HD3	1:B:246:ALA:H	1.83	0.43
1:A:438:ILE:N	1:A:438:ILE:CD1	2.81	0.43
1:B:90:ASN:O	1:B:91:TRP:C	2.59	0.43
1:A:528:ASP:HB3	1:A:531:GLU:HB3	2.00	0.43
1:B:297:VAL:CG2	1:B:369:PHE:CG	3.02	0.43
1:B:583:LEU:O	1:B:584:GLU:C	2.61	0.43
1:A:9:LEU:HD23	1:A:61:LEU:HD21	2.00	0.43
1:A:117:ASP:C	1:A:117:ASP:OD1	2.61	0.43
1:A:462:VAL:O	1:A:462:VAL:HG12	2.18	0.43
1:B:773:ASP:O	1:B:774:GLU:C	2.61	0.43
1:A:118:PRO:HD2	1:A:146:LYS:HG3	2.00	0.43
1:A:464:LEU:HA	1:A:464:LEU:HD12	1.76	0.43
1:A:726:ILE:CD1	1:A:739:CYS:SG	3.07	0.43
1:B:9:LEU:HD23	1:B:61:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:SER:HB3	1:B:410:LEU:HD11	2.00	0.43
1:A:72:MET:HG2	1:A:76:MET:HE3	2.01	0.43
1:A:736:GLY:O	1:A:737:SER:CB	2.67	0.43
1:B:297:VAL:HG21	1:B:369:PHE:CD2	2.54	0.43
1:A:699:SER:OG	1:A:725:MET:HE3	2.19	0.43
1:B:33:LEU:HD22	1:B:37:LEU:CD2	2.41	0.43
1:B:184:LEU:HD21	1:B:540:PHE:HE1	1.83	0.43
1:B:394:LEU:HD21	1:B:785:GLN:NE2	2.33	0.43
1:A:173:LEU:HB3	1:A:182:SER:HB2	2.01	0.42
1:A:390:MET:HE1	1:A:407:ILE:CD1	2.49	0.42
1:A:132:ARG:HA	1:A:135:GLU:HG2	2.01	0.42
1:A:249:TYR:CE1	1:A:451:LEU:HD13	2.54	0.42
1:A:396:GLN:CB	1:A:404:LEU:HD21	2.50	0.42
1:B:257:ALA:HB3	1:B:280:ILE:CD1	2.49	0.42
1:B:288:MET:HE2	1:B:294:ALA:HA	2.00	0.42
1:B:264:LEU:HD13	1:B:377:CYS:SG	2.59	0.42
1:A:245:LYS:CD	1:A:246:ALA:H	2.32	0.42
1:A:245:LYS:HD3	1:A:246:ALA:H	1.84	0.42
1:B:473:PHE:CD1	1:B:473:PHE:C	2.98	0.42
1:A:297:VAL:CG2	1:A:369:PHE:CG	3.03	0.42
1:B:755:ASN:O	1:B:756:ARG:C	2.62	0.42
1:A:606:THR:O	1:A:606:THR:HG23	2.19	0.42
1:A:727:GLN:O	1:A:728:VAL:HB	2.20	0.42
1:B:574:ASN:O	1:B:575:VAL:C	2.62	0.42
1:B:712:LEU:HD23	1:B:714:VAL:HG23	2.00	0.42
1:A:29:MET:HE1	1:A:75:ALA:HB3	2.02	0.42
1:A:623:TYR:CE2	1:A:657:ILE:CD1	3.03	0.42
1:A:110:GLU:CG	1:A:154:ILE:HD11	2.50	0.42
1:A:462:VAL:CG2	1:A:741:LEU:HB3	2.50	0.42
1:B:25:VAL:HG23	1:B:75:ALA:HB1	2.01	0.42
1:B:511:GLU:O	1:B:515:VAL:HG23	2.20	0.42
1:A:372:MET:HE2	1:A:374:PHE:CZ	2.55	0.42
1:A:431:SER:O	1:A:434:SER:OG	2.31	0.42
1:B:327:ILE:CG2	1:B:349:VAL:HG13	2.50	0.42
1:A:487:LEU:O	1:A:490:THR:HB	2.20	0.41
1:B:73:LEU:CD2	1:B:88:ILE:HD11	2.50	0.41
1:B:504:ASP:O	1:B:504:ASP:CG	2.63	0.41
1:A:536:CYS:O	1:A:537:ARG:C	2.62	0.41
1:B:245:LYS:CD	1:B:246:ALA:H	2.34	0.41
1:B:620:ASP:HB2	1:B:653:ILE:HG22	2.03	0.41
1:B:390:MET:HG3	1:B:436:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLN:HB3	1:B:404:LEU:HD21	2.01	0.41
1:A:456:ASN:OD1	1:A:456:ASN:N	2.48	0.41
1:B:116:VAL:HG13	1:B:178:TYR:CZ	2.56	0.41
1:B:118:PRO:HD2	1:B:146:LYS:HG3	2.02	0.41
1:B:565:LEU:O	1:B:566:SER:C	2.64	0.41
1:A:288:MET:HE2	1:A:294:ALA:HA	2.01	0.41
1:B:363:LEU:HD21	1:B:368:ILE:CD1	2.51	0.41
1:A:465:VAL:HG13	1:A:614:GLU:HG3	2.02	0.41
1:B:288:MET:CE	1:B:370:THR:HG21	2.51	0.41
1:B:328:SER:C	1:B:353:ILE:HD11	2.45	0.41
1:B:726:ILE:CG2	1:B:727:GLN:N	2.77	0.41
1:A:416:VAL:HG11	1:A:761:MET:CE	2.51	0.41
1:A:745:LYS:O	1:A:748:VAL:HG12	2.21	0.41
1:B:471:ASN:O	1:B:474:ALA:HB3	2.20	0.41
1:A:110:GLU:OE2	1:A:154:ILE:HD11	2.21	0.41
1:A:381:THR:CG2	1:A:382:GLY:N	2.84	0.41
1:A:620:ASP:HB2	1:A:653:ILE:HG22	2.03	0.41
1:B:9:LEU:HB3	1:B:61:LEU:HD21	2.03	0.41
1:B:96:LEU:HD21	1:B:161:ASP:HB2	2.02	0.41
1:B:306:TYR:CZ	1:B:328:SER:HB2	2.56	0.41
1:B:393:TYR:CZ	1:B:404:LEU:HD13	2.55	0.41
1:B:436:LEU:CB	1:B:438:ILE:HD13	2.51	0.41
1:B:469:ILE:HB	1:B:470:HIS:CD2	2.56	0.41
1:A:310:LYS:HA	1:A:348:VAL:HG21	2.03	0.41
1:A:523:LEU:O	1:A:524:LEU:C	2.63	0.41
1:A:755:ASN:O	1:A:756:ARG:C	2.64	0.41
1:B:288:MET:HE2	1:B:294:ALA:CB	2.51	0.41
1:B:303:VAL:N	1:B:304:PRO:HD2	2.36	0.41
1:B:474:ALA:HA	1:B:553:LEU:CD2	2.50	0.41
1:A:25:VAL:HG23	1:A:75:ALA:HB1	2.03	0.40
1:B:110:GLU:HG3	1:B:154:ILE:CD1	2.50	0.40
1:A:328:SER:CA	1:A:353:ILE:CD1	2.90	0.40
1:A:511:GLU:O	1:A:515:VAL:HG23	2.22	0.40
1:B:558:ASP:CB	1:B:640:LEU:HD11	2.48	0.40
1:A:402:SER:OG	1:A:403:GLN:N	2.53	0.40
1:A:473:PHE:CD1	1:A:473:PHE:C	2.99	0.40
1:A:576:LYS:HZ1	1:B:595:GLU:CD	2.29	0.40
1:B:73:LEU:CG	1:B:88:ILE:HD11	2.51	0.40
1:B:108:ARG:NH1	1:B:521:CYS:O	2.52	0.40
1:B:421:ASN:ND2	1:B:421:ASN:N	2.69	0.40
1:B:436:LEU:HB3	1:B:438:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:ARG:O	1:B:639:ALA:C	2.65	0.40
1:B:29:MET:HE1	1:B:72:MET:HA	2.04	0.40
1:B:99:LEU:HD22	1:B:165:TRP:NE1	2.37	0.40
1:A:32:TRP:CH2	1:A:71:GLY:HA3	2.56	0.40
1:A:122:ILE:N	1:A:123:PRO:HD2	2.37	0.40
1:A:477:ILE:HG21	1:A:553:LEU:HG	2.03	0.40
1:B:565:LEU:HD12	1:B:598:LEU:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LYS:O	1:B:779:LYS:NZ[1_565]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	664/936 (71%)	594 (90%)	61 (9%)	9 (1%)	9	37
1	B	660/936 (70%)	595 (90%)	56 (8%)	9 (1%)	9	37
All	All	1324/1872 (71%)	1189 (90%)	117 (9%)	18 (1%)	9	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	LEU
1	A	737	SER
1	B	524	LEU
1	B	737	SER
1	A	66	ARG
1	B	66	ARG

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Mol	Chain	Res	Type
1	B	774	GLU
1	A	19	SER
1	A	738	LYS
1	A	774	GLU
1	B	19	SER
1	B	246	ALA
1	B	738	LYS
1	A	523	LEU
1	A	699	SER
1	B	163	GLU
1	B	523	LEU
1	A	575	VAL

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	606/831 (73%)	552 (91%)	54 (9%)	9	33
1	B	602/831 (72%)	554 (92%)	48 (8%)	11	37
All	All	1208/1662 (73%)	1106 (92%)	102 (8%)	10	35

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	60	VAL
1	A	64	GLU
1	A	77	LEU
1	A	88	ILE
1	A	113	MET
1	A	122	ILE
1	A	125	ILE
1	A	146	LYS
1	A	164	HIS
1	A	171	LEU

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Mol	Chain	Res	Type
1	A	174	ASP
1	A	186	ASP
1	A	245	LYS
1	A	253	LEU
1	A	264	LEU
1	A	273	LYS
1	A	278	ILE
1	A	288	MET
1	A	297	VAL
1	A	301	THR
1	A	307	GLU
1	A	342	GLU
1	A	367	SER
1	A	421	ASN
1	A	438	ILE
1	A	453	ARG
1	A	456	ASN
1	A	462	VAL
1	A	466	LYS
1	A	469	ILE
1	A	476	ILE
1	A	477	ILE
1	A	507	THR
1	A	524	LEU
1	A	535	ILE
1	A	561	ILE
1	A	581	THR
1	A	602	SER
1	A	606	THR
1	A	607	ASN
1	A	619	LEU
1	A	629	THR
1	A	655	ASN
1	A	693	ARG
1	A	711	ASN
1	A	712	LEU
1	A	713	VAL
1	A	721	ASN
1	A	726	ILE
1	A	743	THR
1	A	744	SER
1	A	754	CYS

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Mol	Chain	Res	Type
1	A	780	LYS
1	B	8	SER
1	B	45	GLU
1	B	60	VAL
1	B	77	LEU
1	B	88	ILE
1	B	113	MET
1	B	122	ILE
1	B	125	ILE
1	B	146	LYS
1	B	164	HIS
1	B	171	LEU
1	B	174	ASP
1	B	186	ASP
1	B	245	LYS
1	B	253	LEU
1	B	264	LEU
1	B	273	LYS
1	B	278	ILE
1	B	288	MET
1	B	297	VAL
1	B	301	THR
1	B	307	GLU
1	B	342	GLU
1	B	367	SER
1	B	421	ASN
1	B	438	ILE
1	B	456	ASN
1	B	462	VAL
1	B	469	ILE
1	B	476	ILE
1	B	477	ILE
1	B	507	THR
1	B	524	LEU
1	B	535	ILE
1	B	561	ILE
1	B	581	THR
1	B	602	SER
1	B	606	THR
1	B	607	ASN
1	B	619	LEU
1	B	629	THR

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Mol	Chain	Res	Type
1	B	655	ASN
1	B	693	ARG
1	B	712	LEU
1	B	718	TYR
1	B	754	CYS
1	B	780	LYS
1	B	793	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	A	399	ASN
1	A	470	HIS
1	A	518	GLN
1	A	586	HIS
1	A	592	GLN
1	B	316	HIS
1	B	320	GLN
1	B	379	ASN
1	B	399	ASN
1	B	586	HIS
1	B	592	GLN
1	B	711	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	678/936 (72%)	-0.72	0 100 100	85, 157, 218, 263	0
1	B	674/936 (72%)	-0.64	0 100 100	95, 185, 265, 315	0
All	All	1352/1872 (72%)	-0.68	0 100 100	85, 169, 253, 315	0

There are no RSRZ outliers to report.

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.