Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:39 PM GMT

PDB ID	:	4A2W
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

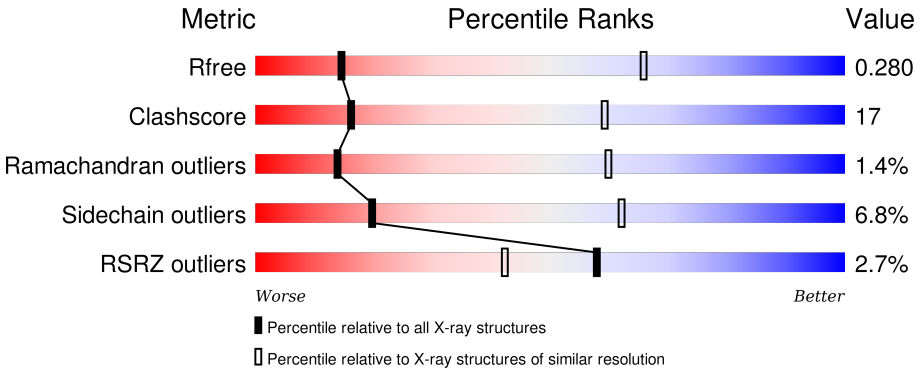
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 47% 23% · 28%
1	B	936	3% 47% 23% · 28%

2 Entry composition (i)

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:

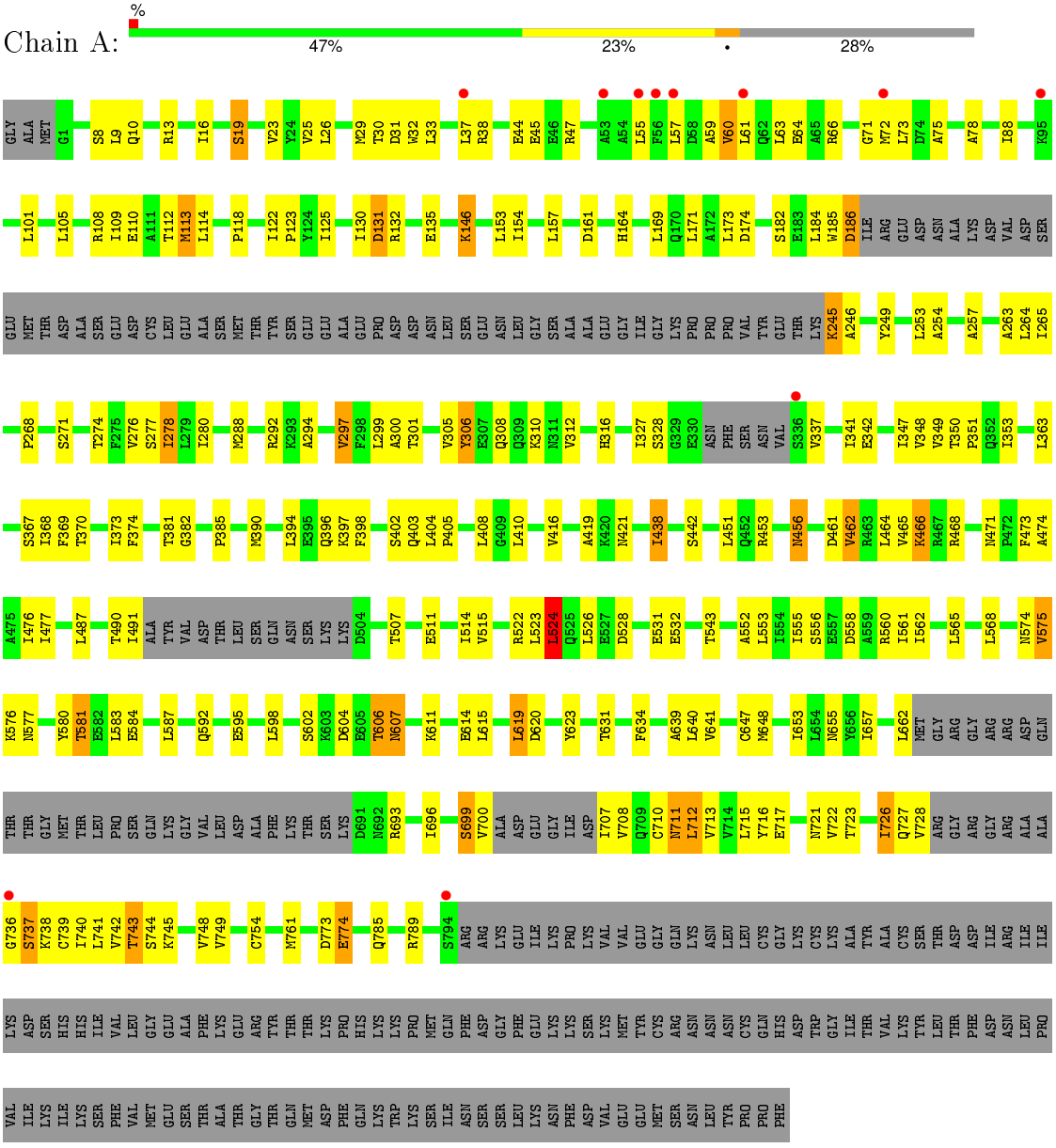
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP D3TI84
A	-1	ALA	-	EXPRESSION TAG	UNP D3TI84
A	0	MET	-	EXPRESSION TAG	UNP D3TI84
A	1	GLY	-	EXPRESSION TAG	UNP D3TI84
B	-2	GLY	-	EXPRESSION TAG	UNP D3TI84
B	-1	ALA	-	EXPRESSION TAG	UNP D3TI84
B	0	MET	-	EXPRESSION TAG	UNP D3TI84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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: RETINOIC ACID INDUCIBLE PROTEIN I

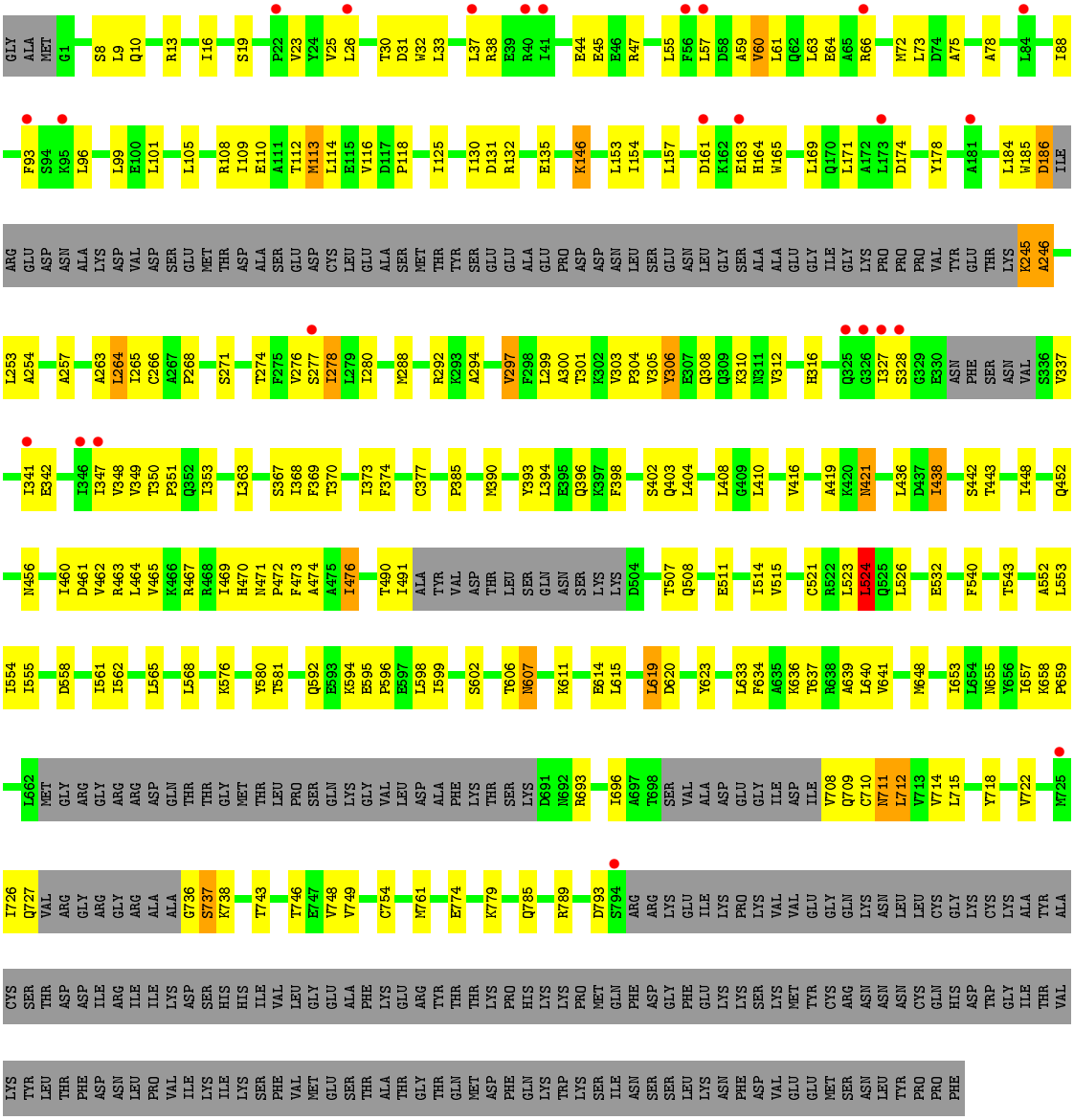
Chain A:



- Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I

Chain B:


3%
47%
23%
28%


GLY ALA MET G1 S8 L9 Q10 R13 I16 S19 P22 V23 Y24 V25 L26 T30 D31 W32 L33 L37 R38 E39 R40 I41 E44 E45 E46 R47 L55 F56 L57 D58 A59 V60 L61 Q62 L63 E64 A65 R66 M72 L73 D74 A75 A78 L84 I88
F93 S94 K95 L96 L99 E100 L101 L105 R108 I109 E110 A111 T112 M113 L114 E115 V116 D117 P118 I125 L130 D131 R132 E135 K146 L153 I154 L157 D161 K162 E163 H164 W165 L169 Q170 L171 A172 L173 D174 Y178 A181 L184 W185 D186 ILE
ARG GLU ASP ASN ALA LYS ASP VAL ASP SER GLU MET THR ASP ALA SER GLU ASP CYS LEU GLU ALA SER MET THR TYR SER GLU GLU ALA GLU PRO ASP ASP ASN LEU SER GLU ASN LEU GLY SER ALA ALA GLU GLY ILE GLY LYS PRO PRO PRO VAL TYR GLU THR LYS K245 A246
L253 A254 A257 A263 I264 I265 C266 A267 P268 S271 T274 F275 V276 S277 I278 L279 I280 M288 R292 K293 A294 V297 P298 L299 A300 T301 K302 V303 P304 V305 Y306 E307 Q308 Q309 K310 N311 V312 H316 Q325 G326 I327 S328 G329 E330 ASN PHE SER ASN VAL S336 V337
I341 E342 I346 I347 V348 V349 T350 P351 Q352 I353 L363 S367 I368 F369 T370 I373 F374 C377 P385 M390 Y393 L394 E395 Q396 K397 F398 S402 Q403 L404 L408 G409 L410 V416 A419 K420 N421 L436 D437 I438 S442 T443 I448 Q452
N456 I460 D461 V462 R463 L464 V465 K466 R467 R468 I469 H470 N471 P472 F473 A474 A475 I476 T490 I491 ALA TYR VAL ASP THR LEU SER GLN ASN SER LYS LYS D504 T507 Q508 E511 I514 V515 C521 R522 L523 L524 Q525 L526 E532 F540 T543 A552 L553
I554 I555 D558 I561 I562 L565 L568 K576 Y580 T581 Q592 E593 K594 E595 P596 E597 L598 I599 S602 T606 N607 K611 E614 L615 L619 D620 Y623 L633 F634 A635 K636 T637 R638 A639 L640 V641 M648 I653 L654 N655 Y656 I657 K658 P659
L662 MET GLY ARG GLY ARG ARG ASP GLN THR THR GLY MET THR LEU PRO SER GLN LYS GLY VAL LEU ASP ALA PHE LYS THR SER LYS D691 N692 R693 I696 A697 T698 SER VAL ALA ASP GLU GLY ILE ASP ILE V708 Q709 C710 N711 L712 V713 V714 L715 Y718 V722 M725
I726 Q727 VAL ARG GLY ARG GLY ARG ALA ALA G736 S737 K738 T743 T746 E747 V748 V749 C754 M761 E774 K779 Q785 R789 D793 S794 ARG ARG LYS GLU ILE LYS PRO LYS VAL VAL GLU GLY GLN LYS ASN LEU LEU CYS GLY LYS CYS LYS ALA TYR ALA
CYS SER THR ASP ASP ILE ARG ILE ILE LYS ASP SER HIS HIS ILE VAL LEU GLY GLU ALA PHE LYS GLU ARG TYR THR THR THR LYS PRO HIS LYS LYS PRO MET GLN PHE ASP GLY PHE GLU LYS LYS SER LYS MET TYR CYS ARG ASN ASN ASN CYS GLN HIS ASP TRP GLY ILE THR VAL
LYS TYR LEU THR PHE ASP ASN LEU PRO VAL ILE ILE LYS ILE LYS SER PHE VAL VAL MET GLU GLU SER THR ALA THR GLY THR GLN MET ASP PHE GLN LYS TRP LYS SER ILE ASN SER SER LEU LYS ASN PHE ASP VAL GLU GLU MET SER ASN LEU TYR PRO PRO PHE

4 Data and refinement statistics (i)

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) 99.9 (42.77-3.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.218 , 0.274 0.222 , 0.280	Depositor DCC
R_{free} test set	1160 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	135.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 117.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 22592 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/5539	0.62	0/7473
1	B	0.46	0/5511	0.58	0/7434
All	All	0.47	0/11050	0.60	0/14907

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.

There are no bond angle outliers.

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	192	1
1	B	5426	0	5466	176	1
All	All	10880	0	10966	367	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 17.

All (367) 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: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: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
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: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:274:THR:O	1:B:278:ILE:HG23	1.88	0.74
1:B:88:ILE:HG22	1:B:93:PHE:CZ	2.23	0.74
1:A:604:ASP:HB3	1:A:606:THR:HB	1.71	0.72
1:B:615:LEU:HD22	1:B:648:MET:HE1	1.69	0.71
1:A:274:THR:O	1:A:278:ILE:HG23	1.91	0.71
1:B:743:THR:HG21	1:B:748:VAL:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD11	1:A:368:ILE:HD11	1.73	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:B:726:ILE:HG22	1:B:727:GLN:N	2.07	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:288:MET:HE2	1:A:370:THR:HG21	1.73	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:615:LEU:HD23	1:B:619:LEU:HD22	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:B:615:LEU:CD2	1:B:619:LEU:HD22	2.25	0.66
1:A:60:VAL:HG11	1:A:72:MET:CE	2.26	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:O	1:B:109:ILE:HG22	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:B:88:ILE:HG22	1:B:93:PHE:HZ	1.63	0.64
1:A:299:LEU:HD12	1:A:374:PHE:CE1	2.32	0.64
1:B:288:MET:HG3	1:B:294:ALA:HB2	1.78	0.64
1:B:288:MET:HE2	1:B:370:THR:HG21	1.78	0.64
1:A:711:ASN:C	1:A:711:ASN:HD22	1.99	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
1:A:278:ILE:HD13	1:A:316:HIS:CD2	2.34	0.63
1:B:328:SER:CA	1:B:353:ILE:HD11	2.25	0.63
1:A:615:LEU:HD23	1:A:619:LEU:HD22	1.80	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:A:308:GLN:O	1:A:312:VAL:HG23	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:60:VAL:HG11	1:A:72:MET:HE1	1.83	0.60
1:B:508:GLN:NE2	1:B:636:LYS:O	2.35	0.60
1:A:710:CYS:SG	1:A:711:ASN:N	2.75	0.59
1:B:363:LEU:HD11	1:B:368:ILE:CD1	2.32	0.59
1:B:125:ILE:HD11	1:B:157:LEU:CD1	2.33	0.59
1:B:109:ILE:HG22	1:B:112:THR:HB	1.85	0.59
1:A:265:ILE:HD13	1:A:442:SER:HB3	1.85	0.59
1:A:615:LEU:HD22	1:A:648:MET:HE1	1.84	0.59
1:A:462:VAL:CG2	1:A:741:LEU:HD23	2.33	0.59
1:A:109:ILE:HG22	1:A:112:THR:HB	1.85	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:HG22	1:A:707:ILE:O	2.02	0.58
1:B:25:VAL:CG2	1:B:75:ALA:HB1	2.33	0.58
1:A:662:LEU:HD11	1:A:708:VAL:HG21	1.85	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:73:LEU:HG	1:B:88:ILE:HD11	1.86	0.58
1:B:55:LEU:HD12	1:B:55:LEU:O	2.04	0.58
1:B:169:LEU:HD23	1:B:185:TRP:CE2	2.39	0.57
1:A:524:LEU:HD21	1:A:526:LEU:HD12	1.80	0.57
1:A:44:GLU:OE1	1:A:47:ARG:NH1	2.38	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:A:55:LEU:HD12	1:A:55:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:268:PRO:O	1:B:271:SER:OG	2.21	0.55
1:B:60:VAL:HG11	1:B:72:MET:HE1	1.89	0.54
1:B:110:GLU:CD	1:B:154:ILE:HD11	2.27	0.54
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:B:25:VAL:HG23	1:B:75:ALA:C	2.27	0.54
1:B:554:ILE:HD13	1:B:637:THR:HG21	1.89	0.54
1:B:108:ARG:NH2	1:B:532:GLU:OE2	2.40	0.54
1:B:472:PRO:O	1:B:476:ILE:HD12	2.08	0.54
1:B:524:LEU:HD21	1:B:526:LEU:HD12	1.82	0.53
1:A:743:THR:HG21	1:A:748:VAL:CG1	2.29	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:25:VAL:HG23	1:A:75:ALA:C	2.30	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:B:347:ILE:HG22	1:B:349:VAL:CG2	2.40	0.52
1:A:634:PHE:HB2	1:A:715:LEU:HD23	1.91	0.52
1:B:710:CYS:SG	1:B:711:ASN:N	2.82	0.52
1:A:23:VAL:HA	1:A:26:LEU:HD12	1.91	0.52
1:B:565:LEU:HD23	1:B:565:LEU:C	2.30	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:277:SER:HB3	1:A:410:LEU:HD11	1.90	0.52
1:A:471:ASN:O	1:A:474:ALA:HB3	2.10	0.51
1:B:448:ILE:HG22	1:B:452:GLN:OE1	2.10	0.51
1:A:723:THR:O	1:A:727:GLN:NE2	2.42	0.51
1:A:576:LYS:HA	1:A:580:TYR:CD1	2.45	0.51
1:A:125:ILE:HD11	1:A:157:LEU:HD22	1.93	0.51
1:A:25:VAL:HG22	1:A:25:VAL:O	2.11	0.51
1:B:300:ALA:HB1	1:B:305:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:PHE:CE2	1:B:390:MET:HE3	2.46	0.50
1:B:23:VAL:HG12	1:B:23:VAL:O	2.12	0.50
1:A:184:LEU:HD12	1:A:522:ARG:HD3	1.92	0.50
1:A:561:ILE:HB	1:A:607:ASN:HB2	1.94	0.50
1:A:257:ALA:HB3	1:A:280:ILE:CD1	2.40	0.50
1:A:125:ILE:CD1	1:A:157:LEU:HD22	2.41	0.50
1:A:466:LYS:NZ	1:A:614:GLU:OE2	2.34	0.50
1:A:125:ILE:CD1	1:A:157:LEU:HD13	2.38	0.50
1:A:641:VAL:HG13	1:A:696:ILE:CG2	2.41	0.50
1:A:25:VAL:HG23	1:A:75:ALA:O	2.11	0.50
1:B:257:ALA:HB3	1:B:280:ILE:HD12	1.93	0.50
1:B:110:GLU:OE2	1:B:154:ILE:HD11	2.12	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: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:A:565:LEU:C	1:A:565:LEU:HD23	2.32	0.49
1:A:288:MET:HE1	1:A:292:ARG:HG2	1.95	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
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: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:25:VAL:HG22	1:B:25:VAL:O	2.13	0.48
1:B:23:VAL:HA	1:B:26:LEU:HD12	1.95	0.48
1:B:416:VAL:HG11	1:B:761:MET:CE	2.44	0.48
1:A:363:LEU:CD1	1:A:368:ILE:HD11	2.43	0.48
1:A:347:ILE:HG22	1:A:349:VAL:CG2	2.43	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:75:ALA:O	1:B:78:ALA:HB3	2.13	0.48
1:A:581:THR:OG1	1:A:584:GLU:HG3	2.13	0.48
1:B:416:VAL:CG1	1:B:419:ALA:HB3	2.41	0.47
1:A:19:SER:OG	1:A:161:ASP:HB3	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HD12	1:A:598:LEU:HB3	1.94	0.47
1:B:105:LEU:O	1:B:108:ARG:HB3	2.14	0.47
1:A:700:VAL:HG11	1:A:728:VAL:HG12	1.95	0.47
1:A:185:TRP:O	1:A:186:ASP:C	2.53	0.47
1:A:60:VAL:HG11	1:A:72:MET:HE2	1.94	0.47
1:A:711:ASN:C	1:A:711:ASN:ND2	2.67	0.47
1:A:473:PHE:CD2	1:A:598:LEU:CD2	2.97	0.47
1:A:396:GLN:HB3	1:A:404:LEU:HD21	1.97	0.47
1:A:416:VAL:CG1	1:A:419:ALA:HB3	2.45	0.47
1:A:606:THR:O	1:A:606:THR:CG2	2.63	0.47
1:B:633:LEU:HD12	1:B:714:VAL:CG1	2.45	0.47
1:A:461:ASP:O	1:A:740:ILE:HA	2.14	0.47
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
1:A:369:PHE:O	1:A:405:PRO:HB3	2.16	0.46
1:B:288:MET:HE1	1:B:292:ARG:HG2	1.97	0.46
1:B:113:MET:O	1:B:114:LEU:C	2.52	0.46
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: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:B:464:LEU:HD23	1:B:464:LEU:O	2.15	0.46
1:B:254:ALA:HB1	1:B:280:ILE:CD1	2.46	0.46
1:B:562:ILE:HD12	1:B:607:ASN:OD1	2.16	0.46
1:B:514:ILE:HG23	1:B:543:THR:HB	1.98	0.46
1:B:464:LEU:CD1	1:B:746:THR:HG23	2.46	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:60:VAL:HG11	1:B:72:MET:HE2	1.97	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:CD1	1:B:438:ILE:N	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:B:185:TRP:O	1:B:186:ASP:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:LEU:HD12	1:B:714:VAL:HG12	1.98	0.45
1:A:114:LEU:HD21	1:A:575:VAL:HA	1.99	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:306:TYR:CZ	1:A:328:SER:HB2	2.52	0.45
1:A:297:VAL:HG21	1:A:369:PHE:CD2	2.52	0.45
1:A:580:TYR:CE2	1:B:599:ILE:HD12	2.52	0.45
1:A:10:GLN:OE1	1:A:61:LEU:HD12	2.16	0.45
1:B:658:LYS:HA	1:B:659:PRO:HD3	1.84	0.45
1:B:746:THR:O	1:B:746:THR:HG22	2.17	0.45
1:A:101:LEU:O	1:A:101:LEU:HD12	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
1:B:402:SER:OG	1:B:403:GLN:N	2.48	0.44
1:B:266:CYS:HB3	1:B:443:THR:HG22	1.99	0.44
1:A:374:PHE:CE2	1:A:390:MET:HE3	2.52	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:110:GLU:CD	1:A:154:ILE:HD11	2.37	0.44
1:A:33:LEU:HD22	1:A:37:LEU:CD2	2.44	0.44
1:B:416:VAL:O	1:B:416:VAL:CG1	2.65	0.44
1:B:461:ASP:OD2	1:B:463:ARG:NE	2.50	0.44
1:A:552:ALA:CB	1:A:568:LEU:HD21	2.46	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:604:ASP:HB3	1:A:606:THR:H	1.83	0.44
1:A:468:ARG:NH2	1:A:607:ASN:O	2.51	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:O	1:B:101:LEU:HD12	2.18	0.44
1:A:327:ILE:CG2	1:A:349:VAL:HG13	2.48	0.44
1:A:722:VAL:O	1:A:723:THR:C	2.56	0.44
1:B:264:LEU:CD1	1:B:377:CYS:SG	3.06	0.44
1:B:132:ARG:HA	1:B:135:GLU:HG2	2.00	0.44
1:A:514:ILE:HG23	1:A:543:THR:HB	2.00	0.43
1:B:169:LEU:HD23	1:B:185:TRP:CZ2	2.53	0.43
1:A:13:ARG:HE	1:A:57:LEU:HD23	1.83	0.43
1:B:245:LYS:HD3	1:B:246:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ILE:CD1	1:A:438:ILE:N	2.81	0.43
1:B:297:VAL:CG2	1:B:369:PHE:CG	3.02	0.43
1:A:528:ASP:HB3	1:A:531:GLU:HB3	2.00	0.43
1:A:462:VAL:HG12	1:A:462:VAL:O	2.18	0.43
1:A:9:LEU:HD23	1:A:61:LEU:HD21	2.00	0.43
1:A:153:LEU:HD23	1:A:153:LEU:C	2.39	0.43
1:B:153:LEU:C	1:B:153:LEU:HD23	2.39	0.43
1:A:464:LEU:HA	1:A:464:LEU:HD12	1.76	0.43
1:B:277:SER:HB3	1:B:410:LEU:HD11	2.00	0.43
1:B:9:LEU:HD23	1:B:61:LEU:HD21	2.00	0.43
1:A:726:ILE:CD1	1:A:739:CYS:SG	3.07	0.43
1:A:118:PRO:HD2	1:A:146:LYS:HG3	2.00	0.43
1:B:297:VAL:HG21	1:B:369:PHE:CD2	2.54	0.43
1:A:736:GLY:O	1:A:737:SER:CB	2.67	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:606:THR:O	1:A:606:THR:HG23	2.19	0.42
1:B:594:LYS:C	1:B:596:PRO:HD2	2.40	0.42
1:A:173:LEU:HB3	1:A:182:SER:HB2	2.01	0.42
1:B:257:ALA:HB3	1:B:280:ILE:CD1	2.49	0.42
1:A:396:GLN:CB	1:A:404:LEU:HD21	2.50	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:B:264:LEU:HD13	1:B:377:CYS:SG	2.59	0.42
1:A:113:MET:O	1:A:114:LEU:C	2.58	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:A:297:VAL:CG2	1:A:369:PHE:CG	3.03	0.42
1:A:727:GLN:O	1:A:728:VAL:HB	2.20	0.42
1:B:712:LEU:HD23	1:B:714:VAL:HG23	2.00	0.42
1:A:623:TYR:CE2	1:A:657:ILE:CD1	3.03	0.42
1:A:615:LEU:C	1:A:615:LEU:HD23	2.40	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:A:110:GLU:CG	1:A:154:ILE:HD11	2.50	0.42
1:B:511:GLU:O	1:B:515:VAL:HG23	2.20	0.42
1:B:327:ILE:CG2	1:B:349:VAL:HG13	2.50	0.42
1:B:73:LEU:CD2	1:B:88:ILE:HD11	2.50	0.41
1:A:487:LEU:O	1:A:490:THR:HB	2.20	0.41
1:B:245:LYS:CD	1:B:246:ALA:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:ASP:HB2	1:B:653:ILE:HG22	2.03	0.41
1:A:288:MET:CE	1:A:370:THR:HG21	2.46	0.41
1:B:390:MET:HG3	1:B:436:LEU:HD23	2.03	0.41
1:B:396:GLN:HB3	1:B:404:LEU:HD21	2.01	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:A:456:ASN:OD1	1:A:456:ASN:N	2.48	0.41
1:B:363:LEU:HD21	1:B:368:ILE:CD1	2.51	0.41
1:A:574:ASN:O	1:A:575:VAL:C	2.59	0.41
1:A:465:VAL:HG13	1:A:614:GLU:HG3	2.02	0.41
1:B:726:ILE:CG2	1:B:727:GLN:N	2.77	0.41
1:A:773:ASP:O	1:A:774:GLU:C	2.59	0.41
1:A:745:LYS:O	1:A:748:VAL:HG12	2.21	0.41
1:A:416:VAL:HG11	1:A:761:MET:CE	2.51	0.41
1:B:471:ASN:O	1:B:474:ALA:HB3	2.20	0.41
1:B:306:TYR:CZ	1:B:328:SER:HB2	2.56	0.41
1:B:436:LEU:CB	1:B:438:ILE:HD13	2.51	0.41
1:B:9:LEU:HB3	1:B:61:LEU:HD21	2.03	0.41
1:A:110:GLU:OE2	1:A:154:ILE:HD11	2.21	0.41
1:B:393:TYR:CZ	1:B:404:LEU:HD13	2.55	0.41
1:A:620:ASP:HB2	1:A:653:ILE:HG22	2.03	0.41
1:B:96:LEU:HD21	1:B:161:ASP:HB2	2.02	0.41
1:A:381:THR:CG2	1:A:382:GLY:N	2.84	0.41
1:B:469:ILE:HB	1:B:470:HIS:CD2	2.56	0.41
1:B:474:ALA:HA	1:B:553:LEU:CD2	2.50	0.41
1:B:303:VAL:N	1:B:304:PRO:HD2	2.36	0.41
1:A:310:LYS:HA	1:A:348:VAL:HG21	2.03	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:B:558:ASP:CB	1:B:640:LEU:HD11	2.48	0.40
1:A:511:GLU:O	1:A:515:VAL:HG23	2.22	0.40
1:B:73:LEU:CG	1:B:88:ILE:HD11	2.51	0.40
1:A:29:MET:HE1	1:A:72:MET:HA	2.03	0.40
1:B:436:LEU:HB3	1:B:438:ILE:HD11	2.03	0.40
1:B:108:ARG:NH1	1:B:521:CYS:O	2.52	0.40
1:A:402:SER:OG	1:A:403:GLN:N	2.53	0.40
1:B:421:ASN:N	1:B:421:ASN:ND2	2.69	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:477:ILE:HG21	1:A:553:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LEU:HD12	1:B:598:LEU:HB3	2.03	0.40
1:A:122:ILE:N	1:A:123:PRO:HD2	2.37	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 (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	664/936 (71%)	594 (90%)	61 (9%)	9 (1%)	14	60
1	B	660/936 (70%)	595 (90%)	56 (8%)	9 (1%)	14	60
All	All	1324/1872 (71%)	1189 (90%)	117 (9%)	18 (1%)	14	60

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
1	B	774	GLU
1	A	19	SER
1	A	738	LYS
1	A	774	GLU
1	B	19	SER

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Mol	Chain	Res	Type
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%)	563 (93%)	43 (7%)	18	60
1	B	602/831 (72%)	563 (94%)	39 (6%)	21	64
All	All	1208/1662 (73%)	1126 (93%)	82 (7%)	20	62

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	45	GLU
1	A	60	VAL
1	A	64	GLU
1	A	113	MET
1	A	131	ASP
1	A	146	LYS
1	A	164	HIS
1	A	171	LEU
1	A	174	ASP
1	A	186	ASP
1	A	245	LYS
1	A	253	LEU
1	A	264	LEU
1	A	278	ILE
1	A	297	VAL

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Mol	Chain	Res	Type
1	A	301	THR
1	A	306	TYR
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	476	ILE
1	A	507	THR
1	A	524	LEU
1	A	581	THR
1	A	602	SER
1	A	606	THR
1	A	607	ASN
1	A	619	LEU
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	754	CYS
1	B	8	SER
1	B	45	GLU
1	B	60	VAL
1	B	64	GLU
1	B	113	MET
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	278	ILE
1	B	297	VAL

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Mol	Chain	Res	Type
1	B	301	THR
1	B	306	TYR
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	467	ARG
1	B	476	ILE
1	B	507	THR
1	B	524	LEU
1	B	581	THR
1	B	602	SER
1	B	606	THR
1	B	607	ASN
1	B	619	LEU
1	B	655	ASN
1	B	693	ARG
1	B	711	ASN
1	B	712	LEU
1	B	718	TYR
1	B	754	CYS
1	B	793	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	711	ASN
1	B	711	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.02	11 (1%)	74	60	85, 157, 218, 263	0
1	B	674/936 (72%)	0.21	25 (3%)	45	31	95, 185, 265, 315	0
All	All	1352/1872 (72%)	0.10	36 (2%)	58	42	85, 169, 253, 315	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	ARG	5.2
1	B	327	ILE	4.0
1	B	56	PHE	3.8
1	A	37	LEU	3.8
1	B	93	PHE	3.7
1	B	725	MET	3.6
1	B	26	LEU	3.5
1	A	56	PHE	3.3
1	B	37	LEU	3.1
1	B	328	SER	3.0
1	B	95	LYS	3.0
1	A	57	LEU	3.0
1	A	736	GLY	2.9
1	B	22	PRO	2.8
1	A	53	ALA	2.8
1	B	57	LEU	2.8
1	B	347	ILE	2.8
1	B	794	SER	2.7
1	B	346	ILE	2.7
1	B	161	ASP	2.6
1	A	95	LYS	2.5
1	B	40	ARG	2.5
1	B	163	GLU	2.4
1	A	794	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	325	GLN	2.3
1	B	84	LEU	2.2
1	B	173	LEU	2.2
1	A	55	LEU	2.2
1	A	72	MET	2.2
1	A	336	SER	2.2
1	B	326	GLY	2.2
1	B	41	ILE	2.2
1	B	277	SER	2.2
1	B	181	ALA	2.1
1	A	61	LEU	2.0
1	B	341	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.