



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:42 PM UTC

PDB ID : 1HCI / pdb_00001hci
Title : CRYSTAL STRUCTURE OF THE ROD DOMAIN OF ALPHA-ACTININ
Authors : Ylanne, J.; Scheffzek, K.; Young, P.; Saraste, M.
Deposited on : 2001-05-04
Resolution : 2.80 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

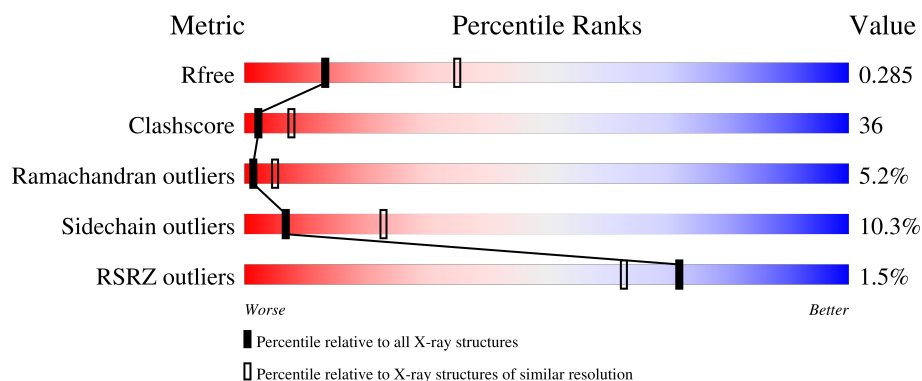
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	476	44% 43% 11% .
1	B	476	2% 45% 43% 11% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7900 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 ALPHA-ACTININ 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3942	2453	714	758	17			
1	B	475	Total	C	N	O	S	0	0	0
			3942	2453	714	758	17			

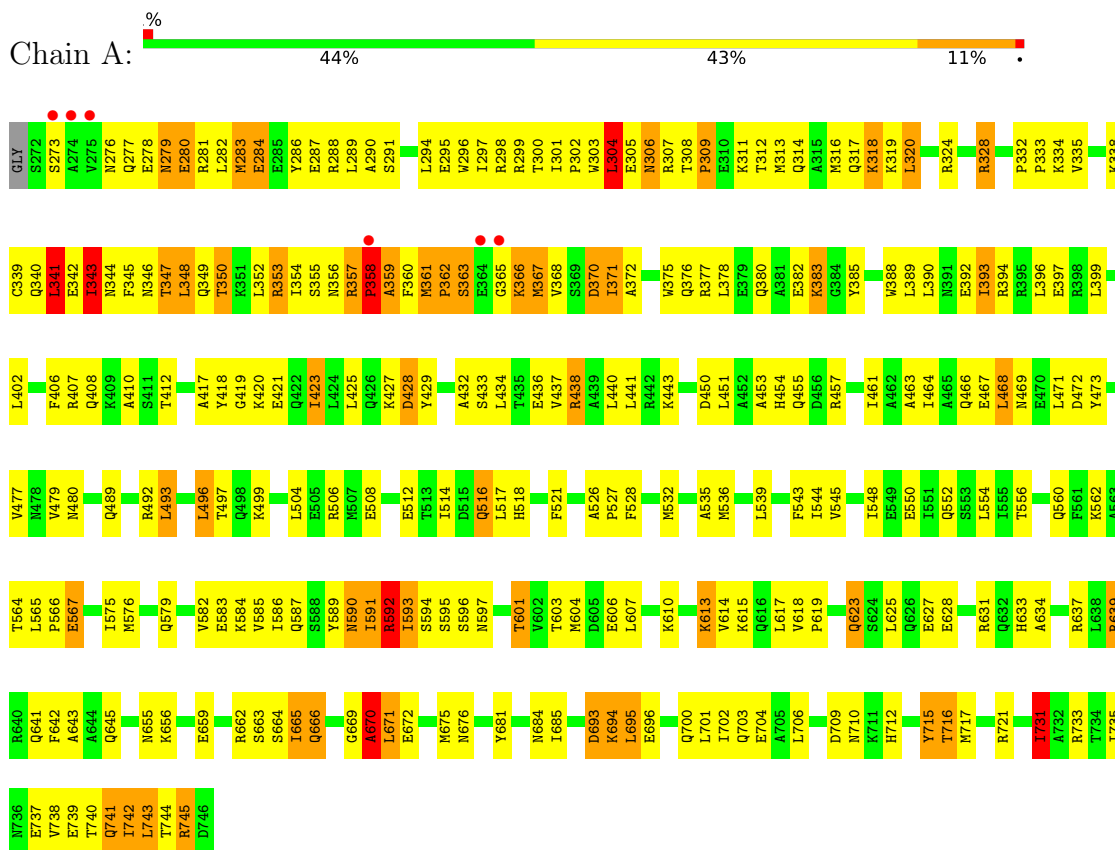
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	9	Total	O	0	0
			9	9		

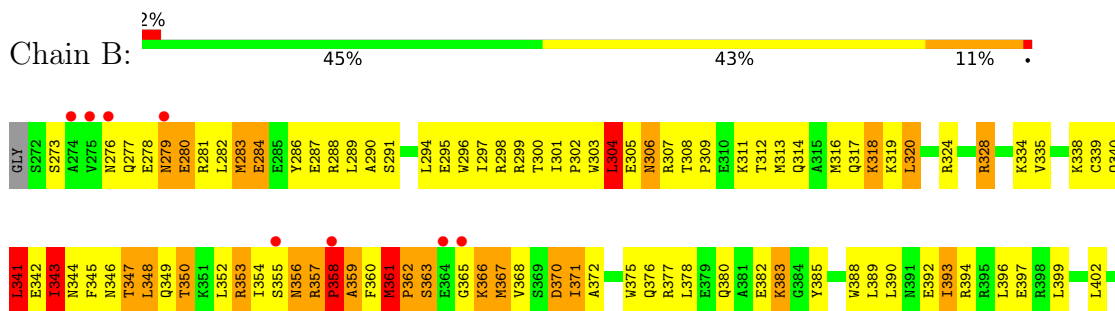
3 Residue-property plots

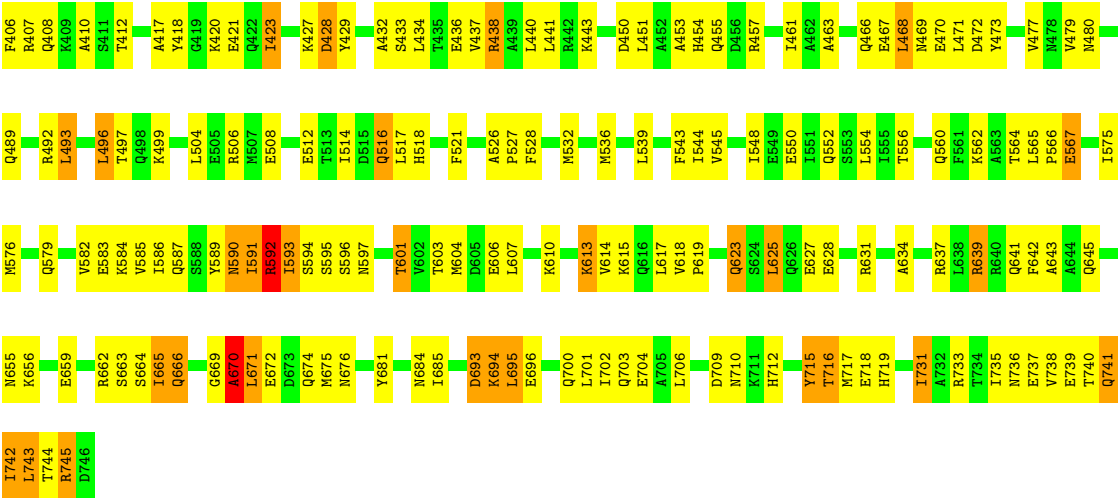
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ALPHA-ACTININ 2



• Molecule 1: ALPHA-ACTININ 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	103.28Å 103.28Å 218.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.78 – 2.80 82.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (82.78-2.80) 98.7 (82.78-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.69Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.270 , 0.295 0.261 , 0.285	Depositor DCC
R_{free} test set	7073 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.450 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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	0.53	0/4008	1.00	20/5401 (0.4%)
1	B	0.53	0/4008	0.99	19/5401 (0.4%)
All	All	0.53	0/8016	0.99	39/10802 (0.4%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	715	TYR	N-CA-C	8.94	124.56	111.96
1	B	343	ILE	N-CA-C	-8.30	100.65	112.35
1	B	284	GLU	N-CA-C	-8.28	103.31	113.41
1	A	284	GLU	N-CA-C	-8.26	103.33	113.41
1	A	343	ILE	N-CA-C	-8.20	100.79	112.35
1	B	341	LEU	N-CA-C	-7.75	100.88	110.41
1	A	341	LEU	N-CA-C	-7.69	100.96	110.41
1	A	361	MET	CA-C-N	7.18	128.82	119.84
1	A	361	MET	C-N-CA	7.18	128.82	119.84
1	B	361	MET	CA-C-N	7.13	128.76	119.84
1	B	361	MET	C-N-CA	7.13	128.76	119.84
1	B	304	LEU	N-CA-C	-7.05	98.81	109.60
1	A	304	LEU	N-CA-C	-6.96	98.96	109.60
1	B	318	LYS	N-CA-C	-6.92	104.10	112.54
1	A	318	LYS	N-CA-C	-6.89	104.13	112.54
1	B	350	THR	N-CA-C	-6.65	104.06	111.71
1	A	350	THR	N-CA-C	-6.63	104.09	111.71
1	B	715	TYR	N-CA-C	6.49	124.63	110.80
1	A	371	ILE	N-CA-C	-6.29	104.77	112.76
1	B	371	ILE	N-CA-C	-6.28	104.78	112.76
1	A	353	ARG	N-CA-C	-5.91	105.16	112.90
1	B	353	ARG	N-CA-C	-5.89	105.18	112.90
1	B	499	LYS	N-CA-C	-5.85	104.59	110.97
1	A	499	LYS	N-CA-C	-5.61	104.85	110.97
1	B	670	ALA	N-CA-C	5.57	122.67	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	LYS	N-CA-C	-5.44	105.51	111.82
1	B	279	ASN	N-CA-C	-5.44	106.42	113.16
1	B	338	LYS	N-CA-C	-5.43	105.52	111.82
1	A	670	ALA	N-CA-C	5.38	122.26	110.80
1	A	279	ASN	N-CA-C	-5.36	106.52	113.16
1	A	283	MET	N-CA-C	-5.33	106.53	114.64
1	A	393	ILE	N-CA-C	-5.31	105.20	110.62
1	B	283	MET	N-CA-C	-5.31	106.58	114.64
1	B	280	GLU	N-CA-C	-5.18	107.02	113.55
1	A	347	THR	N-CA-C	-5.16	106.82	113.01
1	B	393	ILE	N-CA-C	-5.16	105.36	110.62
1	A	731	ILE	CB-CA-C	-5.14	105.39	111.97
1	B	347	THR	N-CA-C	-5.13	106.86	113.01
1	A	280	GLU	N-CA-C	-5.10	107.13	113.55

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	3942	0	3889	290	0
1	B	3942	0	3889	291	0
2	A	7	0	0	0	0
2	B	9	0	0	0	0
All	All	7900	0	7778	562	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 36.

All (562) 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:575:ILE:HG22	1:A:604:MET:HE1	1.39	1.04
1:A:526:ALA:HB3	1:A:527:PRO:HD3	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ALA:HB3	1:B:527:PRO:HD3	1.39	1.02
1:B:575:ILE:HG22	1:B:604:MET:HE1	1.38	1.00
1:B:469:ASN:HD21	1:B:480:ASN:HD21	1.15	0.95
1:A:576:MET:HA	1:A:604:MET:HE3	1.49	0.94
1:B:576:MET:HA	1:B:604:MET:HE3	1.52	0.92
1:A:469:ASN:HD21	1:A:480:ASN:HD21	1.17	0.92
1:B:665:ILE:CD1	1:B:666:GLN:H	1.83	0.91
1:A:350:THR:HG23	1:A:353:ARG:HH12	1.35	0.91
1:A:665:ILE:CD1	1:A:666:GLN:H	1.82	0.91
1:B:350:THR:HG23	1:B:353:ARG:HH12	1.36	0.90
1:B:342:GLU:HA	1:B:345:PHE:HB3	1.54	0.88
1:A:342:GLU:HA	1:A:345:PHE:HB3	1.54	0.87
1:A:665:ILE:HD13	1:A:666:GLN:H	1.41	0.84
1:B:521:PHE:HE2	1:B:604:MET:HE2	1.42	0.83
1:B:665:ILE:HD13	1:B:666:GLN:H	1.42	0.83
1:A:576:MET:HG2	1:A:604:MET:SD	2.19	0.83
1:A:740:THR:HG23	1:B:350:THR:HG21	1.61	0.82
1:B:576:MET:HG2	1:B:604:MET:SD	2.20	0.81
1:A:521:PHE:HE2	1:A:604:MET:HE2	1.44	0.81
1:A:350:THR:HG21	1:B:740:THR:HG23	1.62	0.81
1:B:367:MET:HB2	1:B:370:ASP:HB2	1.63	0.79
1:A:350:THR:HG23	1:A:353:ARG:NH1	1.98	0.78
1:A:367:MET:HB2	1:A:370:ASP:HB2	1.63	0.78
1:B:536:MET:HE3	1:B:613:LYS:HB3	1.66	0.77
1:B:350:THR:HG23	1:B:353:ARG:NH1	1.99	0.76
1:B:700:GLN:O	1:B:704:GLU:HG3	1.85	0.76
1:B:357:ARG:O	1:B:357:ARG:HG3	1.85	0.75
1:B:279:ASN:HD21	1:B:352:LEU:HD21	1.51	0.75
1:A:357:ARG:O	1:A:357:ARG:HG3	1.85	0.75
1:A:279:ASN:HD21	1:A:352:LEU:HD21	1.51	0.75
1:A:536:MET:HE3	1:A:613:LYS:HB3	1.68	0.74
1:B:349:GLN:HE22	1:B:359:ALA:HB1	1.51	0.74
1:A:349:GLN:HE22	1:A:359:ALA:HB1	1.51	0.74
1:B:603:THR:HG23	1:B:606:GLU:H	1.53	0.73
1:A:278:GLU:HA	1:A:281:ARG:HG2	1.72	0.72
1:A:603:THR:HG23	1:A:606:GLU:H	1.54	0.72
1:B:273:SER:HA	1:B:276:ASN:HD22	1.52	0.72
1:A:273:SER:HA	1:A:276:ASN:HD22	1.52	0.72
1:A:681:TYR:O	1:A:685:ILE:HG12	1.89	0.71
1:A:300:THR:C	1:A:302:PRO:HD2	2.15	0.71
1:B:681:TYR:O	1:B:685:ILE:HG12	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:HA	1:B:281:ARG:HG2	1.71	0.71
1:A:694:LYS:HB2	1:A:694:LYS:NZ	2.06	0.71
1:B:671:LEU:HD23	1:B:671:LEU:H	1.56	0.70
1:B:300:THR:C	1:B:302:PRO:HD2	2.16	0.70
1:B:694:LYS:HB2	1:B:694:LYS:NZ	2.05	0.70
1:A:671:LEU:H	1:A:671:LEU:HD23	1.55	0.70
1:A:665:ILE:CD1	1:A:666:GLN:N	2.54	0.70
1:A:589:TYR:HB2	1:A:591:ILE:HG22	1.73	0.69
1:A:696:GLU:CG	1:B:328:ARG:HG3	2.23	0.69
1:A:700:GLN:O	1:A:704:GLU:HG3	1.91	0.69
1:B:565:LEU:N	1:B:566:PRO:HD2	2.08	0.69
1:A:313:MET:CE	1:A:397:GLU:HA	2.23	0.69
1:A:671:LEU:HD23	1:A:671:LEU:N	2.08	0.69
1:A:696:GLU:HG2	1:B:328:ARG:HG3	1.74	0.69
1:B:282:LEU:O	1:B:348:LEU:HG	1.93	0.69
1:B:313:MET:CE	1:B:397:GLU:HA	2.23	0.69
1:B:665:ILE:CD1	1:B:666:GLN:N	2.55	0.69
1:A:306:ASN:ND2	1:A:308:THR:H	1.90	0.69
1:B:589:TYR:HB2	1:B:591:ILE:HG22	1.73	0.69
1:A:576:MET:HA	1:A:604:MET:CE	2.23	0.68
1:B:365:GLY:O	1:B:366:LYS:HG3	1.93	0.68
1:A:742:ILE:HG12	1:A:742:ILE:O	1.94	0.68
1:B:301:ILE:HD13	1:B:377:ARG:HG2	1.75	0.68
1:B:306:ASN:ND2	1:B:308:THR:H	1.91	0.68
1:A:282:LEU:O	1:A:348:LEU:HG	1.94	0.68
1:A:291:SER:OG	1:A:366:LYS:HD2	1.93	0.68
1:B:421:GLU:HG2	1:B:493:LEU:HD13	1.75	0.68
1:A:365:GLY:O	1:A:366:LYS:HG3	1.94	0.67
1:A:301:ILE:HD13	1:A:377:ARG:HG2	1.76	0.67
1:B:671:LEU:HD23	1:B:671:LEU:N	2.09	0.67
1:B:526:ALA:HB3	1:B:527:PRO:CD	2.21	0.67
1:A:328:ARG:HG3	1:B:696:GLU:CG	2.23	0.67
1:B:576:MET:HA	1:B:604:MET:CE	2.24	0.67
1:A:603:THR:HG22	1:A:606:GLU:OE1	1.94	0.67
1:B:291:SER:OG	1:B:366:LYS:HD2	1.95	0.67
1:B:492:ARG:HH11	1:B:492:ARG:HB2	1.60	0.67
1:A:341:LEU:O	1:A:342:GLU:HG2	1.95	0.67
1:B:603:THR:HG22	1:B:606:GLU:OE1	1.94	0.67
1:A:394:ARG:O	1:A:397:GLU:HB3	1.96	0.66
1:A:421:GLU:HG2	1:A:493:LEU:HD13	1.76	0.66
1:A:645:GLN:HE22	1:A:694:LYS:HG2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ARG:HH11	1:B:385:TYR:HD1	1.42	0.66
1:A:564:THR:C	1:A:566:PRO:HD2	2.21	0.66
1:B:341:LEU:O	1:B:342:GLU:HG2	1.95	0.66
1:A:434:LEU:HD21	1:A:438:ARG:NH2	2.09	0.66
1:B:389:LEU:O	1:B:393:ILE:HG12	1.95	0.66
1:A:349:GLN:NE2	1:A:359:ALA:HB1	2.11	0.66
1:B:742:ILE:HG12	1:B:742:ILE:O	1.94	0.66
1:A:517:LEU:HB3	1:A:582:VAL:HG22	1.78	0.66
1:B:360:PHE:CD2	1:B:362:PRO:HD3	2.30	0.66
1:A:441:LEU:HD13	1:A:504:LEU:HB3	1.77	0.66
1:A:360:PHE:CD2	1:A:362:PRO:HD3	2.30	0.66
1:A:469:ASN:ND2	1:A:480:ASN:HD21	1.91	0.66
1:A:389:LEU:O	1:A:393:ILE:HG12	1.96	0.65
1:B:394:ARG:O	1:B:397:GLU:HB3	1.96	0.65
1:A:565:LEU:N	1:A:566:PRO:HD2	2.11	0.65
1:A:685:ILE:HG13	1:A:731:ILE:HD13	1.78	0.65
1:A:328:ARG:HG3	1:B:696:GLU:HG2	1.77	0.65
1:B:564:THR:C	1:B:566:PRO:HD2	2.20	0.65
1:A:307:ARG:HH11	1:A:385:TYR:HD1	1.43	0.65
1:B:349:GLN:NE2	1:B:359:ALA:HB1	2.11	0.65
1:B:685:ILE:HG13	1:B:731:ILE:HD13	1.79	0.65
1:B:376:GLN:HE21	1:B:376:GLN:HA	1.61	0.65
1:A:436:GLU:O	1:A:440:LEU:HG	1.96	0.65
1:B:313:MET:HE1	1:B:397:GLU:OE2	1.97	0.65
1:B:645:GLN:HE22	1:B:694:LYS:HG2	1.62	0.65
1:B:434:LEU:HD21	1:B:438:ARG:NH2	2.11	0.65
1:A:685:ILE:HG13	1:A:731:ILE:CD1	2.27	0.64
1:B:469:ASN:ND2	1:B:480:ASN:HD21	1.90	0.64
1:A:301:ILE:N	1:A:302:PRO:HD2	2.13	0.64
1:B:685:ILE:HG13	1:B:731:ILE:CD1	2.28	0.64
1:B:441:LEU:HD13	1:B:504:LEU:HB3	1.78	0.64
1:B:675:MET:HE2	1:B:738:VAL:HG12	1.79	0.64
1:A:341:LEU:C	1:A:343:ILE:H	2.06	0.63
1:A:313:MET:HE1	1:A:397:GLU:OE2	1.97	0.63
1:A:376:GLN:HE21	1:A:376:GLN:HA	1.62	0.63
1:B:517:LEU:HB3	1:B:582:VAL:HG22	1.80	0.63
1:A:526:ALA:HB3	1:A:527:PRO:CD	2.23	0.63
1:B:341:LEU:C	1:B:343:ILE:H	2.06	0.63
1:B:279:ASN:ND2	1:B:352:LEU:HD21	2.14	0.63
1:A:320:LEU:HA	1:A:389:LEU:HD13	1.81	0.63
1:B:394:ARG:HG3	1:B:394:ARG:HH11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ARG:HH11	1:A:492:ARG:HB2	1.63	0.62
1:A:706:LEU:HD11	1:B:317:GLN:HE22	1.64	0.62
1:B:286:TYR:OH	1:B:368:VAL:HG22	1.99	0.62
1:B:345:PHE:O	1:B:345:PHE:CG	2.52	0.62
1:A:305:GLU:HA	1:A:307:ARG:NH2	2.15	0.62
1:A:317:GLN:HE22	1:B:706:LEU:HD11	1.65	0.62
1:A:675:MET:HE2	1:A:738:VAL:HG12	1.80	0.62
1:B:320:LEU:HA	1:B:389:LEU:HD13	1.81	0.62
1:B:297:ILE:O	1:B:301:ILE:HG13	2.00	0.62
1:A:319:LYS:HG2	1:A:389:LEU:HD21	1.82	0.62
1:B:301:ILE:N	1:B:302:PRO:HD2	2.14	0.61
1:A:592:ARG:HG2	1:A:592:ARG:HH11	1.65	0.61
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.65	0.61
1:A:469:ASN:HD21	1:A:480:ASN:ND2	1.96	0.61
1:A:279:ASN:ND2	1:A:352:LEU:HD21	2.14	0.61
1:B:319:LYS:HG2	1:B:389:LEU:HD21	1.82	0.61
1:A:286:TYR:OH	1:A:368:VAL:HG22	2.01	0.61
1:A:556:THR:O	1:A:560:GLN:HG3	2.01	0.61
1:B:290:ALA:HB3	1:B:366:LYS:NZ	2.16	0.61
1:A:279:ASN:HD21	1:A:352:LEU:CD2	2.14	0.60
1:A:290:ALA:HB3	1:A:366:LYS:NZ	2.16	0.60
1:A:345:PHE:CG	1:A:345:PHE:O	2.53	0.60
1:B:665:ILE:HD12	1:B:666:GLN:N	2.16	0.60
1:A:297:ILE:O	1:A:301:ILE:HG13	2.01	0.60
1:B:517:LEU:HB3	1:B:582:VAL:CG2	2.31	0.60
1:A:735:ILE:O	1:A:739:GLU:HG3	2.00	0.60
1:A:665:ILE:HD12	1:A:666:GLN:N	2.15	0.60
1:A:463:ALA:O	1:A:466:GLN:HB3	2.01	0.60
1:A:639:ARG:HD3	1:A:709:ASP:O	2.01	0.60
1:B:279:ASN:HD21	1:B:352:LEU:CD2	2.14	0.60
1:B:305:GLU:HA	1:B:307:ARG:NH2	2.15	0.60
1:B:592:ARG:HG2	1:B:592:ARG:HH11	1.66	0.60
1:A:370:ASP:C	1:A:372:ALA:H	2.10	0.60
1:A:517:LEU:HB3	1:A:582:VAL:CG2	2.30	0.60
1:A:694:LYS:HB2	1:A:694:LYS:HZ2	1.67	0.60
1:B:436:GLU:O	1:B:440:LEU:HG	2.01	0.60
1:B:735:ILE:O	1:B:739:GLU:HG3	2.01	0.60
1:A:317:GLN:HB3	1:A:393:ILE:HD12	1.84	0.60
1:B:556:THR:O	1:B:560:GLN:HG3	2.02	0.60
1:A:376:GLN:HA	1:A:376:GLN:NE2	2.17	0.59
1:B:339:CYS:O	1:B:341:LEU:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:MET:HE2	1:A:738:VAL:CG1	2.32	0.59
1:B:317:GLN:HB3	1:B:393:ILE:HD12	1.83	0.59
1:A:283:MET:HB2	1:A:360:PHE:CZ	2.38	0.59
1:A:350:THR:HA	1:A:353:ARG:CZ	2.33	0.58
1:B:370:ASP:C	1:B:372:ALA:H	2.10	0.58
1:A:528:PHE:CE2	1:A:532:MET:HE2	2.38	0.58
1:B:283:MET:HB2	1:B:360:PHE:CZ	2.38	0.58
1:B:370:ASP:C	1:B:372:ALA:N	2.60	0.58
1:B:463:ALA:O	1:B:466:GLN:HB3	2.02	0.58
1:A:516:GLN:HE21	1:A:516:GLN:CA	2.16	0.58
1:B:516:GLN:HA	1:B:516:GLN:NE2	2.18	0.58
1:B:376:GLN:HA	1:B:376:GLN:NE2	2.17	0.58
1:B:469:ASN:HD21	1:B:480:ASN:ND2	1.94	0.58
1:A:339:CYS:O	1:A:341:LEU:O	2.21	0.58
1:B:316:MET:HE3	1:B:392:GLU:CB	2.34	0.58
1:B:350:THR:HA	1:B:353:ARG:CZ	2.33	0.58
1:B:516:GLN:HE21	1:B:516:GLN:CA	2.16	0.58
1:A:521:PHE:CE2	1:A:604:MET:HE2	2.34	0.57
1:B:284:GLU:O	1:B:288:ARG:HG2	2.04	0.57
1:B:273:SER:O	1:B:277:GLN:HG3	2.05	0.57
1:B:432:ALA:HB3	1:B:437:VAL:HG23	1.86	0.57
1:A:432:ALA:HB3	1:A:437:VAL:HG23	1.85	0.57
1:A:273:SER:O	1:A:277:GLN:HG3	2.05	0.57
1:A:516:GLN:HA	1:A:516:GLN:NE2	2.19	0.57
1:A:284:GLU:O	1:A:288:ARG:HG2	2.05	0.57
1:B:643:ALA:HB1	1:B:712:HIS:O	2.05	0.57
1:A:370:ASP:C	1:A:372:ALA:N	2.60	0.56
1:B:304:LEU:C	1:B:306:ASN:H	2.13	0.56
1:B:434:LEU:O	1:B:438:ARG:HB2	2.05	0.56
1:A:316:MET:HE3	1:A:392:GLU:CB	2.35	0.56
1:B:521:PHE:CE2	1:B:604:MET:HE2	2.32	0.56
1:A:584:LYS:HD2	1:A:584:LYS:C	2.31	0.56
1:A:304:LEU:C	1:A:306:ASN:H	2.12	0.56
1:B:313:MET:HE3	1:B:397:GLU:HA	1.87	0.56
1:B:584:LYS:HD2	1:B:584:LYS:C	2.31	0.56
1:A:313:MET:HE3	1:A:397:GLU:HA	1.88	0.56
1:A:441:LEU:HD13	1:A:504:LEU:CB	2.35	0.55
1:B:675:MET:HE2	1:B:738:VAL:CG1	2.35	0.55
1:A:282:LEU:HB3	1:A:348:LEU:HD23	1.89	0.55
1:B:639:ARG:HD3	1:B:709:ASP:O	2.06	0.55
1:B:441:LEU:HD13	1:B:504:LEU:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:HIS:HA	1:B:597:ASN:HD21	1.72	0.55
1:B:528:PHE:CE2	1:B:532:MET:HE2	2.41	0.55
1:A:669:GLY:O	1:A:670:ALA:O	2.25	0.55
1:A:354:ILE:HG22	1:A:354:ILE:O	2.07	0.55
1:B:469:ASN:O	1:B:472:ASP:N	2.39	0.55
1:A:434:LEU:O	1:A:438:ARG:HB2	2.07	0.55
1:A:643:ALA:HB1	1:A:712:HIS:O	2.07	0.55
1:A:662:ARG:O	1:A:664:SER:N	2.38	0.55
1:B:354:ILE:HG22	1:B:354:ILE:O	2.07	0.55
1:B:539:LEU:HD23	1:B:617:LEU:CB	2.37	0.55
1:B:694:LYS:HB2	1:B:694:LYS:HZ2	1.72	0.55
1:A:297:ILE:HD12	1:A:297:ILE:C	2.32	0.55
1:A:518:HIS:HA	1:A:597:ASN:HD21	1.72	0.55
1:B:662:ARG:O	1:B:664:SER:N	2.40	0.54
1:A:350:THR:HA	1:A:353:ARG:NH2	2.22	0.54
1:A:342:GLU:CA	1:A:345:PHE:HB3	2.34	0.54
1:A:601:THR:HG23	1:B:443:LYS:HE2	1.89	0.54
1:B:282:LEU:HB3	1:B:348:LEU:HD23	1.89	0.54
1:B:410:ALA:HA	1:B:461:ILE:HD13	1.88	0.54
1:A:539:LEU:HD23	1:A:617:LEU:CB	2.37	0.54
1:B:694:LYS:O	1:B:695:LEU:C	2.51	0.54
1:A:390:LEU:HB3	1:A:394:ARG:HH12	1.73	0.54
1:A:655:ASN:ND2	1:A:659:GLU:OE2	2.41	0.54
1:B:532:MET:O	1:B:536:MET:HG3	2.06	0.54
1:B:585:VAL:O	1:B:589:TYR:HD2	1.91	0.54
1:A:301:ILE:N	1:A:302:PRO:CD	2.70	0.54
1:B:350:THR:HA	1:B:353:ARG:NH2	2.22	0.54
1:B:744:THR:O	1:B:744:THR:HG22	2.08	0.54
1:A:438:ARG:HD2	1:A:508:GLU:OE2	2.07	0.54
1:A:443:LYS:HE2	1:B:601:THR:HG23	1.89	0.54
1:B:301:ILE:N	1:B:302:PRO:CD	2.71	0.54
1:B:297:ILE:C	1:B:297:ILE:HD12	2.33	0.53
1:B:342:GLU:CA	1:B:345:PHE:HB3	2.34	0.53
1:B:592:ARG:O	1:B:593:ILE:HB	2.08	0.53
1:A:316:MET:HE3	1:A:392:GLU:HG3	1.90	0.53
1:B:566:PRO:HG2	1:B:567:GLU:H	1.73	0.53
1:A:324:ARG:NH1	1:B:703:GLN:OE1	2.41	0.53
1:A:410:ALA:HA	1:A:461:ILE:HD13	1.90	0.53
1:B:591:ILE:HG12	1:B:592:ARG:O	2.09	0.53
1:B:438:ARG:HD2	1:B:508:GLU:OE2	2.08	0.53
1:A:585:VAL:O	1:A:589:TYR:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ARG:C	1:A:664:SER:H	2.17	0.53
1:B:669:GLY:O	1:B:670:ALA:O	2.26	0.53
1:A:280:GLU:HA	1:A:283:MET:HG2	1.91	0.53
1:A:363:SER:HB2	1:A:366:LYS:HB2	1.91	0.53
1:B:312:THR:O	1:B:396:LEU:HD13	2.09	0.53
1:A:741:GLN:C	1:A:743:LEU:H	2.17	0.53
1:B:363:SER:HB2	1:B:366:LYS:HB2	1.91	0.53
1:B:468:LEU:HG	1:B:473:TYR:CD1	2.45	0.52
1:B:662:ARG:C	1:B:664:SER:H	2.16	0.52
1:B:410:ALA:HA	1:B:461:ILE:CD1	2.38	0.52
1:A:283:MET:HE3	1:A:360:PHE:CD2	2.44	0.52
1:B:280:GLU:HA	1:B:283:MET:HG2	1.91	0.52
1:B:655:ASN:ND2	1:B:659:GLU:OE2	2.42	0.52
1:B:390:LEU:HB3	1:B:394:ARG:HH12	1.73	0.52
1:A:432:ALA:CB	1:A:437:VAL:HG23	2.40	0.52
1:A:566:PRO:HG2	1:A:567:GLU:H	1.74	0.52
1:B:516:GLN:NE2	1:B:516:GLN:CA	2.73	0.52
1:A:312:THR:O	1:A:396:LEU:HD13	2.10	0.52
1:B:283:MET:HE3	1:B:360:PHE:CD2	2.45	0.52
1:B:634:ALA:HA	1:B:637:ARG:NH2	2.25	0.52
1:A:469:ASN:O	1:A:472:ASP:N	2.40	0.51
1:A:715:TYR:C	1:A:716:THR:HG23	2.35	0.51
1:B:589:TYR:O	1:B:590:ASN:C	2.53	0.51
1:A:417:ALA:O	1:A:418:TYR:C	2.53	0.51
1:A:591:ILE:HG12	1:A:592:ARG:O	2.10	0.51
1:A:592:ARG:O	1:A:593:ILE:HB	2.09	0.51
1:B:316:MET:HE3	1:B:392:GLU:HG3	1.91	0.51
1:B:741:GLN:C	1:B:743:LEU:H	2.18	0.51
1:A:367:MET:CB	1:A:370:ASP:HB2	2.38	0.51
1:A:539:LEU:HD23	1:A:617:LEU:HB2	1.91	0.51
1:A:703:GLN:OE1	1:B:324:ARG:NH1	2.43	0.51
1:A:589:TYR:O	1:A:590:ASN:C	2.53	0.51
1:A:532:MET:O	1:A:536:MET:HG3	2.10	0.51
1:A:516:GLN:CA	1:A:516:GLN:NE2	2.73	0.51
1:A:634:ALA:HA	1:A:637:ARG:NH2	2.26	0.51
1:A:744:THR:HG22	1:A:744:THR:O	2.09	0.51
1:A:399:LEU:HD13	1:A:471:LEU:HB3	1.92	0.50
1:A:548:ILE:O	1:A:552:GLN:HG3	2.11	0.50
1:A:642:PHE:CE1	1:A:695:LEU:HD22	2.46	0.50
1:B:282:LEU:HB3	1:B:348:LEU:CD2	2.42	0.50
1:B:715:TYR:C	1:B:716:THR:HG23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ALA:HA	1:A:461:ILE:CD1	2.42	0.50
1:B:417:ALA:O	1:B:418:TYR:C	2.52	0.50
1:B:642:PHE:CE1	1:B:695:LEU:HD22	2.47	0.50
1:B:733:ARG:HG3	1:B:733:ARG:HH11	1.77	0.50
1:A:544:ILE:HG23	1:A:544:ILE:O	2.10	0.50
1:A:733:ARG:HH11	1:A:733:ARG:HG3	1.76	0.50
1:A:543:PHE:HE1	1:A:628:GLU:HG3	1.77	0.50
1:B:394:ARG:HG3	1:B:394:ARG:NH1	2.27	0.50
1:B:489:GLN:HG2	1:B:493:LEU:HD22	1.94	0.50
1:B:623:GLN:O	1:B:627:GLU:HG3	2.12	0.50
1:B:273:SER:HA	1:B:276:ASN:ND2	2.25	0.50
1:A:457:ARG:O	1:A:461:ILE:HG13	2.12	0.49
1:A:489:GLN:HG2	1:A:493:LEU:HD22	1.93	0.49
1:B:399:LEU:HD13	1:B:471:LEU:HB3	1.93	0.49
1:A:506:ARG:HG3	1:A:506:ARG:HH11	1.76	0.49
1:B:548:ILE:O	1:B:552:GLN:HG3	2.12	0.49
1:A:737:GLU:O	1:A:741:GLN:NE2	2.45	0.49
1:B:594:SER:O	1:B:596:SER:N	2.46	0.49
1:A:623:GLN:O	1:A:627:GLU:HG3	2.13	0.49
1:B:307:ARG:NH1	1:B:385:TYR:HB2	2.27	0.49
1:A:348:LEU:HD12	1:A:360:PHE:CE1	2.47	0.49
1:A:350:THR:HA	1:A:353:ARG:NH1	2.28	0.49
1:B:348:LEU:HD12	1:B:360:PHE:CE1	2.47	0.49
1:B:506:ARG:HG3	1:B:506:ARG:HH11	1.77	0.49
1:A:380:GLN:O	1:A:383:LYS:HB2	2.13	0.49
1:A:468:LEU:HG	1:A:473:TYR:CD1	2.48	0.49
1:A:282:LEU:HB3	1:A:348:LEU:CD2	2.41	0.49
1:A:696:GLU:CD	1:A:717:MET:HE2	2.37	0.49
1:A:615:LYS:O	1:A:619:PRO:HD2	2.12	0.49
1:B:615:LYS:O	1:B:619:PRO:HD2	2.12	0.49
1:B:421:GLU:HG2	1:B:493:LEU:CD1	2.42	0.49
1:A:273:SER:HA	1:A:276:ASN:ND2	2.25	0.49
1:B:296:TRP:C	1:B:298:ARG:N	2.71	0.49
1:B:492:ARG:O	1:B:496:LEU:HB2	2.12	0.49
1:A:307:ARG:NH1	1:A:385:TYR:HB2	2.28	0.48
1:A:394:ARG:HG3	1:A:394:ARG:NH1	2.28	0.48
1:A:427:LYS:O	1:A:428:ASP:C	2.57	0.48
1:B:517:LEU:CB	1:B:582:VAL:HG22	2.43	0.48
1:B:639:ARG:HG2	1:B:710:ASN:CG	2.38	0.48
1:A:352:LEU:HD12	1:A:359:ALA:HA	1.95	0.48
1:A:492:ARG:O	1:A:496:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:SER:C	1:A:596:SER:N	2.71	0.48
1:B:367:MET:CB	1:B:370:ASP:HB2	2.38	0.48
1:B:539:LEU:HD23	1:B:617:LEU:HB2	1.94	0.48
1:B:733:ARG:O	1:B:737:GLU:HG3	2.14	0.48
1:A:639:ARG:HG2	1:A:710:ASN:CG	2.39	0.48
1:B:294:LEU:HD21	1:B:371:ILE:HG12	1.94	0.48
1:B:295:GLU:O	1:B:298:ARG:HB3	2.13	0.48
1:B:348:LEU:HD12	1:B:360:PHE:HE1	1.77	0.48
1:B:350:THR:HA	1:B:353:ARG:NH1	2.28	0.48
1:B:543:PHE:HE1	1:B:628:GLU:HG3	1.79	0.48
1:B:743:LEU:C	1:B:745:ARG:H	2.22	0.48
1:B:380:GLN:O	1:B:383:LYS:HB2	2.13	0.48
1:B:427:LYS:O	1:B:428:ASP:C	2.57	0.48
1:B:352:LEU:HD12	1:B:359:ALA:HA	1.95	0.48
1:B:357:ARG:O	1:B:358:PRO:C	2.57	0.48
1:A:294:LEU:HD21	1:A:371:ILE:HG12	1.95	0.48
1:A:295:GLU:O	1:A:298:ARG:HB3	2.14	0.48
1:A:348:LEU:HD12	1:A:360:PHE:HE1	1.78	0.48
1:A:357:ARG:O	1:A:358:PRO:C	2.57	0.48
1:A:594:SER:O	1:A:596:SER:N	2.46	0.47
1:B:696:GLU:CD	1:B:717:MET:HE2	2.39	0.47
1:B:362:PRO:O	1:B:363:SER:C	2.57	0.47
1:B:427:LYS:O	1:B:429:TYR:N	2.47	0.47
1:A:427:LYS:O	1:A:429:TYR:N	2.48	0.47
1:A:517:LEU:CB	1:A:582:VAL:HG22	2.42	0.47
1:B:281:ARG:HG3	1:B:282:LEU:CD1	2.45	0.47
1:B:303:TRP:HE3	1:B:304:LEU:HD22	1.80	0.47
1:A:362:PRO:O	1:A:363:SER:C	2.58	0.47
1:A:733:ARG:O	1:A:737:GLU:HG3	2.14	0.47
1:B:341:LEU:C	1:B:343:ILE:N	2.73	0.47
1:B:432:ALA:CB	1:B:437:VAL:HG23	2.44	0.47
1:B:737:GLU:O	1:B:741:GLN:NE2	2.47	0.47
1:A:303:TRP:HE3	1:A:304:LEU:HD22	1.80	0.47
1:B:316:MET:HE3	1:B:392:GLU:HB3	1.95	0.47
1:B:544:ILE:HG23	1:B:544:ILE:O	2.15	0.47
1:A:696:GLU:HG2	1:B:328:ARG:CG	2.44	0.47
1:B:613:LYS:O	1:B:614:VAL:C	2.56	0.47
1:B:304:LEU:HD22	1:B:304:LEU:N	2.30	0.47
1:A:304:LEU:HD22	1:A:304:LEU:N	2.30	0.47
1:B:451:LEU:C	1:B:451:LEU:HD13	2.40	0.47
1:B:594:SER:C	1:B:596:SER:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ARG:HG3	1:A:282:LEU:CD1	2.45	0.46
1:A:316:MET:HE3	1:A:392:GLU:HB3	1.97	0.46
1:B:526:ALA:CB	1:B:527:PRO:HD3	2.26	0.46
1:B:585:VAL:CG2	1:B:586:ILE:N	2.78	0.46
1:B:715:TYR:O	1:B:716:THR:HG23	2.15	0.46
1:B:496:LEU:HD12	1:B:496:LEU:HA	1.74	0.46
1:A:743:LEU:C	1:A:745:ARG:H	2.22	0.46
1:A:318:LYS:HD2	1:A:318:LYS:O	2.15	0.46
1:A:585:VAL:CG2	1:A:586:ILE:N	2.78	0.46
1:A:694:LYS:O	1:A:695:LEU:C	2.56	0.46
1:A:706:LEU:HD11	1:B:317:GLN:NE2	2.30	0.46
1:B:716:THR:O	1:B:717:MET:C	2.59	0.46
1:A:278:GLU:CA	1:A:281:ARG:HG2	2.43	0.46
1:A:464:ILE:O	1:A:468:LEU:HB2	2.16	0.45
1:A:341:LEU:C	1:A:343:ILE:N	2.73	0.45
1:A:585:VAL:HG23	1:A:586:ILE:N	2.32	0.45
1:B:304:LEU:O	1:B:306:ASN:N	2.49	0.45
1:A:296:TRP:C	1:A:298:ARG:N	2.71	0.45
1:A:304:LEU:HD22	1:A:304:LEU:H	1.81	0.45
1:A:304:LEU:O	1:A:306:ASN:N	2.48	0.45
1:A:545:VAL:CG1	1:A:550:GLU:HB3	2.47	0.45
1:B:346:ASN:HA	1:B:349:GLN:HB2	1.99	0.45
1:A:575:ILE:HG22	1:A:604:MET:CE	2.29	0.45
1:B:518:HIS:HA	1:B:597:ASN:ND2	2.31	0.45
1:A:340:GLN:O	1:A:343:ILE:HB	2.17	0.45
1:B:304:LEU:HD22	1:B:304:LEU:H	1.82	0.45
1:B:357:ARG:O	1:B:357:ARG:CG	2.60	0.45
1:A:565:LEU:N	1:A:566:PRO:CD	2.80	0.45
1:B:335:VAL:HG22	1:B:375:TRP:CZ2	2.51	0.45
1:B:457:ARG:O	1:B:461:ILE:HG13	2.17	0.45
1:B:575:ILE:HG22	1:B:604:MET:CE	2.28	0.45
1:A:421:GLU:HG2	1:A:493:LEU:CD1	2.43	0.45
1:A:715:TYR:O	1:A:716:THR:HG23	2.16	0.45
1:B:344:ASN:C	1:B:346:ASN:H	2.25	0.45
1:B:382:GLU:O	1:B:383:LYS:C	2.60	0.45
1:B:718:GLU:O	1:B:719:HIS:C	2.60	0.45
1:A:548:ILE:HD13	1:A:633:HIS:CE1	2.52	0.44
1:B:402:LEU:HD11	1:B:467:GLU:CD	2.42	0.44
1:B:543:PHE:CD1	1:B:543:PHE:C	2.95	0.44
1:B:565:LEU:N	1:B:566:PRO:CD	2.77	0.44
1:A:335:VAL:HG22	1:A:375:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:VAL:CG1	1:B:550:GLU:HB3	2.48	0.44
1:A:346:ASN:HA	1:A:349:GLN:HB2	1.99	0.44
1:B:278:GLU:CA	1:B:281:ARG:HG2	2.43	0.44
1:B:340:GLN:O	1:B:343:ILE:HB	2.16	0.44
1:A:454:HIS:O	1:A:455:GLN:C	2.61	0.44
1:B:402:LEU:HB3	1:B:468:LEU:HD13	2.00	0.44
1:B:671:LEU:O	1:B:672:GLU:C	2.58	0.44
1:A:671:LEU:O	1:A:672:GLU:C	2.59	0.44
1:A:344:ASN:C	1:A:346:ASN:H	2.26	0.44
1:A:518:HIS:HA	1:A:597:ASN:ND2	2.33	0.44
1:A:357:ARG:O	1:A:357:ARG:CG	2.61	0.44
1:A:639:ARG:NH1	1:A:709:ASP:OD1	2.51	0.44
1:B:318:LYS:HD2	1:B:318:LYS:O	2.18	0.44
1:A:303:TRP:C	1:A:304:LEU:O	2.58	0.43
1:A:419:GLY:O	1:A:423:ILE:HG23	2.18	0.43
1:B:585:VAL:O	1:B:589:TYR:CD2	2.71	0.43
1:B:585:VAL:HG23	1:B:586:ILE:N	2.32	0.43
1:A:589:TYR:HB2	1:A:591:ILE:CG2	2.45	0.43
1:B:423:ILE:HD12	1:B:423:ILE:O	2.18	0.43
1:A:371:ILE:O	1:A:371:ILE:HG22	2.19	0.43
1:A:743:LEU:HD12	1:B:354:ILE:CD1	2.48	0.43
1:B:468:LEU:HD12	1:B:468:LEU:HA	1.87	0.43
1:B:625:LEU:HD12	1:B:625:LEU:HA	1.90	0.43
1:A:296:TRP:HA	1:A:299:ARG:HG2	2.00	0.43
1:A:313:MET:HB2	1:A:396:LEU:HB3	2.01	0.43
1:A:328:ARG:CG	1:B:696:GLU:HG2	2.46	0.43
1:B:290:ALA:HB3	1:B:366:LYS:HZ1	1.84	0.43
1:A:451:LEU:HD13	1:A:451:LEU:C	2.42	0.43
1:B:514:ILE:HD13	1:B:586:ILE:HG12	2.01	0.43
1:B:388:TRP:O	1:B:389:LEU:C	2.62	0.43
1:B:408:GLN:O	1:B:412:THR:HG23	2.19	0.43
1:B:594:SER:C	1:B:596:SER:H	2.27	0.43
1:A:521:PHE:CD1	1:A:521:PHE:C	2.97	0.43
1:A:585:VAL:O	1:A:589:TYR:CD2	2.70	0.43
1:B:579:GLN:HG3	1:B:583:GLU:OE2	2.19	0.43
1:A:352:LEU:CD1	1:A:359:ALA:HA	2.49	0.43
1:A:388:TRP:O	1:A:389:LEU:C	2.62	0.43
1:B:303:TRP:C	1:B:304:LEU:O	2.57	0.43
1:A:303:TRP:CZ3	1:A:304:LEU:HD13	2.54	0.43
1:A:514:ILE:HD13	1:A:586:ILE:HG12	2.00	0.43
1:A:670:ALA:HB1	1:A:671:LEU:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:LEU:HD12	1:B:354:ILE:HD12	2.01	0.43
1:B:303:TRP:CE3	1:B:304:LEU:HD13	2.54	0.43
1:B:313:MET:HB2	1:B:396:LEU:HB3	2.01	0.43
1:B:433:SER:N	1:B:436:GLU:OE1	2.51	0.42
1:A:347:THR:O	1:A:347:THR:HG22	2.19	0.42
1:A:579:GLN:HG3	1:A:583:GLU:OE2	2.19	0.42
1:B:296:TRP:C	1:B:298:ARG:H	2.27	0.42
1:A:286:TYR:OH	1:A:368:VAL:HG13	2.20	0.42
1:A:543:PHE:C	1:A:543:PHE:CD1	2.96	0.42
1:B:352:LEU:CD1	1:B:359:ALA:HA	2.49	0.42
1:B:371:ILE:O	1:B:371:ILE:HG22	2.19	0.42
1:A:368:VAL:HG12	1:A:368:VAL:O	2.19	0.42
1:A:693:ASP:O	1:A:694:LYS:C	2.59	0.42
1:B:287:GLU:OE1	1:B:362:PRO:HB2	2.19	0.42
1:B:454:HIS:O	1:B:455:GLN:C	2.59	0.42
1:B:695:LEU:HD23	1:B:695:LEU:HA	1.84	0.42
1:A:715:TYR:O	1:A:716:THR:OG1	2.36	0.42
1:A:716:THR:O	1:A:717:MET:C	2.63	0.42
1:B:368:VAL:O	1:B:368:VAL:HG12	2.20	0.42
1:A:296:TRP:C	1:A:298:ARG:H	2.27	0.42
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.84	0.42
1:B:303:TRP:CZ3	1:B:304:LEU:HD13	2.54	0.42
1:A:287:GLU:OE1	1:A:362:PRO:HB2	2.20	0.42
1:A:328:ARG:HG3	1:B:696:GLU:CD	2.45	0.42
1:A:493:LEU:HD12	1:A:493:LEU:HA	1.83	0.42
1:A:593:ILE:N	1:A:593:ILE:HD12	2.35	0.42
1:A:613:LYS:O	1:A:614:VAL:C	2.61	0.42
1:B:296:TRP:HA	1:B:299:ARG:HG2	2.00	0.42
1:B:347:THR:HG22	1:B:347:THR:O	2.20	0.42
1:B:450:ASP:O	1:B:453:ALA:HB3	2.20	0.42
1:B:603:THR:O	1:B:607:LEU:HB2	2.20	0.42
1:A:300:THR:C	1:A:302:PRO:CD	2.91	0.42
1:A:307:ARG:HG3	1:A:388:TRP:CD2	2.55	0.42
1:A:316:MET:HE3	1:A:392:GLU:CG	2.50	0.42
1:A:382:GLU:O	1:A:383:LYS:C	2.61	0.42
1:A:423:ILE:HD12	1:A:423:ILE:O	2.20	0.42
1:B:319:LYS:CG	1:B:389:LEU:HD21	2.49	0.42
1:B:376:GLN:NE2	1:B:376:GLN:CA	2.79	0.42
1:A:294:LEU:O	1:A:297:ILE:HG13	2.20	0.41
1:A:303:TRP:CE3	1:A:304:LEU:HD13	2.54	0.41
1:A:402:LEU:HD11	1:A:467:GLU:CD	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ARG:CZ	1:A:733:ARG:HB2	2.50	0.41
1:B:286:TYR:OH	1:B:368:VAL:HG13	2.20	0.41
1:B:406:PHE:O	1:B:407:ARG:C	2.63	0.41
1:B:521:PHE:CD1	1:B:521:PHE:C	2.98	0.41
1:A:317:GLN:NE2	1:B:706:LEU:HD11	2.31	0.41
1:A:350:THR:CG2	1:A:353:ARG:HH12	2.19	0.41
1:A:715:TYR:O	1:A:716:THR:CB	2.68	0.41
1:B:307:ARG:HG3	1:B:388:TRP:CD2	2.56	0.41
1:B:526:ALA:CB	1:B:527:PRO:CD	2.91	0.41
1:B:693:ASP:O	1:B:694:LYS:C	2.63	0.41
1:A:281:ARG:HG3	1:A:282:LEU:HD12	2.03	0.41
1:B:316:MET:HE3	1:B:392:GLU:CG	2.50	0.41
1:B:641:GLN:O	1:B:645:GLN:HG3	2.21	0.41
1:B:715:TYR:O	1:B:716:THR:CB	2.69	0.41
1:A:506:ARG:HG3	1:A:506:ARG:NH1	2.34	0.41
1:B:296:TRP:CE3	1:B:334:LYS:HG2	2.56	0.41
1:B:301:ILE:HG12	1:B:378:LEU:HA	2.03	0.41
1:B:356:ASN:O	1:B:357:ARG:HB3	2.20	0.41
1:A:287:GLU:CD	1:A:362:PRO:HB2	2.46	0.41
1:A:319:LYS:CG	1:A:389:LEU:HD21	2.49	0.41
1:A:406:PHE:O	1:A:407:ARG:C	2.63	0.41
1:A:594:SER:C	1:A:596:SER:H	2.27	0.41
1:A:603:THR:O	1:A:607:LEU:HB2	2.20	0.41
1:B:733:ARG:O	1:B:736:ASN:HB3	2.21	0.41
1:A:296:TRP:CE3	1:A:334:LYS:HG2	2.55	0.41
1:A:332:PRO:N	1:A:333:PRO:HD2	2.36	0.41
1:A:433:SER:N	1:A:436:GLU:OE1	2.50	0.41
1:A:508:GLU:O	1:A:512:GLU:HB2	2.21	0.41
1:B:434:LEU:CD2	1:B:438:ARG:NH2	2.81	0.41
1:B:506:ARG:HG3	1:B:506:ARG:NH1	2.35	0.41
1:B:562:LYS:HD3	1:B:618:VAL:CG1	2.50	0.41
1:B:361:MET:HA	1:B:362:PRO:HD2	1.91	0.41
1:B:656:LYS:CE	1:B:684:ASN:HD22	2.34	0.41
1:A:300:THR:O	1:A:304:LEU:HD23	2.21	0.41
1:A:390:LEU:O	1:A:393:ILE:N	2.54	0.41
1:A:425:LEU:HD21	1:A:496:LEU:HD11	2.02	0.41
1:A:450:ASP:O	1:A:453:ALA:HB3	2.21	0.41
1:A:468:LEU:HD12	1:A:468:LEU:HA	1.85	0.41
1:B:294:LEU:O	1:B:297:ILE:HG13	2.21	0.41
1:B:298:ARG:HH11	1:B:298:ARG:HG2	1.86	0.41
1:B:438:ARG:CD	1:B:508:GLU:OE2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:LEU:O	1:B:674:GLN:N	2.53	0.41
1:A:301:ILE:HG12	1:A:378:LEU:HA	2.03	0.41
1:A:408:GLN:O	1:A:412:THR:HG23	2.21	0.41
1:A:619:PRO:O	1:A:623:GLN:HB2	2.21	0.41
1:B:281:ARG:HG3	1:B:282:LEU:HD12	2.03	0.41
1:B:302:PRO:O	1:B:304:LEU:O	2.40	0.41
1:B:589:TYR:HB2	1:B:591:ILE:CG2	2.44	0.41
1:B:619:PRO:O	1:B:623:GLN:HB2	2.21	0.41
1:A:309:PRO:HA	1:A:316:MET:HE1	2.03	0.40
1:A:562:LYS:HD3	1:A:618:VAL:CG1	2.51	0.40
1:A:696:GLU:OE2	1:A:721:ARG:NH2	2.47	0.40
1:B:287:GLU:CD	1:B:362:PRO:HB2	2.45	0.40
1:B:423:ILE:HD12	1:B:423:ILE:C	2.47	0.40
1:B:466:GLN:O	1:B:469:ASN:HB2	2.21	0.40
1:B:593:ILE:O	1:B:593:ILE:HG22	2.22	0.40
1:A:280:GLU:O	1:A:283:MET:HG2	2.21	0.40
1:A:308:THR:HA	1:A:309:PRO:HD2	1.89	0.40
1:A:434:LEU:CD2	1:A:438:ARG:NH2	2.81	0.40
1:B:508:GLU:O	1:B:512:GLU:HB2	2.21	0.40
1:A:641:GLN:O	1:A:645:GLN:HG3	2.22	0.40
1:A:438:ARG:CD	1:A:508:GLU:OE2	2.70	0.40
1:A:535:ALA:O	1:A:536:MET:C	2.63	0.40
1:A:656:LYS:CE	1:A:684:ASN:HD22	2.35	0.40
1:B:276:ASN:O	1:B:280:GLU:HG3	2.22	0.40
1:B:300:THR:O	1:B:304:LEU:HD23	2.22	0.40
1:B:350:THR:CG2	1:B:353:ARG:HH12	2.19	0.40
1:B:375:TRP:C	1:B:377:ARG:N	2.79	0.40

There are no symmetry-related clashes.

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	473/476 (99%)	385 (81%)	64 (14%)	24 (5%)	1	5
1	B	473/476 (99%)	386 (82%)	62 (13%)	25 (5%)	1	5
All	All	946/952 (99%)	771 (82%)	126 (13%)	49 (5%)	1	5

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	SER
1	A	356	ASN
1	A	358	PRO
1	A	362	PRO
1	A	363	SER
1	A	383	LYS
1	A	428	ASP
1	A	665	ILE
1	A	670	ALA
1	B	355	SER
1	B	356	ASN
1	B	358	PRO
1	B	362	PRO
1	B	363	SER
1	B	383	LYS
1	B	428	ASP
1	B	665	ILE
1	B	670	ALA
1	A	309	PRO
1	A	311	LYS
1	A	359	ALA
1	A	595	SER
1	A	742	ILE
1	B	309	PRO
1	B	311	LYS
1	B	359	ALA
1	B	595	SER
1	B	742	ILE
1	A	306	ASN
1	A	367	MET
1	A	592	ARG
1	A	663	SER
1	A	666	GLN
1	B	306	ASN
1	B	367	MET

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Mol	Chain	Res	Type
1	B	592	ARG
1	B	663	SER
1	B	666	GLN
1	A	366	LYS
1	A	590	ASN
1	B	366	LYS
1	B	590	ASN
1	A	357	ARG
1	A	593	ILE
1	B	357	ARG
1	B	470	GLU
1	B	593	ILE
1	A	716	THR
1	B	716	THR

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	426/426 (100%)	382 (90%)	44 (10%)	7	23
1	B	426/426 (100%)	382 (90%)	44 (10%)	7	23
All	All	852/852 (100%)	764 (90%)	88 (10%)	7	23

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	LEU
1	A	304	LEU
1	A	314	GLN
1	A	320	LEU
1	A	328	ARG
1	A	341	LEU
1	A	343	ILE
1	A	348	LEU
1	A	358	PRO

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Mol	Chain	Res	Type
1	A	361	MET
1	A	370	ASP
1	A	420	LYS
1	A	423	ILE
1	A	438	ARG
1	A	468	LEU
1	A	477	VAL
1	A	479	VAL
1	A	493	LEU
1	A	496	LEU
1	A	497	THR
1	A	516	GLN
1	A	554	LEU
1	A	567	GLU
1	A	587	GLN
1	A	591	ILE
1	A	592	ARG
1	A	601	THR
1	A	610	LYS
1	A	613	LYS
1	A	623	GLN
1	A	625	LEU
1	A	631	ARG
1	A	639	ARG
1	A	671	LEU
1	A	676	ASN
1	A	693	ASP
1	A	694	LYS
1	A	695	LEU
1	A	701	LEU
1	A	702	ILE
1	A	731	ILE
1	A	741	GLN
1	A	743	LEU
1	A	745	ARG
1	B	289	LEU
1	B	304	LEU
1	B	314	GLN
1	B	320	LEU
1	B	328	ARG
1	B	341	LEU
1	B	343	ILE

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Mol	Chain	Res	Type
1	B	348	LEU
1	B	358	PRO
1	B	361	MET
1	B	370	ASP
1	B	420	LYS
1	B	423	ILE
1	B	438	ARG
1	B	468	LEU
1	B	477	VAL
1	B	479	VAL
1	B	493	LEU
1	B	496	LEU
1	B	497	THR
1	B	516	GLN
1	B	554	LEU
1	B	567	GLU
1	B	587	GLN
1	B	591	ILE
1	B	592	ARG
1	B	601	THR
1	B	610	LYS
1	B	613	LYS
1	B	623	GLN
1	B	625	LEU
1	B	631	ARG
1	B	639	ARG
1	B	671	LEU
1	B	676	ASN
1	B	693	ASP
1	B	694	LYS
1	B	695	LEU
1	B	701	LEU
1	B	702	ILE
1	B	731	ILE
1	B	741	GLN
1	B	743	LEU
1	B	745	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	317	GLN
1	A	344	ASN
1	A	346	ASN
1	A	376	GLN
1	A	401	HIS
1	A	408	GLN
1	A	426	GLN
1	A	460	GLN
1	A	466	GLN
1	A	469	ASN
1	A	484	GLN
1	A	516	GLN
1	A	540	GLN
1	A	579	GLN
1	A	580	ASN
1	A	587	GLN
1	A	597	ASN
1	A	616	GLN
1	A	641	GLN
1	A	645	GLN
1	A	684	ASN
1	A	700	GLN
1	A	736	ASN
1	A	741	GLN
1	B	276	ASN
1	B	306	ASN
1	B	317	GLN
1	B	344	ASN
1	B	346	ASN
1	B	376	GLN
1	B	401	HIS
1	B	408	GLN
1	B	426	GLN
1	B	466	GLN
1	B	480	ASN
1	B	484	GLN
1	B	516	GLN
1	B	530	ASN
1	B	540	GLN
1	B	579	GLN
1	B	580	ASN

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Mol	Chain	Res	Type
1	B	587	GLN
1	B	597	ASN
1	B	616	GLN
1	B	635	ASN
1	B	641	GLN
1	B	645	GLN
1	B	684	ASN
1	B	700	GLN
1	B	736	ASN
1	B	741	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	475/476 (99%)	-0.93	6 (1%) 75 66	39, 64, 131, 156	0
1	B	475/476 (99%)	-0.87	8 (1%) 69 60	33, 64, 132, 156	0
All	All	950/952 (99%)	-0.90	14 (1%) 72 63	33, 64, 132, 156	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	SER	4.5
1	B	358	PRO	4.3
1	B	275	VAL	4.0
1	A	365	GLY	3.9
1	A	364	GLU	3.5
1	A	275	VAL	3.2
1	B	274	ALA	3.1
1	A	274	ALA	2.8
1	B	365	GLY	2.8
1	B	364	GLU	2.7
1	B	279	ASN	2.5
1	A	358	PRO	2.4
1	A	273	SER	2.2
1	B	276	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.