



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:15 AM UTC

PDB ID : 4AM6 / pdb_00004am6
Title : C-TERMINAL DOMAIN OF ACTIN-RELATED PROTEIN ARP8 FROM S. CEREVISIAE
Authors : Wuerges, J.; Saravanan, M.; Bose, D.; Cook, N.J.; Zhang, X.; Wigley, D.B.
Deposited on : 2012-03-07
Resolution : 2.70 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

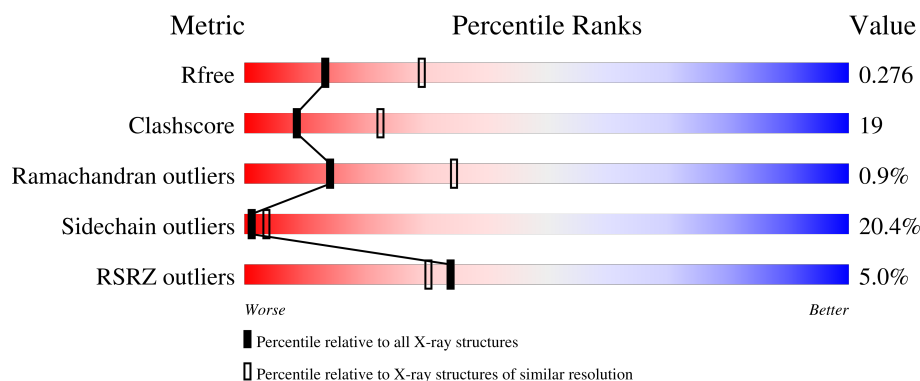
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	655	5% 52% 33% 8% • 5%
1	B	655	5% 53% 31% 9% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10114 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 ACTIN-LIKE PROTEIN ARP8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	0	0
			5036	3219	840	963	14			
1	B	623	Total	C	N	O	S	0	0	0
			5036	3219	840	963	14			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	expression tag	UNP Q12386
A	228	GLY	-	expression tag	UNP Q12386
A	229	SER	-	expression tag	UNP Q12386
A	230	SER	-	expression tag	UNP Q12386
A	231	HIS	-	expression tag	UNP Q12386
A	232	HIS	-	expression tag	UNP Q12386
A	233	HIS	-	expression tag	UNP Q12386
A	234	HIS	-	expression tag	UNP Q12386
A	235	HIS	-	expression tag	UNP Q12386
A	236	HIS	-	expression tag	UNP Q12386
A	237	SER	-	expression tag	UNP Q12386
A	238	SER	-	expression tag	UNP Q12386
A	239	GLY	-	expression tag	UNP Q12386
A	240	LEU	-	expression tag	UNP Q12386
A	241	VAL	-	expression tag	UNP Q12386
A	242	PRO	-	expression tag	UNP Q12386
A	243	ARG	-	expression tag	UNP Q12386
A	244	GLY	-	expression tag	UNP Q12386
A	245	SER	-	expression tag	UNP Q12386
A	246	HIS	-	expression tag	UNP Q12386
A	247	MET	-	expression tag	UNP Q12386
B	227	MET	-	expression tag	UNP Q12386
B	228	GLY	-	expression tag	UNP Q12386
B	229	SER	-	expression tag	UNP Q12386
B	230	SER	-	expression tag	UNP Q12386

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	HIS	-	expression tag	UNP Q12386
B	232	HIS	-	expression tag	UNP Q12386
B	233	HIS	-	expression tag	UNP Q12386
B	234	HIS	-	expression tag	UNP Q12386
B	235	HIS	-	expression tag	UNP Q12386
B	236	HIS	-	expression tag	UNP Q12386
B	237	SER	-	expression tag	UNP Q12386
B	238	SER	-	expression tag	UNP Q12386
B	239	GLY	-	expression tag	UNP Q12386
B	240	LEU	-	expression tag	UNP Q12386
B	241	VAL	-	expression tag	UNP Q12386
B	242	PRO	-	expression tag	UNP Q12386
B	243	ARG	-	expression tag	UNP Q12386
B	244	GLY	-	expression tag	UNP Q12386
B	245	SER	-	expression tag	UNP Q12386
B	246	HIS	-	expression tag	UNP Q12386
B	247	MET	-	expression tag	UNP Q12386

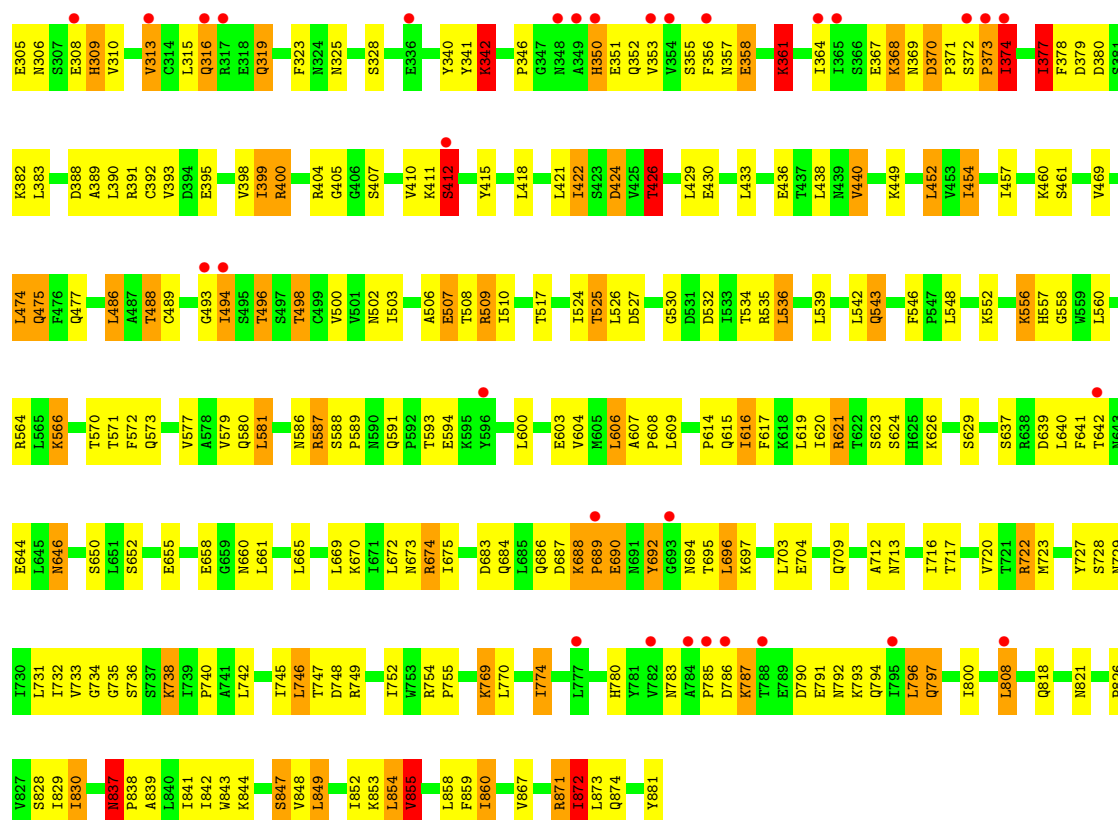
- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	14	Total 14	O 14	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.20Å 87.86Å 149.37Å 90.00° 115.40° 90.00°	Depositor
Resolution (Å)	28.89 – 2.70 28.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.89-2.70) 98.8 (28.89-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.223 , 0.286 0.221 , 0.276	Depositor DCC
R_{free} test set	2190 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10114	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.09	13/5149 (0.3%)	1.30	42/6982 (0.6%)
1	B	0.93	5/5149 (0.1%)	1.18	30/6982 (0.4%)
All	All	1.01	18/10298 (0.2%)	1.24	72/13964 (0.5%)

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	2
1	B	0	1
All	All	0	3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	VAL	CA-C	12.24	1.63	1.52
1	A	331	GLU	CD-OE1	9.04	1.42	1.25
1	A	344	LYS	CE-NZ	8.67	1.75	1.49
1	A	331	GLU	CD-OE2	7.71	1.40	1.25
1	B	494	ILE	CA-CB	7.34	1.64	1.54
1	A	494	ILE	CA-CB	6.70	1.63	1.54
1	A	321	GLU	C-O	6.51	1.31	1.24
1	A	327	LYS	CA-C	6.38	1.61	1.52
1	A	324	ASN	C-O	6.26	1.31	1.24
1	A	291	VAL	CA-CB	-6.20	1.48	1.54
1	A	371	PRO	N-CA	5.55	1.51	1.46
1	A	354	VAL	CA-CB	5.44	1.61	1.54
1	B	848	VAL	CA-CB	5.42	1.60	1.54
1	A	610	ALA	CA-CB	-5.38	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	ILE	CA-CB	5.32	1.59	1.54
1	B	412	SER	N-CA	5.26	1.51	1.45
1	A	341	TYR	CA-C	5.14	1.57	1.52
1	B	260	ILE	CA-CB	5.10	1.59	1.54

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	HIS	N-CA-C	12.48	126.90	109.18
1	A	342	LYS	N-CA-C	12.35	129.74	111.34
1	A	754	ARG	CA-C-N	-9.03	111.09	120.03
1	A	754	ARG	C-N-CA	-9.03	111.09	120.03
1	A	316	GLN	N-CA-C	8.88	122.29	107.20
1	B	790	ASP	N-CA-C	8.53	123.25	111.74
1	A	345	VAL	CA-C-N	8.48	128.61	119.28
1	A	345	VAL	C-N-CA	8.48	128.61	119.28
1	B	297	VAL	N-CA-C	8.06	116.67	107.89
1	B	440	VAL	N-CA-C	7.57	117.60	106.85
1	A	361	LYS	N-CA-C	-7.30	99.42	110.01
1	A	308	GLU	CB-CA-C	-7.27	108.18	116.54
1	B	370	ASP	N-CA-C	7.08	125.46	109.81
1	A	691	ASN	N-CA-C	-7.08	104.22	112.92
1	B	872	ILE	CB-CA-C	-7.05	101.22	112.16
1	A	872	ILE	CB-CA-C	-7.01	101.29	112.16
1	A	369	ASN	N-CA-C	6.90	118.80	108.31
1	A	486	LEU	N-CA-C	-6.85	103.27	111.69
1	A	791	GLU	N-CA-C	-6.81	106.86	114.62
1	B	474	LEU	N-CA-C	-6.68	104.95	113.23
1	B	493	GLY	N-CA-C	-6.65	97.43	113.18
1	A	830	ILE	CA-C-N	-6.39	113.79	120.38
1	A	830	ILE	C-N-CA	-6.39	113.79	120.38
1	B	342	LYS	N-CA-C	6.10	123.79	110.80
1	B	319	GLN	N-CA-C	6.03	119.20	109.79
1	B	837	ASN	N-CA-C	6.03	123.14	109.81
1	A	361	LYS	CB-CA-C	6.01	120.31	109.61
1	B	855	VAL	CB-CA-C	-5.98	102.89	112.16
1	A	371	PRO	N-CA-C	5.97	121.66	111.03
1	A	746	LEU	N-CA-C	-5.79	105.05	111.36
1	B	361	LYS	N-CA-C	5.75	117.83	109.84
1	A	790	ASP	N-CA-C	5.74	117.73	107.80
1	B	291	VAL	N-CA-C	5.74	113.23	107.55
1	A	315	LEU	N-CA-C	5.73	115.59	108.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	CA-C-N	5.72	125.39	119.56
1	A	264	ASP	C-N-CA	5.72	125.39	119.56
1	A	837	ASN	CA-C-N	-5.70	113.94	119.87
1	A	837	ASN	C-N-CA	-5.70	113.94	119.87
1	A	388	ASP	N-CA-C	-5.69	105.15	111.36
1	B	424	ASP	N-CA-C	5.65	117.89	111.11
1	B	306	ASN	N-CA-C	5.62	122.25	113.72
1	B	650	SER	N-CA-C	5.62	118.69	109.76
1	A	438	LEU	CA-C-N	-5.61	115.51	123.03
1	A	438	LEU	C-N-CA	-5.61	115.51	123.03
1	B	299	LYS	N-CA-C	-5.53	106.03	112.89
1	A	377	ILE	N-CA-C	5.52	115.54	107.37
1	B	377	ILE	N-CA-C	5.50	116.20	108.17
1	A	261	ASP	N-CA-C	5.50	117.62	107.73
1	A	865	TRP	N-CA-C	5.47	118.16	111.82
1	B	426	THR	N-CA-CB	5.44	118.31	110.20
1	A	342	LYS	CB-CA-C	-5.38	104.08	112.31
1	B	407	SER	N-CA-CB	-5.36	102.60	110.85
1	A	871	ARG	N-CA-C	5.35	119.30	112.34
1	A	324	ASN	CB-CA-C	5.35	119.20	110.96
1	B	690	GLU	CB-CA-C	5.35	119.11	109.64
1	B	786	ASP	N-CA-C	5.35	117.12	108.41
1	A	394	ASP	N-CA-C	5.28	119.59	113.20
1	A	693	GLY	N-CA-C	-5.26	100.71	113.18
1	A	353	VAL	N-CA-C	-5.26	104.63	110.62
1	B	289	VAL	N-CA-CB	5.24	116.24	110.53
1	B	525	THR	CB-CA-C	5.24	118.52	110.14
1	B	546	PHE	CA-C-N	5.23	124.94	119.82
1	B	546	PHE	C-N-CA	5.23	124.94	119.82
1	A	286	ASP	N-CA-C	-5.18	104.89	111.11
1	A	732	ILE	N-CA-C	5.15	115.38	108.17
1	A	488	THR	N-CA-CB	5.14	118.24	110.28
1	B	374	ILE	N-CA-C	5.13	115.66	108.89
1	B	412	SER	N-CA-CB	5.12	118.37	109.57
1	B	405	GLY	CA-C-N	-5.11	114.58	122.86
1	B	405	GLY	C-N-CA	-5.11	114.58	122.86
1	A	454	ILE	N-CA-CB	-5.03	104.17	111.21
1	A	310	VAL	N-CA-C	-5.00	98.93	109.34

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	ALA	Peptide
1	A	587	ARG	Peptide
1	B	342	LYS	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	5036	0	4985	216	0
1	B	5036	0	4985	164	0
2	A	10	0	0	1	0
3	A	18	0	0	2	0
3	B	14	0	0	0	0
All	All	10114	0	9970	376	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 19.

All (376) 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:344:LYS:CE	1:A:344:LYS:NZ	1.75	1.46
1:A:785:PRO:HB2	1:A:793:LYS:HD2	1.21	1.19
1:A:488:THR:HG22	1:A:842:ILE:CD1	1.79	1.11
1:A:315:LEU:HD23	1:A:316:GLN:N	1.66	1.09
1:A:315:LEU:CG	1:A:316:GLN:H	1.71	1.03
1:A:315:LEU:CD2	1:A:316:GLN:N	2.25	1.00
1:A:315:LEU:HG	1:A:316:GLN:H	1.23	0.99
1:A:355:SER:HB3	1:A:547:PRO:HB3	1.44	0.98
1:A:488:THR:HG22	1:A:842:ILE:HD13	1.46	0.96
1:B:488:THR:HG22	1:B:842:ILE:HG12	1.48	0.94
1:B:738:LYS:H	1:B:738:LYS:HD3	1.31	0.93
1:B:642:THR:HG22	1:B:644:GLU:HB2	1.49	0.92
1:B:374:ILE:HD12	1:B:374:ILE:H	1.33	0.92
1:B:372:SER:HB2	1:B:373:PRO:HD2	1.52	0.91
1:B:316:GLN:HE21	1:B:316:GLN:HA	1.35	0.90
1:A:372:SER:HB3	1:A:373:PRO:HD2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLN:HA	1:B:316:GLN:NE2	1.85	0.89
1:A:490:TYR:HE1	1:A:494:ILE:HD12	1.37	0.88
1:A:372:SER:HB3	1:A:373:PRO:CD	2.03	0.87
1:B:488:THR:HG22	1:B:842:ILE:CG1	2.04	0.87
1:A:315:LEU:CD2	1:A:316:GLN:H	1.84	0.87
1:A:785:PRO:HB2	1:A:793:LYS:CD	2.07	0.85
1:B:684:GLN:O	1:B:688:LYS:HB2	1.78	0.83
1:A:785:PRO:CB	1:A:793:LYS:HD2	2.10	0.79
1:A:490:TYR:CE1	1:A:494:ILE:HD12	2.17	0.79
1:A:315:LEU:CG	1:A:316:GLN:N	2.38	0.78
1:B:502:ASN:HD22	1:B:502:ASN:C	1.92	0.77
1:B:452:LEU:HD13	1:B:454:ILE:CD1	2.15	0.77
1:A:488:THR:CG2	1:A:842:ILE:CD1	2.62	0.76
1:A:795:ILE:HA	1:A:798:ALA:HB3	1.67	0.76
1:A:769:LYS:NZ	1:A:808:LEU:HD11	2.02	0.75
1:A:735:GLY:O	1:A:738:LYS:HD2	1.85	0.74
1:A:836:MET:HE3	1:A:844:LYS:HZ3	1.52	0.74
1:A:315:LEU:HD23	1:A:315:LEU:C	2.12	0.73
1:A:315:LEU:HG	1:A:316:GLN:N	1.98	0.73
1:A:488:THR:HG22	1:A:842:ILE:HD11	1.67	0.73
1:A:392:CYS:O	1:A:556:LYS:NZ	2.21	0.72
1:B:400:ARG:HD2	1:B:424:ASP:OD2	1.88	0.72
1:A:849:LEU:HD22	1:A:855:VAL:HG13	1.70	0.72
1:B:661:LEU:HD23	1:B:709:GLN:HG3	1.69	0.72
1:B:418:LEU:HG	1:B:422:ILE:HD12	1.71	0.72
1:A:817:HIS:HD2	1:A:818:GLN:N	1.87	0.71
1:A:661:LEU:HD23	1:A:709:GLN:HG3	1.73	0.71
1:B:642:THR:CG2	1:B:644:GLU:HB2	2.19	0.71
1:B:733:VAL:HG22	1:B:841:ILE:HD12	1.72	0.71
1:A:427:LYS:NZ	1:B:867:VAL:O	2.21	0.70
1:B:747:THR:OG1	1:B:829:ILE:HD12	1.92	0.70
1:B:769:LYS:HE2	1:B:769:LYS:HA	1.73	0.69
1:A:392:CYS:HB3	1:A:397:PHE:CD2	2.28	0.69
1:B:735:GLY:HA2	1:B:839:ALA:HB2	1.74	0.69
1:A:338:MET:CE	1:A:577:VAL:HB	2.23	0.69
1:A:837:ASN:ND2	1:A:839:ALA:H	1.90	0.69
1:B:304:LEU:O	1:B:308:GLU:HB2	1.93	0.69
1:B:415:TYR:CD2	1:B:421:LEU:HD12	2.28	0.68
1:B:364:ILE:HD12	1:B:593:THR:HG21	1.74	0.68
1:A:541:LEU:HD22	1:A:600:LEU:HD21	1.76	0.68
1:A:702:PRO:HG2	1:A:705:LYS:HE3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:MET:HE3	1:A:844:LYS:NZ	2.07	0.68
1:B:452:LEU:HD13	1:B:454:ILE:HD11	1.76	0.68
1:A:817:HIS:CD2	1:A:818:GLN:N	2.62	0.68
1:B:577:VAL:HG12	1:B:577:VAL:O	1.93	0.67
1:B:587:ARG:HD3	1:B:589:PRO:HD3	1.76	0.67
1:B:797:GLN:O	1:B:800:ILE:HG12	1.94	0.67
1:A:694:ASN:HD22	1:A:697:LYS:HD2	1.60	0.66
1:B:374:ILE:HD12	1:B:374:ILE:N	2.09	0.66
1:A:338:MET:HE1	1:A:577:VAL:HB	1.77	0.66
1:A:837:ASN:C	1:A:837:ASN:HD22	2.04	0.66
1:A:488:THR:CG2	1:A:842:ILE:HD11	2.24	0.65
1:A:355:SER:CB	1:A:547:PRO:HB3	2.21	0.65
1:A:841:ILE:HD12	1:A:841:ILE:H	1.60	0.65
1:B:684:GLN:O	1:B:688:LYS:N	2.30	0.64
1:A:343:ARG:HG3	1:A:344:LYS:N	2.12	0.64
1:A:813:GLN:O	1:A:816:GLU:HB2	1.97	0.64
1:A:871:ARG:HH11	1:A:871:ARG:CG	2.11	0.64
1:B:279:LYS:HG3	1:B:290:VAL:HG22	1.80	0.64
1:A:288:PRO:HB3	1:A:843:TRP:CE2	2.32	0.64
1:B:557:HIS:HB2	1:B:587:ARG:HB3	1.80	0.63
1:A:348:ASN:O	1:A:350:HIS:ND1	2.30	0.63
1:B:532:ASP:HB3	1:B:617:PHE:CD1	2.33	0.63
1:B:358:GLU:HB2	1:B:594:GLU:HG2	1.81	0.63
1:A:769:LYS:HZ3	1:A:808:LEU:HD11	1.64	0.63
1:A:400:ARG:NH1	1:A:424:ASP:OD2	2.31	0.63
1:B:873:LEU:HD13	1:B:881:TYR:CE1	2.33	0.62
1:B:399:ILE:HG13	1:B:556:LYS:HE3	1.81	0.62
1:B:587:ARG:NH1	1:B:591:GLN:OE1	2.33	0.62
1:A:372:SER:CB	1:A:373:PRO:CD	2.78	0.62
1:B:683:ASP:O	1:B:687:ASP:HB3	2.00	0.62
1:A:818:GLN:HG3	1:A:818:GLN:O	2.00	0.62
1:A:793:LYS:O	1:A:793:LYS:HD3	2.00	0.61
1:B:341:TYR:HB3	1:B:342:LYS:HD2	1.81	0.61
1:A:488:THR:CG2	1:A:842:ILE:HD13	2.26	0.61
1:B:271:ILE:HG12	1:B:280:ILE:HD13	1.80	0.61
1:B:603:GLU:HA	1:B:606:LEU:HD12	1.82	0.61
1:B:280:ILE:HD11	1:B:429:LEU:HD22	1.83	0.61
1:B:735:GLY:CA	1:B:839:ALA:HB2	2.30	0.61
1:B:727:TYR:HB3	1:B:826:PRO:O	2.01	0.61
1:A:452:LEU:HD13	1:A:454:ILE:HD12	1.82	0.60
1:B:271:ILE:HG22	1:B:273:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLU:O	1:B:310:VAL:N	2.35	0.60
1:B:792:ASN:O	1:B:793:LYS:HG2	2.00	0.60
1:A:590:ASN:CG	1:A:590:ASN:O	2.43	0.60
1:A:761:ALA:HA	1:A:825:PHE:CE1	2.36	0.60
1:A:871:ARG:HH11	1:A:871:ARG:HG2	1.65	0.60
1:A:286:ASP:OD1	1:A:286:ASP:N	2.30	0.60
1:A:688:LYS:HB3	1:A:690:GLU:HB3	1.82	0.60
1:B:736:SER:HA	1:B:738:LYS:HE2	1.83	0.60
1:B:524:ILE:HD11	1:B:652:SER:HB3	1.83	0.59
1:B:732:ILE:HD11	1:B:746:LEU:HD12	1.85	0.59
1:A:550:ASP:OD1	1:A:550:ASP:N	2.33	0.59
1:B:587:ARG:HD3	1:B:589:PRO:CD	2.32	0.59
1:B:426:THR:O	1:B:430:GLU:HG3	2.02	0.58
1:B:738:LYS:HD3	1:B:738:LYS:N	2.11	0.58
1:A:370:ASP:H	1:A:371:PRO:HD3	1.67	0.58
1:B:496:THR:O	1:B:498:THR:HG22	2.03	0.58
1:A:532:ASP:OD2	1:A:621:ARG:NH1	2.37	0.58
1:B:374:ILE:H	1:B:374:ILE:CD1	2.09	0.58
1:A:567:LYS:HD2	1:A:738:LYS:HE3	1.86	0.58
1:A:805:VAL:O	1:A:809:GLU:HB3	2.04	0.58
1:B:400:ARG:HD3	1:B:415:TYR:CZ	2.39	0.58
1:A:816:GLU:OE1	1:A:816:GLU:HA	2.03	0.57
1:B:733:VAL:HG12	1:B:734:GLY:N	2.18	0.57
1:A:278:ILE:CD1	1:A:428:LEU:HD13	2.34	0.57
1:A:352:GLN:OE1	1:A:599:LYS:O	2.22	0.57
1:A:485:SER:HA	1:A:488:THR:HG23	1.87	0.57
1:A:454:ILE:HG12	1:A:463:VAL:HG22	1.86	0.57
1:A:837:ASN:HD22	1:A:839:ALA:H	1.51	0.56
1:A:580:GLN:O	1:A:599:LYS:HA	2.04	0.56
1:A:838:PRO:HA	1:A:841:ILE:CD1	2.36	0.56
1:A:264:ASP:OD1	1:A:266:THR:HB	2.05	0.56
1:A:351:GLU:HG2	1:A:599:LYS:HG3	1.86	0.56
1:A:837:ASN:HD22	1:A:838:PRO:N	2.02	0.56
1:A:345:VAL:HG12	1:A:346:PRO:HD2	1.87	0.56
1:A:494:ILE:O	1:A:495:SER:C	2.47	0.56
1:A:783:ASN:H	1:A:783:ASN:HD22	1.53	0.56
1:A:841:ILE:HD12	1:A:841:ILE:N	2.21	0.56
1:A:262:LEU:O	1:A:449:LYS:HE3	2.07	0.55
1:A:817:HIS:CD2	1:A:818:GLN:H	2.22	0.55
1:A:330:MET:CE	1:A:606:LEU:O	2.54	0.55
1:A:754:ARG:HG2	1:A:754:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:HD22	1:A:856:GLU:HG3	1.70	0.55
1:A:263:ASN:ND2	1:A:856:GLU:HG3	2.21	0.55
1:A:364:ILE:O	1:A:364:ILE:HG22	2.05	0.55
1:A:732:ILE:HD11	1:A:746:LEU:CD1	2.36	0.55
1:A:471:LEU:HD21	1:A:479:VAL:HG23	1.88	0.55
1:A:852:ILE:HB	1:A:853:LYS:HD2	1.89	0.55
1:B:509:ARG:CB	1:B:509:ARG:HH11	2.20	0.54
1:B:509:ARG:HH11	1:B:509:ARG:N	2.05	0.54
1:B:536:LEU:HD11	1:B:616:ILE:HG21	1.90	0.54
1:A:370:ASP:N	1:A:371:PRO:HD3	2.22	0.54
1:A:588:SER:HB2	1:A:591:GLN:O	2.07	0.54
1:B:729:ASN:HA	1:B:830:ILE:HG12	1.89	0.54
1:B:418:LEU:HG	1:B:422:ILE:CD1	2.37	0.54
1:A:334:PHE:HD1	1:A:605:MET:HE2	1.73	0.54
1:A:727:TYR:HB3	1:A:826:PRO:O	2.07	0.54
1:B:415:TYR:CE1	1:B:421:LEU:HA	2.43	0.54
1:A:337:ARG:NH2	1:A:748:ASP:OD2	2.31	0.53
1:B:527:ASP:O	1:B:621:ARG:NH2	2.26	0.53
1:A:566:LYS:HE3	1:A:738:LYS:HZ1	1.74	0.53
1:B:607:ALA:HB3	1:B:608:PRO:CD	2.38	0.53
1:A:567:LYS:CD	1:A:738:LYS:HE3	2.39	0.53
1:A:661:LEU:CD2	1:A:709:GLN:HG3	2.38	0.53
1:B:372:SER:HB2	1:B:373:PRO:CD	2.32	0.53
1:B:770:LEU:O	1:B:774:ILE:HG23	2.09	0.53
1:B:469:VAL:HG12	1:B:474:LEU:HD12	1.89	0.53
1:A:746:LEU:HD13	1:A:829:ILE:HD13	1.90	0.53
1:B:351:GLU:O	1:B:355:SER:HB2	2.09	0.53
1:B:304:LEU:HD13	1:B:304:LEU:H	1.74	0.52
1:A:319:GLN:HG2	1:A:323:PHE:CG	2.44	0.52
1:A:278:ILE:HD11	1:A:428:LEU:HD13	1.91	0.52
1:A:370:ASP:N	1:A:371:PRO:CD	2.72	0.52
1:A:364:ILE:O	1:A:372:SER:OG	2.28	0.52
1:A:566:LYS:HE3	1:A:738:LYS:NZ	2.24	0.52
1:B:748:ASP:O	1:B:752:ILE:HG13	2.09	0.52
1:B:502:ASN:C	1:B:502:ASN:ND2	2.64	0.52
1:A:426:THR:HG22	1:A:474:LEU:HD11	1.92	0.52
1:A:769:LYS:HZ2	1:A:808:LEU:HD11	1.74	0.52
1:B:508:THR:HB	1:B:526:LEU:HB2	1.92	0.52
1:B:535:ARG:HD3	1:B:620:ILE:HG22	1.91	0.52
1:B:506:ALA:C	1:B:507:GLU:HG3	2.35	0.52
1:A:424:ASP:O	1:A:428:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:ALA:HB3	1:B:608:PRO:HD3	1.90	0.52
1:A:269:ILE:O	1:A:450:VAL:HA	2.09	0.51
1:A:702:PRO:HB2	1:A:704:GLU:OE1	2.11	0.51
1:B:728:SER:HA	1:B:828:SER:OG	2.10	0.51
1:A:853:LYS:HD2	1:A:853:LYS:H	1.76	0.51
1:B:642:THR:HG22	1:B:644:GLU:CB	2.30	0.51
1:A:263:ASN:HD22	1:A:856:GLU:HA	1.76	0.51
1:B:534:THR:OG1	1:B:566:LYS:HG2	2.11	0.51
1:A:426:THR:O	1:A:430:GLU:HG3	2.11	0.51
1:B:716:ILE:HG13	1:B:717:THR:N	2.23	0.51
1:A:279:LYS:HD2	1:A:279:LYS:N	2.26	0.51
1:A:338:MET:HE2	1:A:577:VAL:HB	1.93	0.51
1:A:849:LEU:HD13	1:A:855:VAL:CG1	2.41	0.50
1:A:874:GLN:HB3	1:A:875:TYR:CD2	2.47	0.50
1:B:572:PHE:CD1	1:B:745:ILE:HG21	2.46	0.50
1:A:646:ASN:HD22	1:A:646:ASN:H	1.60	0.50
1:B:852:ILE:HG23	1:B:854:LEU:H	1.76	0.50
1:A:709:GLN:HG2	3:A:2017:HOH:O	2.11	0.49
1:A:755:PRO:HG2	1:A:758:LEU:HD12	1.94	0.49
1:B:460:LYS:HB2	1:B:637:SER:CB	2.42	0.49
1:B:687:ASP:O	1:B:689:PRO:HD3	2.12	0.49
1:B:304:LEU:HA	1:B:308:GLU:HB2	1.94	0.49
1:B:502:ASN:O	1:B:508:THR:HA	2.12	0.49
1:A:505:ALA:O	1:A:531:ASP:HB2	2.11	0.49
1:B:571:THR:OG1	1:B:740:PRO:HB2	2.13	0.49
1:B:509:ARG:N	1:B:509:ARG:NH1	2.60	0.49
1:A:359:ASN:N	1:A:359:ASN:HD22	2.10	0.49
1:B:340:TYR:CD1	1:B:340:TYR:C	2.90	0.49
1:B:372:SER:CB	1:B:373:PRO:HD2	2.36	0.49
1:A:426:THR:HB	1:A:474:LEU:HD21	1.92	0.49
1:B:261:ASP:HB3	1:B:477:GLN:CD	2.38	0.49
1:B:263:ASN:N	1:B:263:ASN:OD1	2.45	0.49
1:A:364:ILE:HG21	1:A:587:ARG:NH1	2.27	0.49
1:B:646:ASN:C	1:B:646:ASN:HD22	2.19	0.49
1:B:655:GLU:OE2	1:B:674:ARG:NH2	2.45	0.49
1:A:332:LYS:O	1:A:333:ASN:C	2.53	0.49
1:A:841:ILE:H	1:A:841:ILE:CD1	2.26	0.49
1:B:300:LYS:HE2	1:B:380:ASP:O	2.12	0.49
1:B:509:ARG:HH11	1:B:509:ARG:CG	2.25	0.49
1:A:460:LYS:HB2	1:A:637:SER:HB2	1.93	0.49
1:B:639:ASP:OD2	1:B:642:THR:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:VAL:HA	1:B:552:LYS:HD3	1.94	0.48
1:B:486:LEU:O	1:B:489:CYS:HB2	2.13	0.48
1:A:457:ILE:HD11	1:A:523:ALA:HB3	1.96	0.48
1:A:809:GLU:O	1:A:813:GLN:HG3	2.13	0.48
1:B:350:HIS:C	1:B:352:GLN:H	2.21	0.48
1:A:444:LYS:HB3	1:A:444:LYS:HE2	1.60	0.48
1:B:733:VAL:CG1	1:B:734:GLY:N	2.77	0.48
1:B:787:LYS:HE2	1:B:796:LEU:HD22	1.95	0.48
1:B:316:GLN:HE21	1:B:316:GLN:CA	2.19	0.47
1:B:426:THR:HB	1:B:474:LEU:HD11	1.96	0.47
1:A:468:ARG:NH1	1:B:641:PHE:CE2	2.81	0.47
1:A:779:GLY:O	1:A:782:VAL:HG13	2.14	0.47
1:B:449:LYS:HD2	1:B:859:PHE:CE2	2.49	0.47
1:B:855:VAL:HA	1:B:858:LEU:HD12	1.96	0.47
1:A:610:ALA:HB3	1:A:617:PHE:CZ	2.49	0.47
1:A:854:LEU:O	1:A:855:VAL:C	2.58	0.47
1:A:874:GLN:HB3	1:A:875:TYR:CE2	2.49	0.47
1:A:750:ILE:HD12	1:A:829:ILE:HD11	1.97	0.47
1:B:378:PHE:CD1	1:B:393:VAL:HG11	2.49	0.47
1:B:783:ASN:O	1:B:785:PRO:HD3	2.14	0.47
1:B:871:ARG:HG3	1:B:871:ARG:HH11	1.78	0.47
1:A:651:LEU:HB2	1:A:682:ILE:HG22	1.97	0.47
1:B:415:TYR:CE2	1:B:421:LEU:HD12	2.49	0.47
1:B:860:ILE:HG23	1:B:872:ILE:HD12	1.97	0.47
1:A:699:ASN:C	1:A:699:ASN:HD22	2.23	0.47
1:B:302:LEU:HB3	1:B:308:GLU:OE2	2.14	0.47
1:B:422:ILE:O	1:B:426:THR:HG23	2.15	0.46
1:B:844:LYS:O	1:B:847:SER:HB2	2.15	0.46
1:A:293:ASN:OD1	1:A:402:PRO:HD2	2.15	0.46
1:A:494:ILE:O	1:A:494:ILE:HG12	2.14	0.46
1:B:316:GLN:NE2	1:B:316:GLN:CA	2.70	0.46
1:A:367:GLU:CD	1:A:564:ARG:HH22	2.20	0.46
1:B:305:GLU:HA	1:B:305:GLU:OE1	2.14	0.46
1:A:818:GLN:O	1:A:818:GLN:CG	2.63	0.46
1:B:581:LEU:O	1:B:581:LEU:HD22	2.16	0.46
1:A:418:LEU:O	1:A:419:ALA:C	2.58	0.46
1:A:344:LYS:O	1:A:345:VAL:HG13	2.16	0.46
1:A:618:LYS:HD2	1:A:700:PHE:CE2	2.51	0.46
1:A:863:SER:O	1:A:864:ASP:C	2.58	0.46
1:A:321:GLU:O	1:A:324:ASN:N	2.49	0.46
1:A:327:LYS:HD2	1:A:540:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LEU:HD23	1:B:709:GLN:CG	2.41	0.46
1:A:368:LYS:HD3	1:A:568:ASN:OD1	2.16	0.46
1:A:812:HIS:O	1:A:816:GLU:HG2	2.16	0.46
1:A:821:ASN:OD1	1:A:822:GLU:N	2.49	0.46
1:A:855:VAL:HA	1:A:858:LEU:HD12	1.98	0.46
1:A:588:SER:HA	1:A:589:PRO:HD2	1.78	0.45
1:A:688:LYS:HG2	1:A:689:PRO:HD2	1.99	0.45
1:A:311:GLU:C	1:A:313:VAL:H	2.24	0.45
1:A:871:ARG:CG	1:A:871:ARG:NH1	2.74	0.45
1:B:289:VAL:CG1	1:B:438:LEU:HD11	2.47	0.45
1:B:389:ALA:O	1:B:392:CYS:HB2	2.16	0.45
1:A:435:SER:O	1:A:436:GLU:C	2.59	0.45
1:B:308:GLU:O	1:B:309:HIS:C	2.54	0.45
1:A:471:LEU:O	1:A:475:GLN:HA	2.15	0.45
1:A:838:PRO:HA	1:A:841:ILE:HD11	1.98	0.45
1:A:614:PRO:HD2	3:A:2015:HOH:O	2.17	0.45
1:A:688:LYS:N	1:A:690:GLU:OE1	2.50	0.45
1:A:539:LEU:HD23	1:A:539:LEU:HA	1.69	0.45
1:A:836:MET:CE	1:A:844:LYS:NZ	2.78	0.45
1:A:738:LYS:H	1:A:738:LYS:HD3	1.81	0.45
1:B:474:LEU:O	1:B:475:GLN:CB	2.64	0.45
1:B:642:THR:CG2	1:B:644:GLU:CB	2.94	0.45
1:A:321:GLU:O	1:A:325:ASN:N	2.48	0.45
1:A:770:LEU:HD21	1:A:805:VAL:HG22	1.98	0.45
1:A:795:ILE:O	1:A:799:GLN:N	2.49	0.45
1:B:733:VAL:CG2	1:B:841:ILE:HD12	2.44	0.45
1:A:283:PRO:HA	1:A:847:SER:HB2	1.99	0.44
1:A:293:ASN:ND2	1:A:401:LYS:HB3	2.32	0.44
1:A:644:GLU:O	1:A:645:LEU:C	2.58	0.44
1:B:390:LEU:O	1:B:556:LYS:CG	2.65	0.44
1:A:276:ASN:HB3	2:A:1883:SO4:O3	2.18	0.44
1:A:328:SER:HA	1:A:331:GLU:OE1	2.17	0.44
1:A:537:PHE:O	1:A:538:ALA:C	2.60	0.44
1:A:732:ILE:HG22	1:A:737:SER:HB2	2.00	0.44
1:B:696:LEU:H	1:B:696:LEU:HD23	1.81	0.44
1:B:849:LEU:O	1:B:855:VAL:HG22	2.17	0.44
1:B:377:ILE:HG13	1:B:392:CYS:HA	1.99	0.44
1:A:321:GLU:O	1:A:322:GLU:C	2.61	0.44
1:A:468:ARG:NH1	1:B:641:PHE:HE2	2.16	0.44
1:A:868:HIS:HB2	1:A:872:ILE:HD13	1.98	0.44
1:B:309:HIS:O	1:B:309:HIS:CG	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:PHE:CE2	1:B:620:ILE:HD11	2.53	0.44
1:B:418:LEU:O	1:B:422:ILE:HD12	2.17	0.44
1:A:738:LYS:HD3	1:A:738:LYS:N	2.33	0.43
1:A:754:ARG:HG2	1:A:759:SER:OG	2.18	0.43
1:B:368:LYS:HE3	1:B:369:ASN:H	1.82	0.43
1:A:456:ASP:OD2	1:A:485:SER:OG	2.33	0.43
1:B:260:ILE:H	1:B:260:ILE:HG13	1.71	0.43
1:A:790:ASP:HB2	1:A:793:LYS:HB3	1.99	0.43
1:A:694:ASN:HB3	1:A:697:LYS:HB2	2.00	0.43
1:B:614:PRO:O	1:B:615:GLN:C	2.61	0.43
1:A:378:PHE:CE1	1:A:393:VAL:HG11	2.54	0.43
1:A:670:LYS:HE2	1:A:674:ARG:NH2	2.34	0.43
1:A:694:ASN:HB3	1:A:697:LYS:CB	2.49	0.43
1:A:688:LYS:C	1:A:690:GLU:N	2.77	0.43
1:A:754:ARG:HG2	1:A:754:ARG:NH1	2.33	0.43
1:B:637:SER:HB3	1:B:646:ASN:HD21	1.84	0.43
1:A:342:LYS:HD2	1:A:574:ASP:C	2.43	0.42
1:A:834:ARG:O	1:A:835:ASP:OD1	2.36	0.42
1:B:368:LYS:HG2	1:B:564:ARG:HG3	2.00	0.42
1:A:468:ARG:HH12	1:B:641:PHE:HE2	1.67	0.42
1:B:543:GLN:H	1:B:543:GLN:HG2	1.60	0.42
1:A:311:GLU:C	1:A:313:VAL:N	2.77	0.42
1:A:364:ILE:HD12	1:A:373:PRO:HB3	2.00	0.42
1:B:361:LYS:H	1:B:361:LYS:HG2	1.60	0.42
1:B:411:LYS:O	1:B:412:SER:C	2.61	0.42
1:B:457:ILE:O	1:B:457:ILE:HG22	2.19	0.42
1:B:692:TYR:HD1	1:B:692:TYR:HA	1.78	0.42
1:B:770:LEU:CD2	1:B:808:LEU:HB3	2.50	0.42
1:A:588:SER:HB2	1:A:591:GLN:H	1.84	0.42
1:A:837:ASN:ND2	1:A:837:ASN:C	2.75	0.42
1:B:871:ARG:HG3	1:B:871:ARG:NH1	2.34	0.42
1:A:761:ALA:HA	1:A:825:PHE:CZ	2.55	0.42
1:A:861:THR:O	1:A:864:ASP:HB2	2.20	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.93	0.42
1:B:548:LEU:HD11	1:B:586:ASN:OD1	2.20	0.42
1:A:608:PRO:C	1:A:610:ALA:N	2.77	0.42
1:A:699:ASN:C	1:A:699:ASN:ND2	2.77	0.42
1:A:317:ARG:NE	1:A:543:GLN:HA	2.35	0.42
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.71	0.42
1:A:790:ASP:HB2	1:A:793:LYS:CB	2.49	0.42
1:A:263:ASN:HA	1:A:449:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:C	1:A:345:VAL:HG22	2.45	0.42
1:A:740:PRO:O	1:A:741:ALA:HB3	2.19	0.42
1:A:855:VAL:HB	1:A:859:PHE:CE2	2.55	0.42
1:B:325:ASN:O	1:B:328:SER:HB2	2.20	0.42
1:A:816:GLU:OE1	1:A:816:GLU:CA	2.68	0.41
1:B:646:ASN:C	1:B:646:ASN:ND2	2.77	0.41
1:B:552:LYS:O	1:B:558:GLY:HA3	2.20	0.41
1:A:344:LYS:O	1:A:345:VAL:HG22	2.20	0.41
1:B:502:ASN:HD22	1:B:503:ILE:N	2.16	0.41
1:A:335:ARG:NH1	1:A:339:ARG:HH22	2.19	0.41
1:B:288:PRO:HB3	1:B:843:TRP:CE2	2.56	0.41
1:B:500:VAL:O	1:B:510:ILE:HA	2.20	0.41
1:B:665:LEU:HD22	1:B:670:LYS:HD3	2.02	0.41
1:A:352:GLN:NE2	1:A:544:SER:O	2.54	0.41
1:B:388:ASP:O	1:B:389:ALA:C	2.64	0.41
1:B:713:ASN:O	1:B:717:THR:HG23	2.21	0.41
1:A:567:LYS:HD2	1:A:738:LYS:CE	2.51	0.41
1:A:746:LEU:HD22	1:A:750:ILE:HD11	2.03	0.41
1:A:792:ASN:HD22	1:A:792:ASN:HA	1.78	0.41
1:A:808:LEU:HD13	1:A:808:LEU:HA	1.92	0.41
1:B:323:PHE:CD1	1:B:323:PHE:C	2.99	0.41
1:B:754:ARG:HA	1:B:755:PRO:HD3	1.91	0.41
1:A:418:LEU:HD11	1:A:634:LEU:HG	2.02	0.41
1:A:797:GLN:HA	1:A:800:ILE:HG22	2.03	0.40
1:B:722:ARG:O	1:B:723:MET:C	2.63	0.40
1:A:317:ARG:HE	1:A:543:GLN:HA	1.86	0.40
1:B:280:ILE:HD12	1:B:280:ILE:HG21	1.90	0.40
1:B:712:ALA:O	1:B:716:ILE:HG23	2.22	0.40
1:A:823:HIS:O	1:A:823:HIS:CG	2.73	0.40
1:B:304:LEU:HD13	1:B:304:LEU:N	2.35	0.40
1:B:530:GLY:O	1:B:566:LYS:NZ	2.55	0.40
1:B:837:ASN:HA	1:B:838:PRO:HD2	1.82	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	621/655 (95%)	554 (89%)	64 (10%)	3 (0%)	24	48
1	B	621/655 (95%)	544 (88%)	69 (11%)	8 (1%)	9	25
All	All	1242/1310 (95%)	1098 (88%)	133 (11%)	11 (1%)	14	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	346	PRO
1	A	372	SER
1	B	373	PRO
1	B	688	LYS
1	B	371	PRO
1	B	379	ASP
1	A	579	VAL
1	B	579	VAL
1	B	313	VAL
1	A	345	VAL
1	B	689	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	569/595 (96%)	459 (81%)	110 (19%)	1	4
1	B	569/595 (96%)	447 (79%)	122 (21%)	1	3
All	All	1138/1190 (96%)	906 (80%)	232 (20%)	1	3

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	ILE

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Mol	Chain	Res	Type
1	A	262	LEU
1	A	264	ASP
1	A	286	ASP
1	A	287	HIS
1	A	309	HIS
1	A	311	GLU
1	A	314	CYS
1	A	315	LEU
1	A	318	GLU
1	A	332	LYS
1	A	333	ASN
1	A	337	ARG
1	A	338	MET
1	A	342	LYS
1	A	343	ARG
1	A	344	LYS
1	A	345	VAL
1	A	348	ASN
1	A	350	HIS
1	A	351	GLU
1	A	353	VAL
1	A	355	SER
1	A	357	ASN
1	A	359	ASN
1	A	361	LYS
1	A	365	ILE
1	A	372	SER
1	A	387	SER
1	A	391	ARG
1	A	395	GLU
1	A	398	VAL
1	A	400	ARG
1	A	404	ARG
1	A	411	LYS
1	A	428	LEU
1	A	433	LEU
1	A	438	LEU
1	A	444	LYS
1	A	449	LYS
1	A	452	LEU
1	A	454	ILE
1	A	459	LYS

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Mol	Chain	Res	Type
1	A	468	ARG
1	A	473	GLU
1	A	486	LEU
1	A	488	THR
1	A	494	ILE
1	A	495	SER
1	A	496	THR
1	A	498	THR
1	A	503	ILE
1	A	515	GLU
1	A	517	THR
1	A	536	LEU
1	A	539	LEU
1	A	548	LEU
1	A	550	ASP
1	A	553	ILE
1	A	556	LYS
1	A	560	LEU
1	A	561	LEU
1	A	566	LYS
1	A	571	THR
1	A	573	GLN
1	A	580	GLN
1	A	588	SER
1	A	606	LEU
1	A	619	LEU
1	A	625	HIS
1	A	626	LYS
1	A	630	LEU
1	A	640	LEU
1	A	646	ASN
1	A	669	LEU
1	A	672	LEU
1	A	696	LEU
1	A	703	LEU
1	A	704	GLU
1	A	715	SER
1	A	720	VAL
1	A	722	ARG
1	A	732	ILE
1	A	733	VAL
1	A	738	LYS

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Mol	Chain	Res	Type
1	A	746	LEU
1	A	754	ARG
1	A	771	THR
1	A	780	HIS
1	A	782	VAL
1	A	783	ASN
1	A	789	GLU
1	A	791	GLU
1	A	792	ASN
1	A	794	GLN
1	A	796	LEU
1	A	797	GLN
1	A	804	ILE
1	A	808	LEU
1	A	815	ILE
1	A	824	ILE
1	A	828	SER
1	A	837	ASN
1	A	849	LEU
1	A	853	LYS
1	A	854	LEU
1	A	855	VAL
1	A	871	ARG
1	A	872	ILE
1	A	874	GLN
1	B	260	ILE
1	B	263	ASN
1	B	264	ASP
1	B	280	ILE
1	B	287	HIS
1	B	289	VAL
1	B	304	LEU
1	B	309	HIS
1	B	315	LEU
1	B	316	GLN
1	B	319	GLN
1	B	342	LYS
1	B	350	HIS
1	B	353	VAL
1	B	356	PHE
1	B	357	ASN
1	B	358	GLU

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Mol	Chain	Res	Type
1	B	361	LYS
1	B	367	GLU
1	B	368	LYS
1	B	370	ASP
1	B	374	ILE
1	B	377	ILE
1	B	382	LYS
1	B	383	LEU
1	B	391	ARG
1	B	395	GLU
1	B	398	VAL
1	B	399	ILE
1	B	400	ARG
1	B	404	ARG
1	B	410	VAL
1	B	412	SER
1	B	422	ILE
1	B	426	THR
1	B	433	LEU
1	B	436	GLU
1	B	440	VAL
1	B	452	LEU
1	B	454	ILE
1	B	461	SER
1	B	475	GLN
1	B	486	LEU
1	B	488	THR
1	B	494	ILE
1	B	496	THR
1	B	498	THR
1	B	507	GLU
1	B	509	ARG
1	B	517	THR
1	B	525	THR
1	B	536	LEU
1	B	539	LEU
1	B	542	LEU
1	B	543	GLN
1	B	556	LYS
1	B	560	LEU
1	B	566	LYS
1	B	570	THR

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Mol	Chain	Res	Type
1	B	573	GLN
1	B	580	GLN
1	B	581	LEU
1	B	587	ARG
1	B	588	SER
1	B	600	LEU
1	B	604	VAL
1	B	606	LEU
1	B	609	LEU
1	B	616	ILE
1	B	619	LEU
1	B	621	ARG
1	B	623	SER
1	B	624	SER
1	B	626	LYS
1	B	629	SER
1	B	640	LEU
1	B	646	ASN
1	B	658	GLU
1	B	660	ASN
1	B	669	LEU
1	B	672	LEU
1	B	673	ASN
1	B	674	ARG
1	B	675	ILE
1	B	686	GLN
1	B	690	GLU
1	B	692	TYR
1	B	694	ASN
1	B	695	THR
1	B	696	LEU
1	B	697	LYS
1	B	703	LEU
1	B	704	GLU
1	B	720	VAL
1	B	722	ARG
1	B	731	LEU
1	B	738	LYS
1	B	742	LEU
1	B	746	LEU
1	B	749	ARG
1	B	769	LYS

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Mol	Chain	Res	Type
1	B	774	ILE
1	B	780	HIS
1	B	787	LYS
1	B	791	GLU
1	B	794	GLN
1	B	796	LEU
1	B	797	GLN
1	B	808	LEU
1	B	818	GLN
1	B	821	ASN
1	B	830	ILE
1	B	837	ASN
1	B	847	SER
1	B	849	LEU
1	B	853	LYS
1	B	854	LEU
1	B	855	VAL
1	B	860	ILE
1	B	871	ARG
1	B	872	ILE
1	B	874	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	316	GLN
1	A	348	ASN
1	A	359	ASN
1	A	369	ASN
1	A	434	ASN
1	A	439	ASN
1	A	502	ASN
1	A	573	GLN
1	A	615	GLN
1	A	633	GLN
1	A	646	ASN
1	A	666	ASN
1	A	686	GLN
1	A	694	ASN
1	A	699	ASN
1	A	783	ASN

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Mol	Chain	Res	Type
1	A	792	ASN
1	A	794	GLN
1	A	812	HIS
1	A	813	GLN
1	A	817	HIS
1	A	818	GLN
1	A	837	ASN
1	A	851	GLN
1	B	316	GLN
1	B	325	ASN
1	B	369	ASN
1	B	434	ASN
1	B	439	ASN
1	B	447	GLN
1	B	502	ASN
1	B	583	ASN
1	B	646	ASN
1	B	666	ASN
1	B	684	GLN
1	B	686	GLN
1	B	691	ASN
1	B	724	ASN
1	B	794	GLN
1	B	797	GLN
1	B	818	GLN
1	B	821	ASN
1	B	868	HIS

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 [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1882	-	4,4,4	0.41	0	6,6,6	0.42	0
2	SO4	A	1883	-	4,4,4	0.45	0	6,6,6	0.37	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1883	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	623/655 (95%)	-0.03	30 (4%) 35 32	32, 64, 146, 240	0
1	B	623/655 (95%)	0.22	32 (5%) 33 29	41, 85, 174, 263	0
All	All	1246/1310 (95%)	0.10	62 (4%) 34 30	32, 74, 162, 263	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	PRO	5.3
1	B	784	ALA	3.9
1	B	782	VAL	3.8
1	B	374	ILE	3.8
1	A	260	ILE	3.7
1	A	310	VAL	3.6
1	B	689	PRO	3.5
1	A	371	PRO	3.4
1	B	372	SER	3.3
1	A	349	ALA	3.3
1	B	308	GLU	3.3
1	A	346	PRO	3.1
1	A	315	LEU	3.1
1	B	795	ILE	3.1
1	A	696	LEU	3.0
1	B	364	ILE	3.0
1	A	494	ILE	3.0
1	A	347	GLY	3.0
1	A	782	VAL	3.0
1	A	627	ASN	2.9
1	B	353	VAL	2.9
1	A	365	ILE	2.9
1	A	693	GLY	2.9
1	B	354	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	808	LEU	2.8
1	B	316	GLN	2.8
1	B	262	LEU	2.8
1	A	364	ILE	2.7
1	B	356	PHE	2.7
1	B	785	PRO	2.7
1	A	366	SER	2.7
1	A	781	TYR	2.6
1	B	494	ILE	2.6
1	A	689	PRO	2.6
1	B	493	GLY	2.5
1	B	350	HIS	2.5
1	A	823	HIS	2.5
1	B	777	LEU	2.4
1	A	794	GLN	2.4
1	A	368	LYS	2.4
1	B	412	SER	2.3
1	B	786	ASP	2.3
1	A	589	PRO	2.3
1	A	353	VAL	2.3
1	A	367	GLU	2.3
1	A	361	LYS	2.2
1	B	349	ALA	2.2
1	B	365	ILE	2.2
1	B	313	VAL	2.2
1	A	806	GLU	2.2
1	B	336	GLU	2.2
1	A	695	THR	2.2
1	B	642	THR	2.2
1	A	350	HIS	2.2
1	A	342	LYS	2.1
1	A	688	LYS	2.1
1	A	804	ILE	2.1
1	B	317	ARG	2.1
1	B	693	GLY	2.1
1	B	348	ASN	2.0
1	B	596	TYR	2.0
1	B	788	THR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1883	5/5	0.93	0.12	70,73,73,73	0
2	SO4	A	1882	5/5	0.96	0.06	62,63,64,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.