



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:48 pm GMT

PDB ID : 4AM6
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

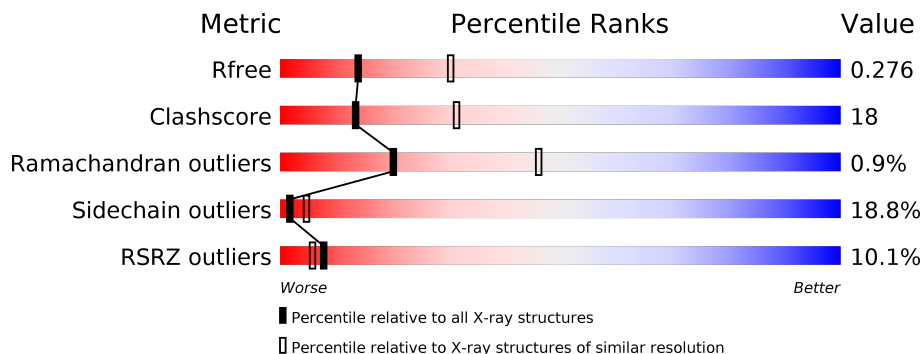
1 Overall quality at a glance

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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 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 $\leq 5\%$. 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	<div> <div>9%</div> <div> <div></div> <div>55%</div> <div>30%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	655	<div> <div>11%</div> <div> <div></div> <div>56%</div> <div>30%</div> <div>9%</div> <div>5%</div> </div> </div>

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:

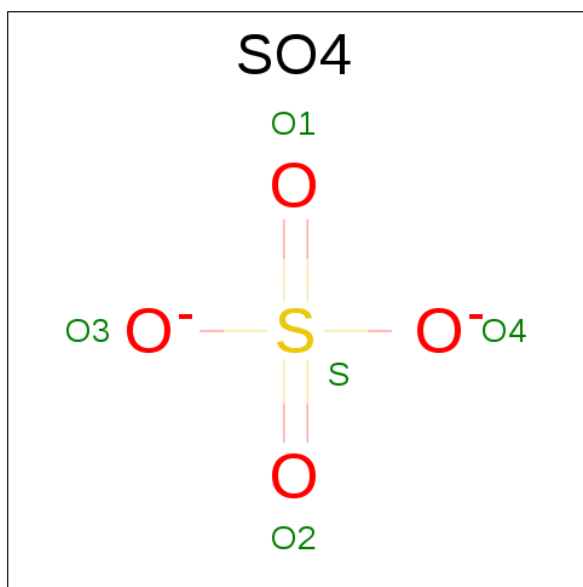
Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	EXPRESSION TAG	UNP Q12386
A	228	GLY	-	EXPRESSION TAG	UNP Q12386
A	229	SER	-	EXPRESSION TAG	UNP Q12386
A	230	SER	-	EXPRESSION TAG	UNP Q12386
A	231	HIS	-	EXPRESSION TAG	UNP Q12386
A	232	HIS	-	EXPRESSION TAG	UNP Q12386
A	233	HIS	-	EXPRESSION TAG	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

Continued on next page...

Continued from previous page...

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 (three-letter code: 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		

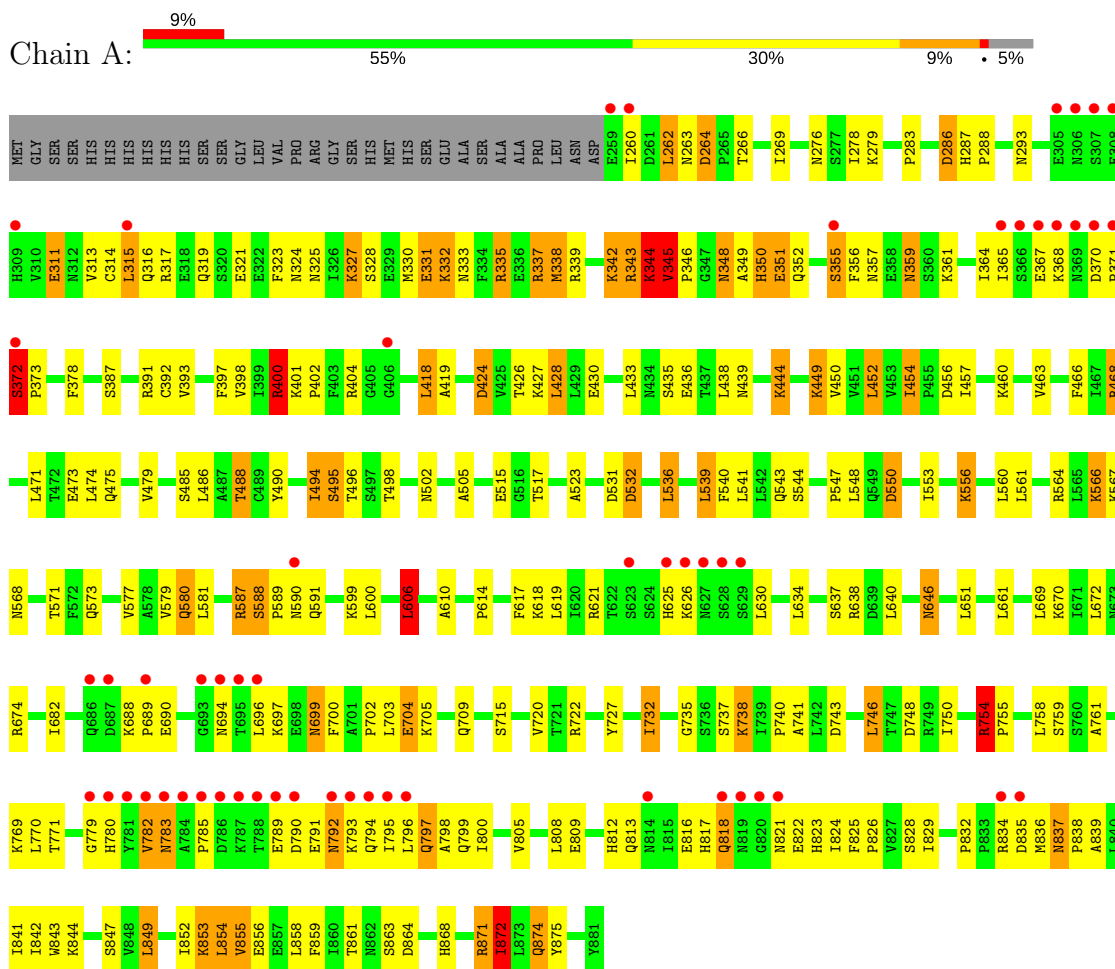
- Molecule 3 is water.

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

3 Residue-property plots

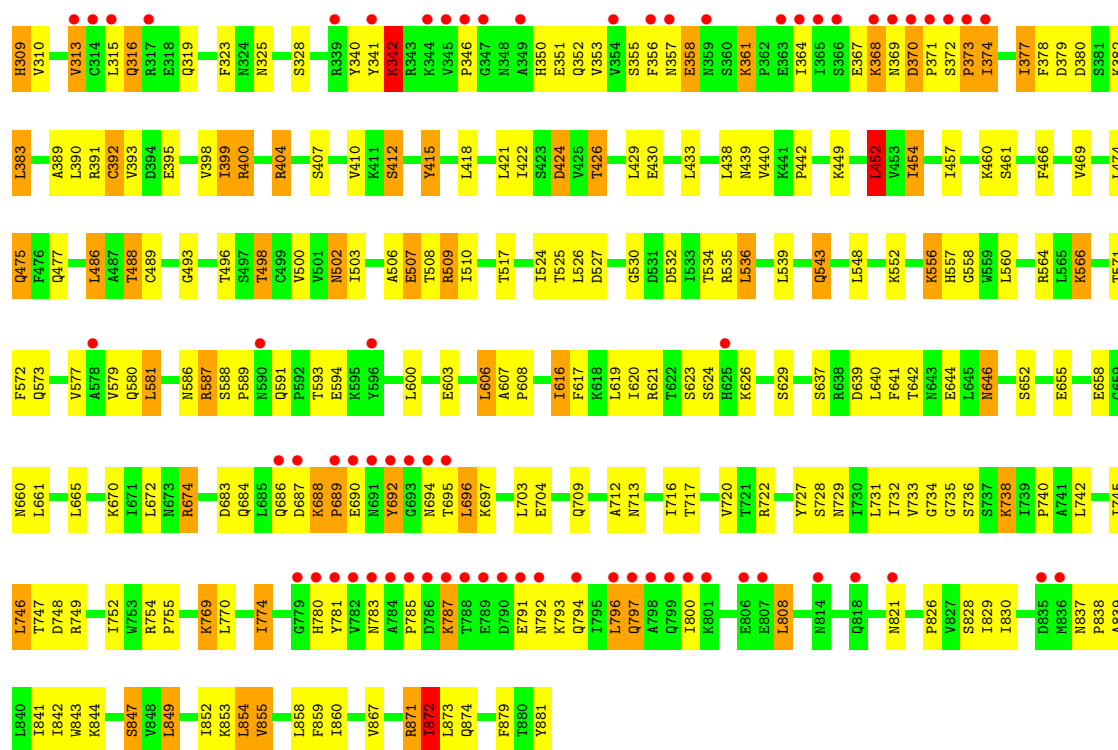
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ACTIN-LIKE PROTEIN ARP8



• Molecule 1: ACTIN-LIKE PROTEIN ARP8





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) 98.9 (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 (5.23%)	DCC
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.4	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 [i](#)

5.1 Standard geometry [i](#)

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	0.90	4/5149 (0.1%)	0.94	14/6982 (0.2%)
1	B	0.75	5/5149 (0.1%)	0.86	11/6982 (0.2%)
All	All	0.83	9/10298 (0.1%)	0.90	25/13964 (0.2%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	GLU	CD-OE1	15.34	1.42	1.25
1	A	331	GLU	CD-OE2	13.05	1.40	1.25
1	A	344	LYS	CE-NZ	10.53	1.75	1.49
1	A	327	LYS	CD-CE	6.42	1.67	1.51
1	B	424	ASP	CB-CG	6.02	1.64	1.51
1	B	412	SER	CB-OG	5.88	1.49	1.42
1	B	879	PHE	CD2-CE2	5.19	1.49	1.39
1	B	392	CYS	CB-SG	-5.16	1.73	1.81
1	B	415	TYR	CE2-CZ	5.07	1.45	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	ASP	CB-CG-OD1	10.67	127.91	118.30
1	A	424	ASP	CB-CG-OD1	-7.80	111.28	118.30
1	A	754	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	342	LYS	N-CA-C	6.94	129.74	111.00
1	A	344	LYS	CD-CE-NZ	6.92	127.63	111.70
1	A	581	LEU	CA-CB-CG	6.72	130.75	115.30
1	A	335	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	493	GLY	N-CA-C	-6.27	97.43	113.10
1	A	754	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	350	HIS	N-CA-C	5.89	126.90	111.00
1	A	400	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	418	LEU	CB-CG-CD1	-5.55	101.57	111.00
1	A	638	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	606	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	B	370	ASP	N-CA-C	5.36	125.46	111.00
1	B	452	LEU	CB-CG-CD2	5.36	120.11	111.00
1	B	383	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	400	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	407	SER	N-CA-CB	-5.27	102.60	110.50
1	B	412	SER	N-CA-CB	5.25	118.37	110.50
1	B	415	TYR	CZ-CE2-CD2	-5.23	115.09	119.80
1	B	872	ILE	CB-CA-C	-5.19	101.22	111.60
1	A	872	ILE	CB-CA-C	-5.16	101.29	111.60
1	B	404	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	872	ILE	CG1-CB-CG2	5.02	122.44	111.40

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	206	0
1	B	5036	0	4985	159	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	361	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 18.

All (361) 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:HD3	1:B:738:LYS:H	1.31	0.93
1:B:642:THR:HG22	1:B:644:GLU:HB2	1.49	0.92
1:B:374:ILE:H	1:B:374:ILE:HD12	1.33	0.92
1:B:372:SER:HB2	1:B:373:PRO:HD2	1.52	0.91
1:B:316:GLN:HA	1:B:316:GLN:HE21	1.35	0.90
1:A:372:SER:HB3	1:A:373:PRO:HD2	1.54	0.89
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:452:LEU:HD13	1:B:454:ILE:CD1	2.15	0.77
1:A:795:ILE:HA	1:A:798:ALA:HB3	1.67	0.76
1:A:488:THR:CG2	1:A:842:ILE:CD1	2.62	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:502:ASN:HD22	1:B:502:ASN:C	1.92	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:315:LEU:C	1:A:315:LEU:HD23	2.12	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
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:O	1:B:577:VAL:HG12	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:N	1:B:374:ILE:HD12	2.09	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:CG	1:A:871:ARG:HH11	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:A:793:LYS:O	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:A:837:ASN:HD22	1:A:837:ASN:C	2.04	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:338:MET:HE1	1:A:577:VAL:HB	1.82	0.60
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
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: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:N	1:A:550:ASP:OD1	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:N	1:B:738:LYS:HD3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:SER:HA	1:A:488:THR:HG23	1.87	0.57
1:A:352:GLN:OE1	1:A:599:LYS:O	2.22	0.57
1:A:590:ASN:O	1:A:590:ASN:CG	2.43	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:783:ASN:H	1:A:783:ASN:HD22	1.53	0.56
1:A:841:ILE:N	1:A:841:ILE:HD12	2.21	0.56
1:A:262:LEU:O	1:A:449:LYS:HE3	2.07	0.55
1:A:338:MET:HE2	1:A:577:VAL:HB	1.88	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:HH11	1:A:754:ARG:HG2	1.72	0.55
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:N	1:B:509:ARG:HH11	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:A:832:PRO:HB3	1:A:836:MET:HE2	1.89	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:727:TYR:HB3	1:A:826:PRO:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:B:304:LEU:HD13	1.74	0.52
1:A:319:GLN:HG2	1:A:323:PHE:CG	2.44	0.52
1:A:370:ASP:N	1:A:371:PRO:CD	2.72	0.52
1:A:278:ILE:HD11	1:A:428:LEU:HD13	1.91	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: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:A:424:ASP:O	1:A:428:LEU:HB2	2.10	0.52
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:494:ILE:O	1:A:495:SER:C	2.47	0.51
1:A:853:LYS:H	1:A:853:LYS:HD2	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:N	1:A:279:LYS:HD2	2.26	0.51
1:A:849:LEU:HD13	1:A:855:VAL:CG1	2.41	0.50
1:B:747:THR:HG1	1:B:829:ILE:HD12	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:655:GLU:OE2	1:B:674:ARG:NH2	2.45	0.49
1:A:841:ILE:CD1	1:A:841:ILE:H	2.26	0.49
1:B:300:LYS:HE2	1:B:380:ASP:O	2.12	0.49
1:B:509:ARG:CG	1:B:509:ARG:HH11	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
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: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:A:364:ILE:O	1:A:372:SER:OG	2.28	0.47
1:B:316:GLN:CA	1:B:316:GLN:HE21	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:A:836:MET:CE	1:A:844:LYS:NZ	2.78	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:874:GLN:HB3	1:A:875:TYR:CE2	2.49	0.47
1:B:305:GLU:HA	1:B:305:GLU:OE1	2.14	0.47
1:B:378:PHE:CD1	1:B:393:VAL:HG11	2.49	0.47
1:B:506:ALA:C	1:B:507:GLU:HG3	2.35	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ILE:HD12	1:A:829:ILE:HD11	1.97	0.47
1:A:823:HIS:HD1	1:A:823:HIS:H	1.63	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: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:HG12	1:A:494:ILE:O	2.14	0.46
1:B:316:GLN:CA	1:B:316:GLN:NE2	2.70	0.46
1:A:818:GLN:O	1:A:818:GLN:CG	2.63	0.46
1:B:581:LEU:HD22	1:B:581:LEU:O	2.16	0.46
1:A:332:LYS:O	1:A:333:ASN:C	2.53	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: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
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: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: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:HA	1:A:539:LEU:HD23	1.69	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:B:646:ASN:C	1:B:646:ASN:HD22	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:TYR:CD1	1:B:340:TYR:C	2.90	0.44
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:B:261:ASP:HB3	1:B:477:GLN:CD	2.38	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:732:ILE:HG22	1:A:737:SER:HB2	2.00	0.44
1:B:696:LEU:HD23	1:B:696:LEU:H	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: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
1:B:418:LEU:O	1:B:422:ILE:HD12	2.17	0.44
1:B:323:PHE:CE2	1:B:620:ILE:HD11	2.53	0.44
1:A:738:LYS:N	1:A:738:LYS:HD3	2.33	0.43
1:A:754:ARG:HG2	1:A:759:SER:OG	2.18	0.43
1:B:350:HIS:C	1:B:352:GLN:H	2.21	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:HG13	1:B:260:ILE:H	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: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:754:ARG:NH1	1:A:754:ARG:HG2	2.33	0.43
1:B:637:SER:HB3	1:B:646:ASN:HD21	1.84	0.43
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:A:854:LEU:O	1:A:855:VAL:C	2.58	0.42
1:B:543:GLN:HG2	1:B:543:GLN:H	1.60	0.42
1:A:364:ILE:HD12	1:A:373:PRO:HB3	2.00	0.42
1:B:361:LYS:HG2	1:B:361:LYS:H	1.60	0.42
1:A:699:ASN:C	1:A:699:ASN:HD22	2.23	0.42
1:B:457:ILE:O	1:B:457:ILE:HG22	2.19	0.42
1:B:692:TYR:HA	1:B:692:TYR:HD1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:536:LEU:HA	1:A:536:LEU:HD23	1.71	0.42
1:A:317:ARG:NE	1:A:543:GLN:HA	2.35	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
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:CA	1:A:816:GLU:OE1	2.68	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:A:367:GLU:CD	1:A:564:ARG:HH22	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:A:418:LEU:O	1:A:419:ALA:C	2.58	0.41
1:A:863:SER:O	1:A:864:ASP:C	2.58	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:B:288:PRO:HB3	1:B:843:TRP:CE2	2.56	0.41
1:A:352:GLN:NE2	1:A:544:SER:O	2.54	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:B:577:VAL:O	1:B:577:VAL:CG1	2.62	0.41
1:B:754:ARG:HA	1:B:755:PRO:HD3	1.91	0.41
1:A:746:LEU:HD22	1:A:750:ILE:HD11	2.03	0.41
1:A:792:ASN:HA	1:A:792:ASN:HD22	1.78	0.41
1:A:808:LEU:HA	1:A:808:LEU:HD13	1.92	0.41
1:A:435:SER:O	1:A:436:GLU:C	2.59	0.41
1:A:418:LEU:HD11	1:A:634:LEU:HG	2.02	0.41
1:B:308:GLU:O	1:B:309:HIS:C	2.54	0.41
1:A:797:GLN:HA	1:A:800:ILE:HG22	2.03	0.40
1:A:317:ARG:HE	1:A:543:GLN:HA	1.86	0.40
1:B:280:ILE:HG21	1:B:280:ILE:HD12	1.90	0.40
1:B:712:ALA:O	1:B:716:ILE:HG23	2.22	0.40
1:A:315:LEU:C	1:A:315:LEU:CD2	2.82	0.40
1:A:823:HIS:CG	1:A:823:HIS:O	2.73	0.40
1:B:304:LEU:N	1:B:304:LEU:HD13	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:311:GLU:C	1:A:313:VAL:H	2.24	0.40
1:A:566:LYS:HE3	1:A:738:LYS:HZ2	1.87	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%)	32	60
1	B	621/655 (95%)	544 (88%)	69 (11%)	8 (1%)	14	35
All	All	1242/1310 (95%)	1098 (88%)	133 (11%)	11 (1%)	20	46

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%)	464 (82%)	105 (18%)	2	5
1	B	569/595 (96%)	460 (81%)	109 (19%)	1	4
All	All	1138/1190 (96%)	924 (81%)	214 (19%)	2	5

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	ILE
1	A	262	LEU
1	A	264	ASP
1	A	286	ASP
1	A	287	HIS
1	A	311	GLU
1	A	314	CYS
1	A	315	LEU
1	A	332	LYS
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	351	GLU
1	A	355	SER
1	A	356	PHE
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	398	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	400	ARG
1	A	404	ARG
1	A	428	LEU
1	A	433	LEU
1	A	438	LEU
1	A	439	ASN
1	A	444	LYS
1	A	449	LYS
1	A	452	LEU
1	A	454	ILE
1	A	466	PHE
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	502	ASN
1	A	515	GLU
1	A	517	THR
1	A	532	ASP
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	646	ASN
1	A	669	LEU
1	A	672	LEU
1	A	696	LEU
1	A	699	ASN
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	738	LYS
1	A	743	ASP
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	818	GLN
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	263	ASN
1	B	264	ASP
1	B	280	ILE
1	B	287	HIS
1	B	289	VAL
1	B	304	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	309	HIS
1	B	315	LEU
1	B	316	GLN
1	B	319	GLN
1	B	342	LYS
1	B	353	VAL
1	B	356	PHE
1	B	357	ASN
1	B	358	GLU
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	426	THR
1	B	433	LEU
1	B	439	ASN
1	B	440	VAL
1	B	442	PRO
1	B	452	LEU
1	B	454	ILE
1	B	461	SER
1	B	466	PHE
1	B	475	GLN
1	B	486	LEU
1	B	488	THR
1	B	498	THR
1	B	502	ASN
1	B	507	GLU
1	B	509	ARG
1	B	517	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	525	THR
1	B	536	LEU
1	B	539	LEU
1	B	543	GLN
1	B	556	LYS
1	B	560	LEU
1	B	566	LYS
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	606	LEU
1	B	616	ILE
1	B	619	LEU
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	672	LEU
1	B	674	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	769	LYS
1	B	774	ILE
1	B	780	HIS
1	B	781	TYR
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	821	ASN
1	B	847	SER
1	B	849	LEU
1	B	853	LYS
1	B	854	LEU
1	B	855	VAL
1	B	871	ARG
1	B	872	ILE
1	B	874	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	309	HIS
1	A	316	GLN
1	A	359	ASN
1	A	369	ASN
1	A	434	ASN
1	A	439	ASN
1	A	502	ASN
1	A	646	ASN
1	A	666	ASN
1	A	684	GLN
1	A	686	GLN
1	A	694	ASN
1	A	699	ASN
1	A	783	ASN
1	A	792	ASN
1	A	794	GLN
1	A	817	HIS
1	A	818	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	837	ASN
1	B	316	GLN
1	B	369	ASN
1	B	434	ASN
1	B	439	ASN
1	B	447	GLN
1	B	502	ASN
1	B	549	GLN
1	B	646	ASN
1	B	666	ASN
1	B	686	GLN
1	B	691	ASN
1	B	794	GLN
1	B	797	GLN
1	B	818	GLN
1	B	821	ASN
1	B	851	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 carbohydrates 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	0.31	0	6,6,6	0.49	0
2	SO4	A	1883	-	4,4,4	0.42	0	6,6,6	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1882	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1883	-	-	0/0/0/0	0/0/0/0

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%)	0.39	56 (8%) 10 8	32, 64, 146, 240	0
1	B	623/655 (95%)	0.60	70 (11%) 6 4	41, 85, 174, 263	0
All	All	1246/1310 (95%)	0.50	126 (10%) 8 6	32, 74, 162, 263	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	786	ASP	14.9
1	B	373	PRO	13.8
1	B	689	PRO	12.3
1	B	372	SER	11.6
1	A	782	VAL	11.4
1	A	371	PRO	10.0
1	B	782	VAL	9.8
1	B	787	LYS	9.2
1	A	368	LYS	9.1
1	A	783	ASN	8.9
1	B	781	TYR	8.4
1	B	371	PRO	8.3
1	A	366	SER	8.3
1	B	370	ASP	8.1
1	B	797	GLN	7.6
1	B	369	ASN	7.2
1	B	788	THR	6.8
1	A	786	ASP	6.7
1	B	690	GLU	6.5
1	A	369	ASN	6.4
1	B	366	SER	5.9
1	A	788	THR	5.8
1	B	356	PHE	5.8
1	A	779	GLY	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	308	GLU	5.6
1	A	696	LEU	5.4
1	B	693	GLY	5.4
1	B	687	ASP	5.3
1	B	363	GLU	5.1
1	A	784	ALA	5.1
1	A	307	SER	5.0
1	A	628	SER	5.0
1	A	787	LYS	5.0
1	B	796	LEU	4.9
1	A	794	GLN	4.9
1	B	783	ASN	4.9
1	A	370	ASP	4.8
1	A	627	ASN	4.8
1	B	307	SER	4.7
1	B	821	ASN	4.6
1	A	781	TYR	4.6
1	B	317	ARG	4.6
1	B	791	GLU	4.6
1	B	365	ILE	4.5
1	A	306	ASN	4.4
1	A	626	LYS	4.4
1	A	625	HIS	4.3
1	B	313	VAL	4.3
1	B	801	LYS	4.2
1	A	689	PRO	4.2
1	A	780	HIS	4.2
1	B	691	ASN	4.1
1	B	368	LYS	4.1
1	B	792	ASN	4.1
1	B	345	VAL	4.1
1	B	780	HIS	4.1
1	B	692	TYR	4.0
1	A	305	GLU	3.9
1	A	793	LYS	3.8
1	B	785	PRO	3.8
1	B	314	CYS	3.8
1	A	821	ASN	3.8
1	A	309	HIS	3.7
1	A	785	PRO	3.7
1	B	344	LYS	3.7
1	B	359	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	260	ILE	3.6
1	A	796	LEU	3.6
1	A	686	GLN	3.6
1	A	695	THR	3.6
1	A	792	ASN	3.6
1	B	354	VAL	3.6
1	A	789	GLU	3.5
1	B	799	GLN	3.4
1	B	789	GLU	3.4
1	A	365	ILE	3.3
1	B	794	GLN	3.3
1	B	596	TYR	3.2
1	B	784	ALA	3.2
1	B	578	ALA	3.2
1	A	819	ASN	3.2
1	A	820	GLY	3.1
1	A	835	ASP	3.1
1	B	347	GLY	3.0
1	B	694	ASN	3.0
1	B	790	ASP	3.0
1	A	590	ASN	3.0
1	B	590	ASN	2.9
1	A	259	GLU	2.9
1	A	790	ASP	2.9
1	A	308	GLU	2.9
1	B	349	ALA	2.9
1	B	779	GLY	2.8
1	B	818	GLN	2.8
1	B	836	MET	2.7
1	B	341	TYR	2.7
1	B	357	ASN	2.7
1	B	686	GLN	2.7
1	B	798	ALA	2.7
1	A	795	ILE	2.7
1	A	834	ARG	2.7
1	B	346	PRO	2.6
1	A	355	SER	2.6
1	B	800	ILE	2.6
1	A	315	LEU	2.6
1	A	687	ASP	2.6
1	B	374	ILE	2.6
1	B	625	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	315	LEU	2.6
1	A	372	SER	2.5
1	B	339	ARG	2.5
1	B	814	ASN	2.5
1	B	364	ILE	2.4
1	A	367	GLU	2.4
1	B	695	THR	2.4
1	A	694	ASN	2.3
1	B	260	ILE	2.3
1	A	623	SER	2.3
1	A	693	GLY	2.2
1	A	814	ASN	2.2
1	B	807	GLU	2.2
1	A	818	GLN	2.1
1	B	806	GLU	2.1
1	B	835	ASP	2.1
1	A	406	GLY	2.0
1	A	629	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	1882	5/5	0.96	0.22	1.26	62,63,64,67	0
2	SO4	A	1883	5/5	0.95	0.11	-1.87	70,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.