



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 AM UTC

PDB ID : 5Z16 / pdb_00005z16
Title : A novel dimeric isocitrate dehydrogenase from *Acinetobacter baumannii*
Authors : Song, P.; Huang, S.P.; Wang, P.; Zhu, G.P.
Deposited on : 2017-12-25
Resolution : 3.00 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

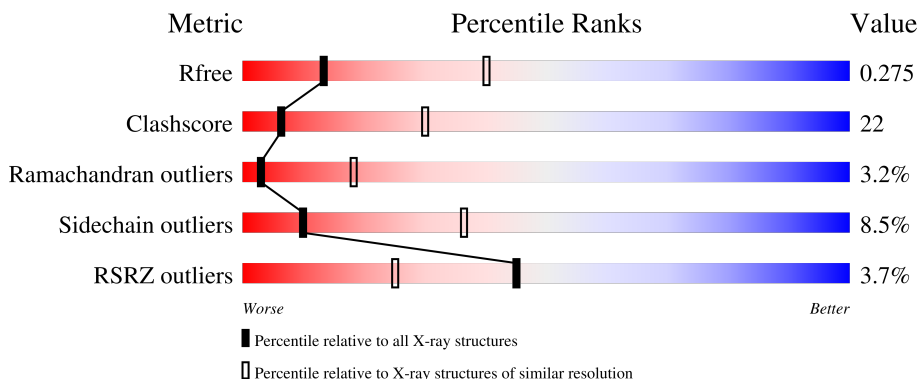
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	751	
1	B	751	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11788 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.

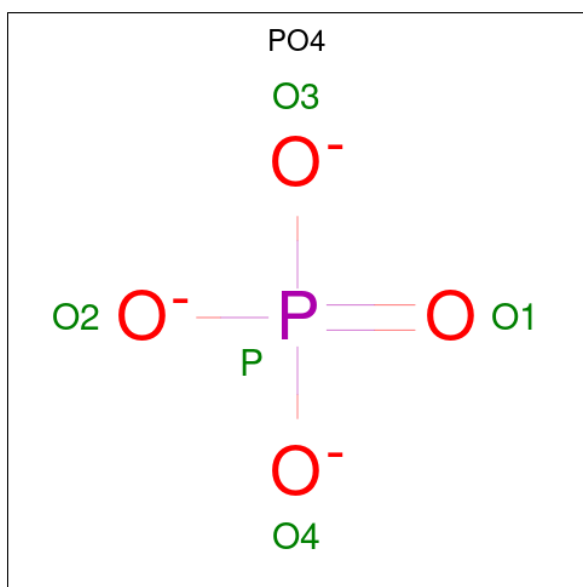
- Molecule 1 is a protein called Isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5666	3571	969	1091	35			
1	B	739	Total	C	N	O	S	0	0	0
			5741	3626	978	1102	35			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP V5VCI0
A	-4	HIS	-	expression tag	UNP V5VCI0
A	-3	HIS	-	expression tag	UNP V5VCI0
A	-2	HIS	-	expression tag	UNP V5VCI0
A	-1	HIS	-	expression tag	UNP V5VCI0
A	0	HIS	-	expression tag	UNP V5VCI0
A	629	THR	ALA	conflict	UNP V5VCI0
B	-5	HIS	-	expression tag	UNP V5VCI0
B	-4	HIS	-	expression tag	UNP V5VCI0
B	-3	HIS	-	expression tag	UNP V5VCI0
B	-2	HIS	-	expression tag	UNP V5VCI0
B	-1	HIS	-	expression tag	UNP V5VCI0
B	0	HIS	-	expression tag	UNP V5VCI0
B	629	THR	ALA	conflict	UNP V5VCI0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

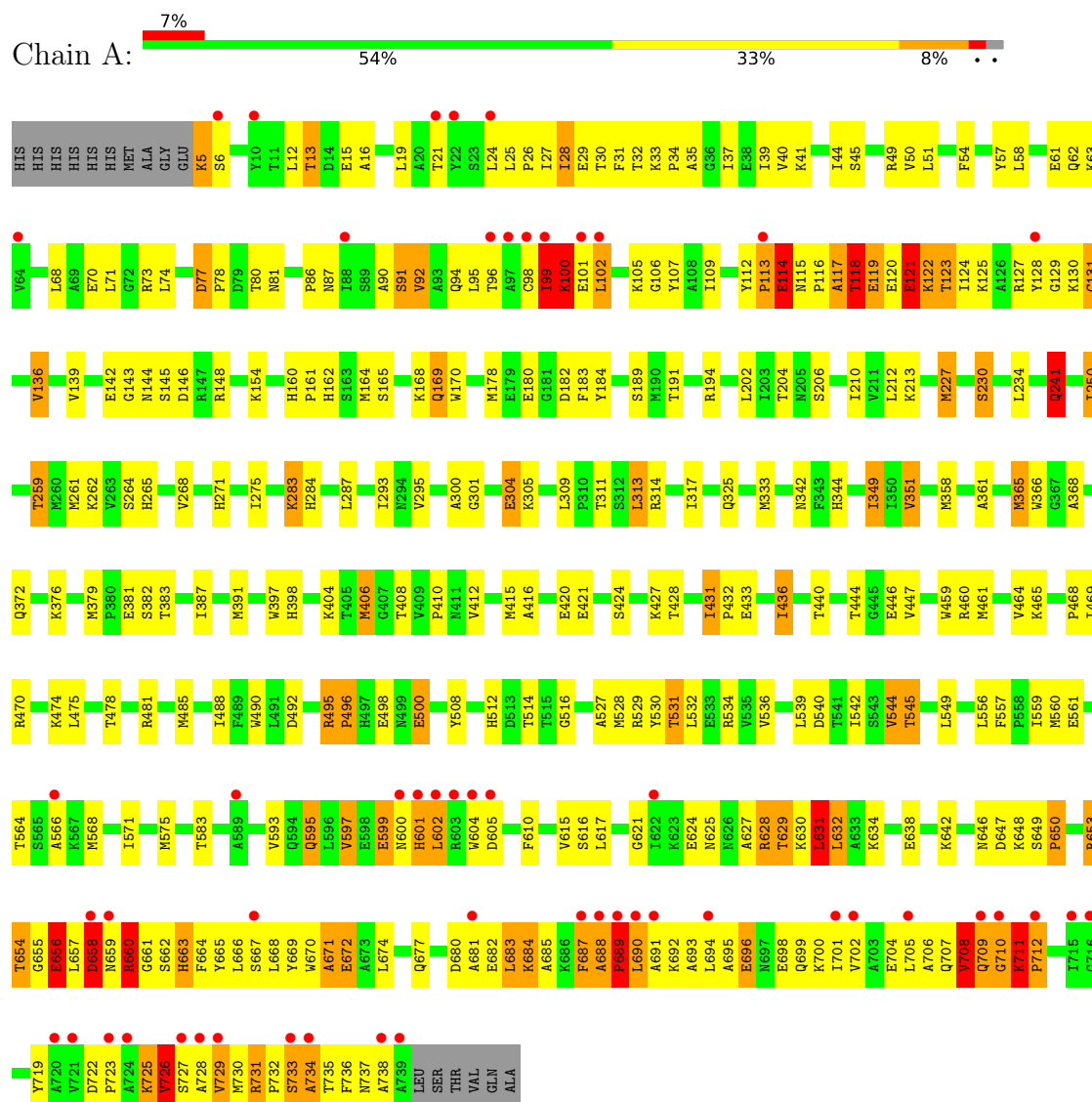
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total	O	0	0
			201	201		
4	B	168	Total	O	0	0
			168	168		

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: Isocitrate dehydrogenase



• Molecule 1: Isocitrate dehydrogenase



I715	L602	L491	Y373	K257	D111	HIS
Y718	E609	D492	M379	T259	A117	HIS
V721		P493	P380	M260	T118	HIS
V726	L613	H497	E381	M261	E119	HIS
V729	V615	E498	S382	I267	E120	HIS
R730	E619	N499	S382	I267	E121	MET
R731	M620	E500		I275	K122	ALA
T742	K623	L509	I387	I276	T123	GLY
V743		T515	Y388	Y277	T123	GLY
Q744		L517	Q389		I124	GLU
ALA			E390			LYS
					R127	S6
					</	

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.16Å 137.16Å 238.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 3.00 48.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-3.00) 99.9 (48.54-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.276 0.210 , 0.275	Depositor DCC
R_{free} test set	2267 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11788	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: PO4, MG

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	0.70	2/5773 (0.0%)	1.19	50/7810 (0.6%)
1	B	0.63	0/5855	0.99	12/7923 (0.2%)
All	All	0.66	2/11628 (0.0%)	1.09	62/15733 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	HIS	CE1-NE2	-8.96	1.23	1.32
1	A	160	HIS	CD2-NE2	8.64	1.47	1.37

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	LYS	CA-C-N	-15.35	100.65	119.84
1	A	711	LYS	C-N-CA	-15.35	100.65	119.84
1	A	119	GLU	N-CA-C	9.92	128.86	113.28
1	A	689	PRO	N-CA-C	-9.41	93.08	112.47
1	A	709	GLN	N-CA-C	9.36	130.74	110.80
1	A	649	SER	CA-C-N	8.68	130.69	119.84
1	A	649	SER	C-N-CA	8.68	130.69	119.84
1	A	660	ARG	CB-CG-CD	8.12	129.98	111.30
1	A	431	ILE	CA-C-N	8.11	127.41	118.97
1	A	431	ILE	C-N-CA	8.11	127.41	118.97
1	A	595	GLN	N-CA-C	-7.99	103.52	113.18
1	B	485	MET	CA-C-N	-7.94	112.17	120.03
1	B	485	MET	C-N-CA	-7.94	112.17	120.03
1	A	122	LYS	N-CA-C	-7.86	103.92	113.97
1	A	722	ASP	C-N-CD	-7.69	93.48	125.00
1	A	61	GLU	N-CA-C	-7.25	104.29	113.72
1	A	129	GLY	N-CA-C	-7.25	105.82	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	GLY	N-CA-C	-7.12	96.30	113.18
1	A	160	HIS	ND1-CG-CD2	6.71	112.81	106.10
1	A	77	ASP	CA-C-N	6.61	126.30	119.82
1	A	77	ASP	C-N-CA	6.61	126.30	119.82
1	A	495	ARG	CA-C-N	6.59	128.07	119.84
1	A	495	ARG	C-N-CA	6.59	128.07	119.84
1	A	13	THR	CB-CA-C	-6.52	107.68	117.07
1	A	557	PHE	CA-C-N	-6.37	113.13	119.56
1	A	557	PHE	C-N-CA	-6.37	113.13	119.56
1	A	689	PRO	CA-C-N	6.25	133.47	121.54
1	A	689	PRO	C-N-CA	6.25	133.47	121.54
1	A	687	PHE	N-CA-C	-6.22	102.98	111.56
1	A	689	PRO	CA-C-O	6.18	131.85	120.60
1	A	241	GLN	CA-CB-CG	-6.10	101.89	114.10
1	A	13	THR	N-CA-C	6.09	113.78	108.78
1	B	355	MET	CA-C-N	-6.00	112.31	118.85
1	B	355	MET	C-N-CA	-6.00	112.31	118.85
1	A	102	LEU	CA-CB-CG	6.00	137.28	116.30
1	A	99	ILE	N-CA-C	-5.99	96.89	109.34
1	A	601	HIS	N-CA-C	5.94	123.45	110.80
1	A	13	THR	CA-C-O	5.91	121.37	117.94
1	B	555	ASP	N-CA-C	-5.84	105.16	112.93
1	A	545	THR	N-CA-C	5.83	117.08	108.86
1	A	683	LEU	CA-CB-CG	-5.83	95.91	116.30
1	A	213	LYS	CA-C-N	5.72	124.92	118.97
1	A	213	LYS	C-N-CA	5.72	124.92	118.97
1	B	16	ALA	CA-C-N	-5.68	113.96	119.87
1	B	16	ALA	C-N-CA	-5.68	113.96	119.87
1	A	91	SER	N-CA-C	5.63	115.72	108.34
1	A	726	VAL	N-CA-C	-5.60	97.69	109.34
1	A	351	VAL	N-CA-C	5.54	116.17	110.36
1	B	143	GLY	N-CA-C	5.52	126.26	113.18
1	B	517	LEU	N-CA-C	5.50	117.18	110.41
1	A	194	ARG	CA-C-N	-5.48	114.28	119.76
1	A	194	ARG	C-N-CA	-5.48	114.28	119.76
1	B	453	VAL	N-CA-C	5.31	116.97	108.89
1	A	264	SER	N-CA-C	5.29	116.73	110.97
1	A	118	THR	N-CA-C	5.26	115.96	108.54
1	B	189	SER	N-CA-C	5.25	117.04	109.07
1	A	632	LEU	N-CA-C	-5.23	105.76	111.82
1	A	189	SER	N-CA-C	5.18	116.16	108.60
1	B	396	LYS	N-CA-C	-5.16	105.73	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	GLU	N-CA-C	-5.10	104.80	111.02
1	A	660	ARG	CG-CD-NE	-5.04	100.92	112.00
1	A	631	LEU	N-CA-C	5.02	116.44	110.97

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	5666	0	5620	380	0
1	B	5741	0	5699	126	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	201	0	0	22	0
4	B	168	0	0	22	0
All	All	11788	0	11319	503	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 22.

All (503) 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:24:LEU:CD2	1:A:663:HIS:ND1	1.81	1.43
1:A:24:LEU:HD23	1:A:663:HIS:ND1	1.14	1.40
1:A:688:ALA:C	1:A:690:LEU:H	1.04	1.39
1:A:96:THR:HA	1:A:99:ILE:CG2	1.56	1.35
1:A:96:THR:O	1:A:100:LYS:HD2	1.25	1.31
1:A:731:ARG:HG3	1:A:736:PHE:CE1	1.66	1.29
1:A:725:LYS:CE	1:A:726:VAL:HG13	1.63	1.28
1:A:659:ASN:O	1:A:663:HIS:CB	1.83	1.24
1:A:659:ASN:O	1:A:663:HIS:HB2	1.33	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:CA	1:A:99:ILE:HG22	1.67	1.23
1:A:24:LEU:HD23	1:A:663:HIS:CE1	1.76	1.21
1:A:24:LEU:HD11	1:A:659:ASN:OD1	1.42	1.20
1:A:96:THR:O	1:A:100:LYS:CD	1.91	1.18
1:A:688:ALA:C	1:A:690:LEU:N	1.83	1.18
1:A:725:LYS:HE2	1:A:726:VAL:HG13	1.15	1.15
1:A:705:LEU:HA	1:A:708:VAL:HG13	1.35	1.07
1:A:725:LYS:HE2	1:A:726:VAL:CG1	1.85	1.06
1:A:729:VAL:HG13	1:A:730:MET:H	1.18	1.06
1:A:101:GLU:OE1	1:A:719:TYR:HB2	1.56	1.05
1:A:731:ARG:CG	1:A:736:PHE:HE1	1.70	1.04
1:A:24:LEU:HD23	1:A:663:HIS:CG	1.93	1.03
1:A:96:THR:HA	1:A:99:ILE:HG22	1.04	1.02
1:A:687:PHE:C	1:A:689:PRO:HD2	1.84	1.01
1:A:24:LEU:CD2	1:A:663:HIS:CG	2.43	1.01
1:A:729:VAL:O	1:A:732:PRO:HD3	1.60	1.00
1:A:657:LEU:O	1:A:658:ASP:O	1.79	0.99
1:B:117:ALA:O	1:B:118:THR:HB	1.61	0.99
1:A:729:VAL:HG13	1:A:730:MET:N	1.73	0.99
1:A:101:GLU:CD	1:A:719:TYR:HB2	1.88	0.97
1:A:391:MET:HE3	1:A:528:MET:HE1	1.45	0.97
1:A:725:LYS:NZ	1:A:726:VAL:HG13	1.80	0.97
1:A:729:VAL:CG1	1:A:730:MET:H	1.77	0.96
1:A:655:GLY:H	1:A:656:GLU:HB3	1.31	0.96
1:B:254:LEU:H	1:B:342:ASN:HD21	1.13	0.94
1:A:659:ASN:O	1:A:663:HIS:HB3	1.68	0.94
1:A:101:GLU:OE1	1:A:719:TYR:CD2	2.21	0.93
1:A:101:GLU:OE1	1:A:719:TYR:HD2	1.52	0.91
1:A:24:LEU:HD21	1:A:663:HIS:HA	1.52	0.91
1:A:96:THR:HA	1:A:99:ILE:HG21	1.52	0.91
1:B:534:ARG:NH2	1:B:540:ASP:O	2.04	0.90
1:A:24:LEU:CD1	1:A:659:ASN:OD1	2.21	0.89
1:A:25:LEU:HD23	1:A:41:LYS:HE3	1.55	0.89
1:A:96:THR:C	1:A:99:ILE:HG22	1.97	0.88
1:A:695:ALA:HA	1:A:698:GLU:HB3	1.54	0.87
1:A:101:GLU:OE1	1:A:719:TYR:CB	2.23	0.86
1:A:24:LEU:HD21	1:A:663:HIS:CB	2.06	0.86
1:A:24:LEU:HD21	1:A:663:HIS:CA	2.05	0.85
1:A:688:ALA:N	1:A:689:PRO:CD	2.38	0.85
1:A:628:ARG:HD3	1:A:683:LEU:HD11	1.59	0.84
1:A:99:ILE:CD1	4:A:954:HOH:O	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LEU:CA	1:A:708:VAL:HG13	2.07	0.84
1:A:631:LEU:HD12	1:A:632:LEU:H	1.43	0.83
1:A:115:ASN:N	1:A:116:PRO:HD3	1.93	0.82
1:A:731:ARG:O	4:A:901:HOH:O	1.95	0.82
1:A:564:THR:HG22	1:A:566:ALA:H	1.45	0.82
1:A:24:LEU:HD21	1:A:663:HIS:CG	2.13	0.81
1:B:19:LEU:HD13	1:B:596:LEU:HD22	1.61	0.81
1:A:655:GLY:N	1:A:656:GLU:HB3	1.95	0.81
1:A:688:ALA:O	1:A:690:LEU:N	2.14	0.81
1:A:704:GLU:OE1	1:A:733:SER:OG	1.97	0.81
1:A:725:LYS:CE	1:A:726:VAL:CG1	2.50	0.80
1:A:687:PHE:C	1:A:689:PRO:CD	2.54	0.79
1:A:420:GLU:H	1:A:464:VAL:HG22	1.46	0.79
1:A:731:ARG:HG3	1:A:736:PHE:HE1	0.74	0.79
1:A:99:ILE:C	1:A:100:LYS:HD3	2.10	0.77
1:A:631:LEU:HD21	1:A:683:LEU:HD13	1.67	0.77
1:B:117:ALA:O	1:B:118:THR:CB	2.33	0.77
1:A:725:LYS:HD3	1:A:725:LYS:N	2.00	0.77
1:A:118:THR:N	1:A:121:GLU:OE2	2.18	0.76
1:A:96:THR:CA	1:A:99:ILE:CG2	2.41	0.76
1:A:658:ASP:HB2	1:A:660:ARG:NH2	2.02	0.74
1:B:119:GLU:OE2	4:B:901:HOH:O	2.04	0.74
1:A:99:ILE:HG12	4:A:954:HOH:O	1.88	0.74
1:B:204:THR:HG22	1:B:206:SER:H	1.53	0.74
1:A:668:LEU:HG	1:A:669:TYR:CE1	2.23	0.73
1:A:28:ILE:O	1:A:30:THR:N	2.22	0.73
1:A:96:THR:C	1:A:100:LYS:HD2	2.14	0.72
1:A:656:GLU:CD	1:A:660:ARG:HH21	1.97	0.72
1:A:692:LYS:HA	1:A:695:ALA:HB3	1.72	0.72
1:A:729:VAL:O	1:A:732:PRO:CD	2.37	0.72
1:A:77:ASP:HB3	1:A:80:THR:HG23	1.72	0.72
1:B:15:GLU:OE2	1:B:718:TYR:OH	2.05	0.71
1:A:102:LEU:O	1:A:106:GLY:N	2.23	0.71
1:A:182:ASP:OD2	1:A:382:SER:HB3	1.91	0.71
1:A:51:LEU:HD21	1:A:102:LEU:HD11	1.72	0.71
1:B:402:ASP:OD1	1:B:404:LYS:HD3	1.89	0.71
1:A:646:ASN:HD22	1:A:648:LYS:NZ	1.89	0.70
1:A:646:ASN:O	1:A:648:LYS:N	2.21	0.70
1:A:481:ARG:HH22	1:A:516:GLY:H	1.40	0.70
1:A:261:MET:HE1	1:A:421:GLU:HB3	1.75	0.69
1:B:191:THR:HG22	1:B:500:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:O	1:A:100:LYS:HD3	1.89	0.68
1:A:293:ILE:HG13	4:A:968:HOH:O	1.93	0.68
1:A:100:LYS:HD3	1:A:100:LYS:N	2.09	0.68
1:A:99:ILE:H	1:A:100:LYS:HD3	1.58	0.68
1:A:123:THR:O	1:A:127:ARG:HB2	1.94	0.68
1:B:254:LEU:H	1:B:342:ASN:ND2	1.89	0.68
1:A:527:ALA:O	1:A:531:THR:HG23	1.94	0.67
1:A:693:ALA:HA	1:A:696:GLU:HG2	1.77	0.67
1:B:436:ILE:HG23	1:B:450:THR:HG23	1.76	0.67
1:B:37:ILE:HD11	1:B:629:THR:HG22	1.76	0.67
1:A:406:MET:HE2	1:A:561:GLU:HG2	1.76	0.67
1:B:416:ALA:HB3	1:B:468:PRO:HB3	1.76	0.67
1:A:99:ILE:HD11	4:A:954:HOH:O	1.94	0.67
1:A:664:PHE:HE1	1:A:694:LEU:HB3	1.59	0.67
1:B:150:PRO:HG2	1:B:153:VAL:HG23	1.76	0.67
1:A:692:LYS:O	1:A:696:GLU:N	2.28	0.66
1:B:44:ILE:HG12	4:B:946:HOH:O	1.95	0.66
1:A:688:ALA:C	1:A:690:LEU:CA	2.68	0.66
1:A:62:GLN:NE2	1:A:106:GLY:O	2.29	0.66
1:A:127:ARG:C	1:A:130:LYS:HD3	2.21	0.65
1:A:601:HIS:HA	1:A:660:ARG:NH2	2.11	0.65
1:A:685:ALA:HA	1:A:687:PHE:H	1.62	0.65
1:A:96:THR:O	1:A:99:ILE:HG22	1.96	0.65
1:A:646:ASN:HD22	1:A:648:LYS:HZ1	1.45	0.64
1:B:653:ARG:O	1:B:654:THR:CB	2.45	0.64
1:A:729:VAL:CG1	1:A:730:MET:N	2.40	0.64
1:A:727:SER:O	1:A:729:VAL:N	2.28	0.64
1:A:26:PRO:HB2	1:A:731:ARG:HH12	1.62	0.63
1:A:169:GLN:HB2	1:B:174:HIS:CD2	2.33	0.63
1:A:685:ALA:CA	1:A:687:PHE:H	2.11	0.63
1:B:148:ARG:HB3	1:B:410:PRO:HB3	1.81	0.63
1:B:191:THR:CG2	1:B:500:GLU:HG3	2.28	0.63
1:A:427:LYS:HD2	1:A:461:MET:HE3	1.79	0.63
1:A:112:TYR:HE1	1:A:125:LYS:HG3	1.62	0.62
1:A:602:LEU:CB	1:A:658:ASP:OD2	2.47	0.62
1:A:311:THR:HG22	1:A:314:ARG:NH1	2.15	0.62
1:A:358:MET:HB2	1:A:365:MET:HE3	1.81	0.62
1:A:113:PRO:O	1:A:114:GLU:O	2.17	0.61
1:A:101:GLU:HG3	1:A:101:GLU:O	1.99	0.61
1:A:112:TYR:HD1	1:A:125:LYS:HD2	1.63	0.61
1:A:127:ARG:O	1:A:128:TYR:CD1	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:ALA:HA	1:A:687:PHE:N	2.15	0.61
1:A:733:SER:OG	1:A:734:ALA:N	2.32	0.61
1:A:344:HIS:ND1	2:A:801:PO4:O4	2.24	0.61
1:A:305:LYS:HD2	4:A:968:HOH:O	2.00	0.61
1:B:301:GLY:O	1:B:305:LYS:HG3	2.01	0.61
1:A:96:THR:O	1:A:99:ILE:CG2	2.48	0.61
1:A:631:LEU:HD12	1:A:632:LEU:N	2.14	0.61
1:A:601:HIS:C	1:A:660:ARG:HH22	2.09	0.61
1:A:148:ARG:HB3	1:A:410:PRO:HB3	1.82	0.60
1:A:655:GLY:H	1:A:656:GLU:CB	2.09	0.60
1:A:704:GLU:OE1	1:A:735:THR:OG1	2.16	0.60
1:B:531:THR:O	1:B:535:VAL:HG23	2.00	0.60
1:A:342:ASN:OD1	1:A:349:ILE:HD12	2.01	0.60
1:A:731:ARG:HD2	1:A:736:PHE:HD1	1.65	0.60
1:B:200:MET:SD	1:B:461:MET:HE2	2.42	0.60
1:A:351:VAL:HG21	1:A:379:MET:HE3	1.84	0.60
1:A:99:ILE:CG1	4:A:954:HOH:O	2.44	0.59
1:B:626:ASN:O	1:B:629:THR:OG1	2.19	0.59
1:A:736:PHE:CG	1:A:737:ASN:N	2.70	0.59
1:A:24:LEU:CD2	1:A:663:HIS:HA	2.29	0.59
1:B:707:GLN:O	1:B:711:LYS:NZ	2.35	0.59
1:A:27:ILE:HD11	1:A:667:SER:CB	2.32	0.59
1:A:664:PHE:CE1	1:A:694:LEU:HB3	2.37	0.59
1:A:731:ARG:HD2	1:A:736:PHE:CD1	2.38	0.59
1:A:687:PHE:O	1:A:689:PRO:HD2	2.01	0.59
1:A:101:GLU:OE1	1:A:719:TYR:CG	2.55	0.59
1:A:705:LEU:HB2	1:A:708:VAL:HG11	1.85	0.59
1:A:120:GLU:HA	1:A:123:THR:HG22	1.85	0.58
1:A:730:MET:C	1:A:732:PRO:HD3	2.28	0.58
1:B:653:ARG:O	1:B:654:THR:HB	2.02	0.58
1:A:661:GLY:O	1:A:665:TYR:N	2.25	0.58
1:A:688:ALA:HA	1:A:690:LEU:HA	1.85	0.58
1:A:130:LYS:H	1:A:130:LYS:HD2	1.69	0.58
1:A:112:TYR:CD1	1:A:125:LYS:HD2	2.38	0.58
1:A:688:ALA:N	1:A:689:PRO:HD2	2.06	0.58
1:A:70:GLU:HA	1:A:73:ARG:HH11	1.68	0.57
1:A:144:ASN:HA	1:A:415:MET:HG2	1.85	0.57
1:A:259:THR:O	1:A:262:LYS:HE3	2.04	0.57
1:A:283:LYS:HE2	1:A:284:HIS:NE2	2.19	0.57
1:B:336:SER:OG	1:B:367:GLY:O	2.21	0.57
1:A:81:ASN:OD1	1:A:616:SER:OG	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HG	1:A:659:ASN:HD21	1.68	0.57
1:A:727:SER:C	1:A:729:VAL:H	2.12	0.57
1:A:130:LYS:HD2	1:A:130:LYS:N	2.18	0.57
1:A:474:LYS:O	1:A:478:THR:HG23	2.04	0.57
1:A:534:ARG:NH2	1:A:540:ASP:O	2.33	0.57
1:A:90:ALA:HB3	1:A:131:CYS:O	2.04	0.57
1:A:736:PHE:H	1:A:736:PHE:HD2	1.52	0.57
1:A:333:MET:HG3	1:A:368:ALA:HA	1.87	0.57
1:B:91:SER:OG	1:B:94:GLN:HG3	2.05	0.57
1:A:726:VAL:HA	1:A:729:VAL:HG12	1.86	0.56
1:A:40:VAL:HG23	4:A:917:HOH:O	2.04	0.56
1:A:5:LYS:N	4:A:915:HOH:O	2.39	0.56
1:A:227:MET:HE2	1:A:460:ARG:HG3	1.88	0.56
1:B:596:LEU:HD13	1:B:602:LEU:HB2	1.88	0.56
1:A:115:ASN:N	1:A:116:PRO:CD	2.63	0.56
1:B:311:THR:HG22	1:B:314:ARG:HH11	1.71	0.56
1:B:659:ASN:O	1:B:662:SER:OG	2.22	0.56
1:A:428:THR:HG23	1:A:460:ARG:HB3	1.87	0.56
1:B:387:ILE:HG13	4:B:986:HOH:O	2.06	0.56
1:A:709:GLN:O	1:A:709:GLN:HG2	2.06	0.55
1:A:731:ARG:CG	1:A:736:PHE:CE1	2.58	0.55
1:B:365:MET:HG2	4:B:928:HOH:O	2.05	0.55
1:A:650:PRO:HB3	1:A:658:ASP:HA	1.88	0.55
1:A:99:ILE:N	1:A:100:LYS:HD3	2.21	0.55
1:A:470:ARG:NH1	1:A:508:TYR:OH	2.40	0.55
1:A:688:ALA:O	1:A:690:LEU:HB2	2.06	0.55
1:A:114:GLU:OE1	1:A:114:GLU:N	2.40	0.55
1:A:725:LYS:HZ3	1:A:726:VAL:HG13	1.70	0.55
1:A:122:LYS:HD3	4:A:967:HOH:O	2.06	0.54
1:A:632:LEU:HD22	1:A:670:TRP:CZ2	2.41	0.54
1:A:658:ASP:HB2	1:A:660:ARG:CZ	2.37	0.54
1:A:604:TRP:HA	1:A:650:PRO:HG2	1.90	0.54
1:A:731:ARG:N	1:A:732:PRO:HD3	2.23	0.54
1:A:119:GLU:N	1:A:121:GLU:OE1	2.41	0.54
1:B:191:THR:HG22	1:B:223:ILE:HG12	1.88	0.54
1:B:225:ASP:OD1	1:B:497:HIS:ND1	2.36	0.54
1:B:223:ILE:HD13	1:B:500:GLU:HB3	1.89	0.54
1:B:634:LYS:O	1:B:637:ASP:HB2	2.07	0.54
1:A:669:TYR:O	1:A:672:GLU:HB3	2.08	0.54
1:A:40:VAL:N	4:A:917:HOH:O	2.40	0.53
1:A:705:LEU:HB2	1:A:708:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HA	1:A:105:LYS:HB2	1.90	0.53
1:B:257:LYS:NZ	1:B:551:ASP:OD2	2.41	0.53
1:B:267:ILE:HA	1:B:296:ASN:ND2	2.22	0.53
1:A:24:LEU:O	1:A:27:ILE:HG22	2.09	0.53
1:A:534:ARG:HB3	1:A:539:LEU:HB2	1.91	0.53
1:B:355:MET:O	1:B:359:ILE:HG13	2.07	0.53
1:A:96:THR:C	1:A:99:ILE:CG2	2.79	0.53
1:A:99:ILE:H	1:A:100:LYS:CD	2.20	0.53
1:A:648:LYS:NZ	1:A:669:TYR:OH	2.36	0.53
1:A:688:ALA:N	1:A:689:PRO:HD3	2.23	0.53
1:A:130:LYS:HB2	1:A:131:CYS:SG	2.49	0.53
1:A:311:THR:HG22	1:A:314:ARG:HH12	1.74	0.53
1:B:175:VAL:HB	1:B:389:GLN:HB2	1.90	0.53
1:B:225:ASP:OD2	1:B:462:CYS:HB2	2.09	0.53
1:B:547:ASN:OD1	1:B:550:ARG:NH1	2.41	0.53
1:A:31:PHE:N	4:A:920:HOH:O	2.42	0.53
1:A:387:ILE:HD13	1:A:490:TRP:HZ3	1.73	0.53
1:A:659:ASN:HA	1:A:662:SER:OG	2.08	0.53
1:A:726:VAL:CA	1:A:729:VAL:HG12	2.39	0.52
1:B:21:THR:HB	4:B:997:HOH:O	2.09	0.52
1:B:300:ALA:O	1:B:304:GLU:HG3	2.10	0.52
1:B:369:ASP:OD2	1:B:373:TYR:OH	2.27	0.52
1:A:54:PHE:HA	1:A:127:ARG:NH2	2.24	0.52
1:A:681:ALA:O	1:A:684:LYS:HB3	2.10	0.52
1:A:250:ILE:HG21	4:A:930:HOH:O	2.09	0.52
1:B:281:PHE:O	1:B:285:GLY:N	2.42	0.52
1:B:306:ILE:HD12	4:B:981:HOH:O	2.10	0.52
1:A:733:SER:HB3	1:A:736:PHE:CD2	2.45	0.52
1:A:102:LEU:HB3	1:A:107:TYR:HB2	1.91	0.51
1:B:277:TYR:CE2	1:B:299:MET:HE2	2.44	0.51
1:A:283:LYS:HG2	1:A:284:HIS:CD2	2.45	0.51
1:A:115:ASN:H	1:A:116:PRO:HD3	1.74	0.51
1:A:397:TRP:CD1	1:A:398:HIS:CD2	2.99	0.51
1:A:120:GLU:N	1:A:121:GLU:HG3	2.26	0.51
1:A:204:THR:HG22	1:A:206:SER:H	1.75	0.51
1:A:653:ARG:O	1:A:654:THR:OG1	2.22	0.51
1:B:660:ARG:NH1	1:B:729:VAL:O	2.44	0.51
1:A:24:LEU:HD22	1:A:663:HIS:ND1	2.10	0.51
1:A:21:THR:HB	4:A:902:HOH:O	2.10	0.50
1:A:658:ASP:CB	1:A:660:ARG:CZ	2.89	0.50
1:B:26:PRO:HG2	1:B:731:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ASN:CB	1:A:648:LYS:HE3	2.41	0.50
1:A:99:ILE:O	1:A:99:ILE:HG13	2.12	0.50
1:A:391:MET:HB2	1:A:528:MET:HE2	1.92	0.50
1:A:707:GLN:O	1:A:709:GLN:N	2.43	0.50
1:B:705:LEU:O	1:B:708:VAL:HG22	2.11	0.50
1:A:117:ALA:HB3	1:A:121:GLU:OE2	2.10	0.50
1:A:184:TYR:CE2	1:A:495:ARG:HB2	2.46	0.50
1:A:366:TRP:CZ3	1:A:372:GLN:HG3	2.46	0.50
1:A:528:MET:HE3	1:A:532:LEU:HD11	1.92	0.50
1:B:15:GLU:OE1	1:B:588:SER:OG	2.27	0.50
1:A:168:LYS:HD2	1:A:170:TRP:CH2	2.47	0.50
1:A:495:ARG:HD3	1:A:498:GLU:HG3	1.94	0.50
1:A:692:LYS:NZ	1:A:696:GLU:OE2	2.33	0.50
1:A:683:LEU:C	1:A:685:ALA:H	2.18	0.50
1:A:230:SER:OG	1:A:230:SER:O	2.30	0.49
1:A:424:SER:HA	1:A:427:LYS:HE2	1.93	0.49
1:A:490:TRP:HB2	1:A:545:THR:HG22	1.93	0.49
1:B:257:LYS:HE2	1:B:260:MET:HG3	1.94	0.49
1:B:257:LYS:HE2	1:B:260:MET:CG	2.42	0.49
1:B:601:HIS:CE1	1:B:658:ASP:HB3	2.47	0.49
1:A:309:LEU:HD13	1:A:313:LEU:HD13	1.93	0.49
1:B:550:ARG:CZ	4:B:961:HOH:O	2.59	0.49
1:A:665:TYR:HB3	1:A:669:TYR:CE2	2.46	0.49
1:A:21:THR:O	4:A:902:HOH:O	2.20	0.49
1:A:412:VAL:HB	1:A:544:VAL:HG13	1.93	0.49
1:B:53:GLU:OE2	1:B:127:ARG:HD2	2.12	0.49
1:A:440:THR:OG1	1:A:447:VAL:HG22	2.13	0.49
1:A:646:ASN:HB3	1:A:648:LYS:HE3	1.94	0.49
1:A:35:ALA:HA	1:A:628:ARG:HD2	1.93	0.48
1:A:529:ARG:HH12	1:B:390:GLU:CD	2.20	0.48
1:A:658:ASP:CB	1:A:660:ARG:NH2	2.74	0.48
1:A:162:HIS:CD2	4:A:965:HOH:O	2.66	0.48
1:A:657:LEU:C	1:A:658:ASP:O	2.55	0.48
1:B:603:ARG:CD	1:B:652:ARG:HG3	2.43	0.48
1:B:603:ARG:HD3	1:B:652:ARG:HG3	1.93	0.48
1:A:627:ALA:O	1:A:631:LEU:HG	2.13	0.48
1:B:25:LEU:HD22	4:B:997:HOH:O	2.13	0.48
1:B:171:SER:HB3	1:B:396:LYS:HE2	1.96	0.48
1:B:328:ARG:HD3	4:B:911:HOH:O	2.12	0.48
1:A:13:THR:O	1:A:45:SER:HB3	2.14	0.48
1:B:250:ILE:HG21	4:B:1044:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:HIS:ND1	4:B:903:HOH:O	2.35	0.48
1:B:294:ASN:OD1	1:B:296:ASN:HB2	2.13	0.48
1:A:146:ASP:HB3	1:A:571:ILE:HB	1.95	0.48
1:A:677:GLN:NE2	1:A:680:ASP:HB3	2.29	0.48
1:A:661:GLY:O	1:A:664:PHE:N	2.47	0.48
1:A:164:MET:HE1	1:A:560:MET:HA	1.95	0.48
1:A:683:LEU:C	1:A:685:ALA:N	2.72	0.48
1:B:11:THR:HB	4:B:946:HOH:O	2.14	0.48
1:B:137:ASN:CG	1:B:141:ARG:HH21	2.21	0.47
1:B:534:ARG:HH21	1:B:540:ASP:N	2.11	0.47
1:A:19:LEU:HA	4:A:974:HOH:O	2.14	0.47
1:B:137:ASN:N	1:B:138:PRO:HD2	2.28	0.47
1:A:387:ILE:HB	4:A:950:HOH:O	2.14	0.47
1:A:120:GLU:C	1:A:121:GLU:HG3	2.38	0.47
1:A:128:TYR:HA	1:A:130:LYS:HG2	1.96	0.47
1:B:643:LEU:HD12	1:B:648:LYS:HB2	1.96	0.47
1:A:595:GLN:O	1:A:601:HIS:N	2.47	0.47
1:A:726:VAL:C	1:A:729:VAL:HG12	2.39	0.47
1:B:119:GLU:O	1:B:122:LYS:HD3	2.15	0.47
1:B:432:PRO:O	1:B:455:GLU:HG3	2.15	0.47
1:B:597:VAL:HG13	4:B:1014:HOH:O	2.13	0.47
1:A:94:GLN:NE2	1:A:719:TYR:OH	2.47	0.47
1:A:387:ILE:HD13	1:A:490:TRP:CZ3	2.50	0.47
1:A:488:ILE:HD11	1:A:530:TYR:CE2	2.50	0.47
1:A:49:ARG:HD3	1:A:68:LEU:HD13	1.97	0.47
1:A:568:MET:HE3	1:A:568:MET:HB3	1.76	0.47
1:A:650:PRO:HA	1:A:658:ASP:N	2.30	0.47
1:A:729:VAL:O	1:A:732:PRO:CG	2.63	0.47
1:B:466:ASP:OD2	1:B:470:ARG:HD2	2.15	0.46
1:B:550:ARG:HG2	1:B:551:ASP:N	2.29	0.46
1:A:631:LEU:CD1	1:A:632:LEU:N	2.78	0.46
1:A:699:GLN:OE1	1:A:699:GLN:N	2.48	0.46
1:A:118:THR:N	1:A:121:GLU:CD	2.73	0.46
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.80	0.46
1:A:465:LYS:O	1:A:469:ILE:HG13	2.15	0.46
1:B:523:SER:HB3	1:B:526:ARG:HG3	1.97	0.46
1:A:287:LEU:HD21	1:A:309:LEU:HD11	1.98	0.46
1:A:444:THR:OG1	1:A:446:GLU:HG3	2.15	0.46
1:B:62:GLN:NE2	1:B:106:GLY:O	2.47	0.46
1:B:284:HIS:CE1	1:B:317:ILE:HG12	2.50	0.46
1:A:112:TYR:CE1	1:A:125:LYS:HG3	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:HG2	1:A:464:VAL:HG21	1.98	0.46
1:A:729:VAL:C	1:A:732:PRO:HD3	2.37	0.46
1:A:26:PRO:HD2	1:A:731:ARG:HH11	1.81	0.46
1:A:100:LYS:CD	1:A:100:LYS:N	2.78	0.46
1:A:410:PRO:HG2	1:A:542:ILE:HA	1.97	0.46
1:A:628:ARG:C	1:A:631:LEU:HD11	2.41	0.46
1:A:665:TYR:O	1:A:668:LEU:HB3	2.16	0.46
1:A:700:LYS:O	1:A:704:GLU:N	2.34	0.46
1:B:23:SER:O	1:B:731:ARG:NH2	2.48	0.46
1:B:189:SER:HB2	1:B:224:ILE:O	2.15	0.46
1:A:12:LEU:HD11	1:A:41:LYS:HD3	1.97	0.46
1:A:701:ILE:O	1:A:705:LEU:HG	2.16	0.46
1:A:731:ARG:HA	1:A:731:ARG:HD3	1.62	0.46
1:B:15:GLU:HB3	1:B:593:VAL:HG21	1.97	0.46
1:A:183:PHE:HB2	1:A:381:GLU:CD	2.42	0.45
1:A:92:VAL:HG23	4:A:1047:HOH:O	2.16	0.45
1:A:212:LEU:HD12	1:A:459:TRP:HZ3	1.81	0.45
1:B:227:MET:CE	1:B:460:ARG:HE	2.29	0.45
1:A:101:GLU:OE2	1:A:719:TYR:HB2	2.13	0.45
1:A:660:ARG:C	1:A:663:HIS:HB3	2.41	0.45
1:A:677:GLN:NE2	1:A:680:ASP:H	2.14	0.45
1:A:26:PRO:HD2	1:A:731:ARG:NH1	2.32	0.45
1:A:77:ASP:HB3	1:A:80:THR:CG2	2.44	0.45
1:A:87:ASN:ND2	1:A:136:VAL:HG21	2.31	0.45
1:A:154:LYS:HE2	1:A:408:THR:HG23	1.97	0.45
1:A:599:GLU:OE1	4:A:903:HOH:O	2.21	0.45
1:B:143:GLY:O	1:B:144:ASN:HB2	2.17	0.45
1:B:479:ARG:HH21	1:B:483:SER:HB3	1.80	0.45
1:A:621:GLY:HA2	1:A:629:THR:OG1	2.16	0.45
1:A:727:SER:C	1:A:729:VAL:N	2.75	0.45
1:B:183:PHE:HB2	1:B:381:GLU:OE2	2.17	0.45
1:A:736:PHE:CD2	1:A:736:PHE:N	2.85	0.45
1:B:636:LEU:O	1:B:640:THR:OG1	2.32	0.45
1:A:300:ALA:O	1:A:304:GLU:HG3	2.16	0.45
1:A:130:LYS:H	1:A:130:LYS:CD	2.29	0.45
1:A:191:THR:HG1	1:A:500:GLU:HG3	1.82	0.45
1:A:481:ARG:HA	1:A:481:ARG:HD3	1.80	0.45
1:A:656:GLU:OE2	1:A:660:ARG:NE	2.50	0.45
1:A:671:ALA:HA	1:A:674:LEU:HB2	1.98	0.45
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.81	0.45
1:A:690:LEU:CD2	1:A:692:LYS:HD3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:SER:HB3	1:A:736:PHE:CG	2.52	0.45
1:A:736:PHE:CZ	1:A:737:ASN:HB2	2.52	0.45
1:B:693:ALA:O	1:B:697:ASN:ND2	2.43	0.44
1:A:71:LEU:HD23	1:A:74:LEU:HD22	1.98	0.44
1:A:114:GLU:CD	1:A:114:GLU:H	2.25	0.44
1:A:301:GLY:O	1:A:305:LYS:HG3	2.17	0.44
1:A:725:LYS:HD3	1:A:725:LYS:H	1.77	0.44
1:A:485:MET:HE2	1:A:540:ASP:CB	2.47	0.44
1:A:412:VAL:HG13	1:A:475:LEU:HD23	1.99	0.44
1:A:734:ALA:HA	1:A:736:PHE:HE2	1.82	0.44
1:A:25:LEU:HD11	1:A:39:ILE:HG21	2.00	0.44
1:A:142:GLU:O	1:A:575:MET:HG2	2.18	0.44
1:B:657:LEU:HD11	1:B:661:GLY:HA3	1.99	0.44
1:A:37:ILE:HD11	1:A:629:THR:CG2	2.46	0.44
1:A:731:ARG:N	1:A:732:PRO:CD	2.81	0.44
1:B:408:THR:HA	1:B:561:GLU:OE1	2.18	0.44
1:A:161:PRO:HG3	1:A:404:LYS:HE2	2.00	0.44
1:A:512:HIS:O	1:A:514:THR:HG23	2.18	0.44
1:A:600:ASN:N	1:A:710:GLY:HA2	2.32	0.44
1:A:659:ASN:O	1:A:660:ARG:C	2.61	0.44
1:A:690:LEU:HD23	1:A:692:LYS:HB3	2.00	0.44
1:A:325:GLN:OE1	4:A:904:HOH:O	2.21	0.44
1:A:726:VAL:HA	1:A:729:VAL:CG1	2.46	0.44
1:B:124:ILE:HA	4:B:905:HOH:O	2.18	0.44
1:B:742:THR:OG1	1:B:743:VAL:N	2.38	0.44
1:A:112:TYR:HA	1:A:125:LYS:HZ2	1.81	0.43
1:B:414:LEU:HB2	1:B:472:TRP:CE2	2.53	0.43
1:A:95:LEU:O	1:A:99:ILE:N	2.51	0.43
1:A:202:LEU:HB3	1:A:210:ILE:HB	2.00	0.43
1:A:485:MET:HE2	1:A:540:ASP:OD2	2.18	0.43
1:A:646:ASN:C	1:A:648:LYS:H	2.19	0.43
1:A:699:GLN:C	1:A:700:LYS:HD3	2.42	0.43
1:B:122:LYS:H	1:B:122:LYS:HG3	1.57	0.43
1:A:191:THR:OG1	1:A:500:GLU:HG3	2.17	0.43
1:A:692:LYS:O	1:A:696:GLU:HG2	2.18	0.43
1:A:28:ILE:C	1:A:30:THR:N	2.77	0.43
1:B:314:ARG:HB2	4:B:981:HOH:O	2.18	0.43
1:A:57:TYR:O	1:A:58:LEU:HD23	2.18	0.43
1:A:241:GLN:CA	1:A:241:GLN:HE21	2.32	0.43
1:B:261:MET:HE1	4:B:920:HOH:O	2.19	0.43
1:A:391:MET:HB2	1:A:528:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASP:HB2	1:A:498:GLU:OE1	2.18	0.43
1:A:495:ARG:HA	1:A:496:PRO:HD2	1.76	0.43
1:B:358:MET:HB2	1:B:365:MET:HE2	1.99	0.43
1:A:27:ILE:HG21	1:A:663:HIS:CE1	2.54	0.43
1:A:634:LYS:O	1:A:638:GLU:HG3	2.19	0.43
1:A:33:LYS:N	1:A:34:PRO:HD2	2.34	0.43
1:A:32:THR:HB	1:A:37:ILE:HB	2.01	0.43
1:A:661:GLY:HA2	1:A:664:PHE:HB3	2.01	0.43
1:B:387:ILE:HG23	1:B:528:MET:HE2	2.01	0.43
1:A:617:LEU:HD13	1:A:632:LEU:HB3	2.00	0.42
1:B:491:LEU:O	1:B:493:PRO:HD3	2.19	0.42
1:B:509:LEU:HD12	4:B:1060:HOH:O	2.18	0.42
1:A:165:SER:HB2	1:A:361:ALA:C	2.44	0.42
1:A:431:ILE:HA	1:A:432:PRO:HD3	1.69	0.42
1:A:669:TYR:HA	1:A:672:GLU:HB2	2.02	0.42
1:B:12:LEU:C	4:B:946:HOH:O	2.62	0.42
1:B:143:GLY:HA2	1:B:575:MET:HE2	2.00	0.42
1:B:401:PHE:O	1:B:403:PRO:HD3	2.19	0.42
1:B:404:LYS:HE2	4:B:1035:HOH:O	2.19	0.42
1:B:674:LEU:HD13	1:B:687:PHE:CE2	2.54	0.42
1:B:715:ILE:HB	1:B:726:VAL:HG22	2.01	0.42
1:A:77:ASP:HA	1:A:78:PRO:HD3	1.76	0.42
1:A:86:PRO:HD3	1:A:583:THR:OG1	2.20	0.42
1:A:664:PHE:O	1:A:667:SER:N	2.52	0.42
1:B:665:TYR:HD1	4:B:1038:HOH:O	2.02	0.42
1:A:98:CYS:HB2	1:A:719:TYR:CD2	2.55	0.42
1:A:416:ALA:HB3	1:A:468:PRO:HB3	2.02	0.42
1:A:27:ILE:HG21	1:A:27:ILE:HD13	1.83	0.42
1:A:284:HIS:ND1	1:A:317:ILE:HG12	2.35	0.42
1:B:183:PHE:HD2	1:B:381:GLU:CG	2.33	0.42
1:B:283:LYS:HG2	1:B:284:HIS:CD2	2.55	0.42
1:A:488:ILE:HD11	1:A:530:TYR:CD2	2.55	0.41
1:A:170:TRP:HZ3	1:B:244:ASP:CG	2.28	0.41
1:A:705:LEU:CB	1:A:708:VAL:HG13	2.48	0.41
1:B:437:ALA:HB3	1:B:451:GLN:HB2	2.02	0.41
1:B:570:SER:HB3	1:B:582:GLU:HB2	2.01	0.41
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.87	0.41
1:A:690:LEU:CD2	1:A:692:LYS:HB3	2.50	0.41
1:B:28:ILE:HG23	1:B:613:LEU:HD21	2.02	0.41
1:B:267:ILE:HA	1:B:296:ASN:HD21	1.83	0.41
1:A:102:LEU:HD22	1:A:107:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:SER:HB3	1:A:736:PHE:HB3	2.03	0.41
1:B:400:ASN:OD1	1:B:401:PHE:N	2.50	0.41
1:A:96:THR:O	1:A:99:ILE:HG23	2.21	0.41
1:A:271:HIS:O	1:A:275:ILE:HG12	2.21	0.41
1:A:659:ASN:O	1:A:663:HIS:N	2.54	0.41
1:A:729:VAL:HG13	1:A:730:MET:HG2	2.02	0.41
1:B:33:LYS:N	1:B:34:PRO:HD2	2.36	0.41
1:A:24:LEU:HA	1:A:663:HIS:CE1	2.56	0.41
1:A:117:ALA:C	1:A:121:GLU:OE1	2.64	0.41
1:A:119:GLU:N	1:A:121:GLU:CD	2.79	0.41
1:B:657:LEU:HD12	1:B:657:LEU:HA	1.96	0.41
1:A:15:GLU:HB3	1:A:16:ALA:H	1.54	0.41
1:A:44:ILE:HD11	4:A:1064:HOH:O	2.20	0.41
1:A:68:LEU:HD21	1:A:139:VAL:HG21	2.02	0.41
1:A:91:SER:OG	1:A:94:GLN:HB2	2.21	0.41
1:A:178:MET:HE2	1:A:180:GLU:O	2.20	0.41
1:A:234:LEU:HD21	1:A:268:VAL:HG13	2.03	0.41
1:A:261:MET:HG3	1:A:265:HIS:CE1	2.55	0.41
1:A:301:GLY:HA2	1:A:304:GLU:HG3	2.02	0.41
1:A:420:GLU:HG2	1:A:464:VAL:CG2	2.50	0.41
1:A:642:LYS:HE3	1:A:669:TYR:CG	2.56	0.41
1:A:702:VAL:O	1:A:706:ALA:HB2	2.21	0.41
1:B:284:HIS:ND1	1:B:317:ILE:HG12	2.35	0.41
1:B:551:ASP:HA	4:B:961:HOH:O	2.20	0.41
1:B:711:LYS:NZ	4:B:919:HOH:O	2.53	0.41
1:A:376:LYS:HB2	1:A:376:LYS:HE2	1.76	0.41
1:B:619:GLU:O	1:B:623:LYS:HG2	2.20	0.41
1:A:24:LEU:HD13	1:A:610:PHE:HE1	1.87	0.40
1:A:461:MET:HE2	1:A:461:MET:HB3	1.91	0.40
1:A:559:ILE:HD13	1:A:559:ILE:HA	1.95	0.40
1:A:650:PRO:CB	1:A:658:ASP:HA	2.50	0.40
1:A:699:GLN:OE1	1:A:700:LYS:HE2	2.21	0.40
1:A:102:LEU:HD22	1:A:107:TYR:CE1	2.55	0.40
1:A:227:MET:CE	1:A:460:ARG:HE	2.33	0.40
1:B:23:SER:HG	1:B:663:HIS:CE1	2.28	0.40
1:B:379:MET:HB3	1:B:379:MET:HE2	1.72	0.40
1:B:534:ARG:NE	1:B:541:THR:HG23	2.36	0.40
1:A:241:GLN:HE21	1:A:241:GLN:N	2.19	0.40
1:A:556:LEU:O	1:A:560:MET:HG2	2.21	0.40
1:A:711:LYS:HB3	1:A:712:PRO:CD	2.52	0.40
1:B:302:LEU:HD23	1:B:306:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASP:O	1:A:183:PHE:C	2.64	0.40
1:A:184:TYR:HB2	1:A:383:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/751 (98%)	626 (85%)	70 (10%)	37 (5%)	1	10
1	B	737/751 (98%)	673 (91%)	54 (7%)	10 (1%)	9	36
All	All	1470/1502 (98%)	1299 (88%)	124 (8%)	47 (3%)	3	18

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	117	ALA
1	A	647	ASP
1	A	654	THR
1	A	658	ASP
1	A	690	LEU
1	A	691	ALA
1	A	711	LYS
1	A	728	ALA
1	A	729	VAL
1	A	733	SER
1	B	118	THR
1	A	29	GLU
1	A	92	VAL
1	A	602	LEU
1	A	625	ASN

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Mol	Chain	Res	Type
1	A	663	HIS
1	A	671	ALA
1	A	723	PRO
1	A	726	VAL
1	A	738	ALA
1	B	143	GLY
1	B	654	THR
1	A	28	ILE
1	A	100	LYS
1	A	113	PRO
1	A	605	ASP
1	A	650	PRO
1	A	656	GLU
1	A	684	LYS
1	A	712	PRO
1	A	734	ALA
1	B	119	GLU
1	B	361	ALA
1	B	523	SER
1	A	283	LYS
1	A	496	PRO
1	A	708	VAL
1	B	13	THR
1	B	111	ASP
1	B	743	VAL
1	A	121	GLU
1	A	143	GLY
1	A	688	ALA
1	B	46	VAL
1	A	597	VAL
1	A	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/628 (96%)	548 (91%)	53 (9%)	9	35
1	B	614/628 (98%)	564 (92%)	50 (8%)	11	38
All	All	1215/1256 (97%)	1112 (92%)	103 (8%)	10	36

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	SER
1	A	50	VAL
1	A	63	LYS
1	A	99	ILE
1	A	100	LYS
1	A	109	ILE
1	A	114	GLU
1	A	118	THR
1	A	121	GLU
1	A	123	THR
1	A	124	ILE
1	A	131	CYS
1	A	136	VAL
1	A	145	SER
1	A	169	GLN
1	A	227	MET
1	A	230	SER
1	A	241	GLN
1	A	250	ILE
1	A	259	THR
1	A	295	VAL
1	A	304	GLU
1	A	313	LEU
1	A	349	ILE
1	A	365	MET
1	A	406	MET
1	A	433	GLU
1	A	436	ILE
1	A	500	GLU
1	A	531	THR
1	A	536	VAL

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Mol	Chain	Res	Type
1	A	544	VAL
1	A	593	VAL
1	A	597	VAL
1	A	599	GLU
1	A	615	VAL
1	A	624	GLU
1	A	628	ARG
1	A	629	THR
1	A	630	LYS
1	A	631	LEU
1	A	653	ARG
1	A	656	GLU
1	A	658	ASP
1	A	660	ARG
1	A	666	LEU
1	A	672	GLU
1	A	682	GLU
1	A	708	VAL
1	A	711	LYS
1	A	725	LYS
1	A	731	ARG
1	B	12	LEU
1	B	50	VAL
1	B	59	SER
1	B	76	GLN
1	B	83	ILE
1	B	100	LYS
1	B	120	GLU
1	B	122	LYS
1	B	142	GLU
1	B	145	SER
1	B	153	VAL
1	B	189	SER
1	B	191	THR
1	B	225	ASP
1	B	227	MET
1	B	238	TYR
1	B	250	ILE
1	B	256	VAL
1	B	259	THR
1	B	275	ILE
1	B	286	LYS

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Mol	Chain	Res	Type
1	B	295	VAL
1	B	319	GLU
1	B	349	ILE
1	B	358	MET
1	B	365	MET
1	B	382	SER
1	B	436	ILE
1	B	442	LEU
1	B	499	ASN
1	B	515	THR
1	B	521	ILE
1	B	524	GLN
1	B	525	VAL
1	B	536	VAL
1	B	541	THR
1	B	544	VAL
1	B	548	ILE
1	B	549	LEU
1	B	550	ARG
1	B	609	GLU
1	B	615	VAL
1	B	619	GLU
1	B	620	MET
1	B	623	LYS
1	B	640	THR
1	B	652	ARG
1	B	668	LEU
1	B	721	VAL
1	B	743	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	115	ASN
1	A	160	HIS
1	A	241	GLN
1	A	411	ASN
1	A	594	GLN
1	A	595	GLN
1	A	646	ASN
1	A	663	HIS

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Mol	Chain	Res	Type
1	A	677	GLN
1	A	707	GLN
1	B	296	ASN
1	B	342	ASN
1	B	372	GLN
1	B	512	HIS

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	PO4	B	801	-	4,4,4	1.02	0	6,6,6	0.67	0
2	PO4	A	801	-	4,4,4	0.92	0	6,6,6	0.67	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	801	PO4	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	735/751 (97%)	0.23	53 (7%)	21 11	28, 50, 130, 141	0
1	B	739/751 (98%)	-0.46	1 (0%)	92 86	22, 38, 64, 100	0
All	All	1474/1502 (98%)	-0.11	54 (3%)	45 25	22, 42, 125, 141	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	605	ASP	7.4
1	A	728	ALA	6.8
1	A	101	GLU	5.9
1	A	22	TYR	5.8
1	A	739	ALA	4.9
1	A	701	ILE	4.8
1	A	604	TRP	4.1
1	A	99	ILE	4.0
1	A	98	CYS	3.9
1	A	710	GLY	3.9
1	A	658	ASP	3.9
1	A	720	ALA	3.9
1	A	724	ALA	3.8
1	A	721	VAL	3.7
1	A	128	TYR	3.6
1	A	716	GLY	3.4
1	A	729	VAL	3.3
1	A	734	ALA	3.2
1	A	24	LEU	3.1
1	A	687	PHE	3.1
1	A	689	PRO	3.0
1	A	712	PRO	3.0
1	A	709	GLN	3.0
1	A	589	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	715	ILE	2.9
1	A	723	PRO	2.9
1	A	659	ASN	2.9
1	A	602	LEU	2.8
1	A	603	ARG	2.7
1	A	691	ALA	2.6
1	A	667	SER	2.6
1	A	64	VAL	2.6
1	A	600	ASN	2.5
1	A	690	LEU	2.5
1	A	727	SER	2.5
1	A	601	HIS	2.5
1	A	688	ALA	2.4
1	A	733	SER	2.4
1	A	113	PRO	2.4
1	A	738	ALA	2.4
1	A	566	ALA	2.4
1	A	681	ALA	2.3
1	A	102	LEU	2.3
1	A	622	ILE	2.3
1	A	96	THR	2.3
1	A	694	LEU	2.2
1	B	118	THR	2.2
1	A	6	SER	2.2
1	A	705	LEU	2.2
1	A	21	THR	2.1
1	A	97	ALA	2.1
1	A	702	VAL	2.1
1	A	88	ILE	2.0
1	A	10	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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	PO4	A	801	5/5	0.94	0.08	52,53,59,66	0
3	MG	A	802	1/1	0.95	0.14	27,27,27,27	0
3	MG	B	802	1/1	0.95	0.15	38,38,38,38	0
2	PO4	B	801	5/5	0.96	0.09	41,41,49,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.