



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 AM GMT

PDB ID : 2JHR
Title : CRYSTAL STRUCTURE OF MYOSIN-2 MOTOR DOMAIN IN COMPLEX WITH ADP-METAVANADATE AND PENTABROMOPSEUDILIN
Authors : Fedorov, R.; Boehl, M.; Tsiavaliaris, G.; Hartmann, F.K.; Baruch, P.; Brenner, B.; Martin, R.; Knoelker, H.J.; Gutzeit, H.O.; Manstein, D.J.
Deposited on : 2008-03-25
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

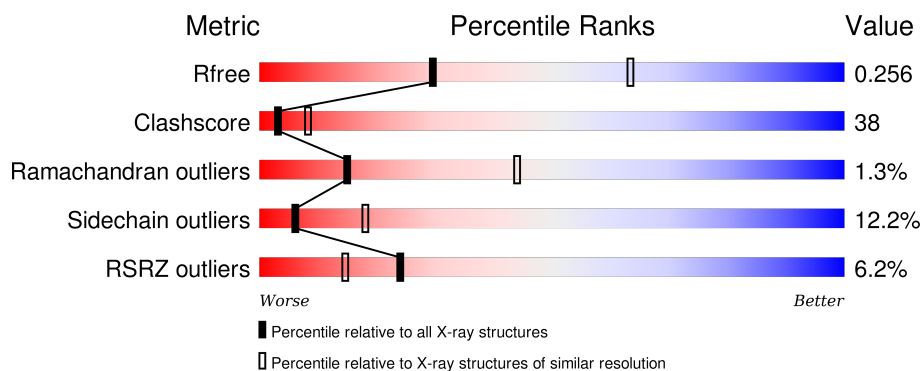
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	788	<div> <div>6%</div> <div>47%</div> <div>41%</div> <div>7%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PBQ	A	1780	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6761 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 MYOSIN-2 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	776	6239	3961	1076	1185	17	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

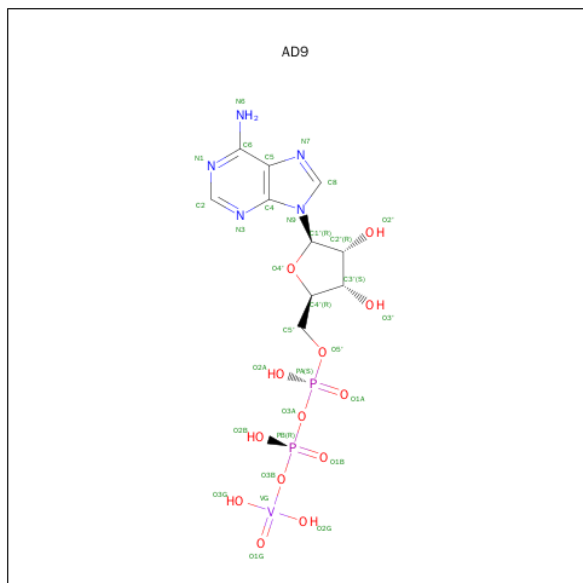
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P08799
A	-9	HIS	-	EXPRESSION TAG	UNP P08799
A	-8	HIS	-	EXPRESSION TAG	UNP P08799
A	-7	HIS	-	EXPRESSION TAG	UNP P08799
A	-6	HIS	-	EXPRESSION TAG	UNP P08799
A	-5	HIS	-	EXPRESSION TAG	UNP P08799
A	-4	HIS	-	EXPRESSION TAG	UNP P08799
A	-3	HIS	-	EXPRESSION TAG	UNP P08799
A	-2	ASP	-	EXPRESSION TAG	UNP P08799
A	-1	GLY	-	EXPRESSION TAG	UNP P08799
A	0	THR	-	EXPRESSION TAG	UNP P08799
A	1	GLU	-	EXPRESSION TAG	UNP P08799
A	762	LEU	-	EXPRESSION TAG	UNP P08799
A	763	GLU	-	EXPRESSION TAG	UNP P08799
A	764	SER	-	EXPRESSION TAG	UNP P08799
A	765	ASN	-	EXPRESSION TAG	UNP P08799
A	766	GLU	-	EXPRESSION TAG	UNP P08799
A	767	PRO	-	EXPRESSION TAG	UNP P08799
A	768	PRO	-	EXPRESSION TAG	UNP P08799
A	769	MET	-	EXPRESSION TAG	UNP P08799
A	770	ASP	-	EXPRESSION TAG	UNP P08799
A	771	PHE	-	EXPRESSION TAG	UNP P08799
A	772	ASP	-	EXPRESSION TAG	UNP P08799
A	773	ASP	-	EXPRESSION TAG	UNP P08799
A	774	ASP	-	EXPRESSION TAG	UNP P08799
A	775	ILE	-	EXPRESSION TAG	UNP P08799
A	776	PRO	-	EXPRESSION TAG	UNP P08799

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Chain	Residue	Modelled	Actual	Comment	Reference
A	777	PHE	-	EXPRESSION TAG	UNP P08799

- Molecule 2 is ADP METAVANADATE (three-letter code: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).

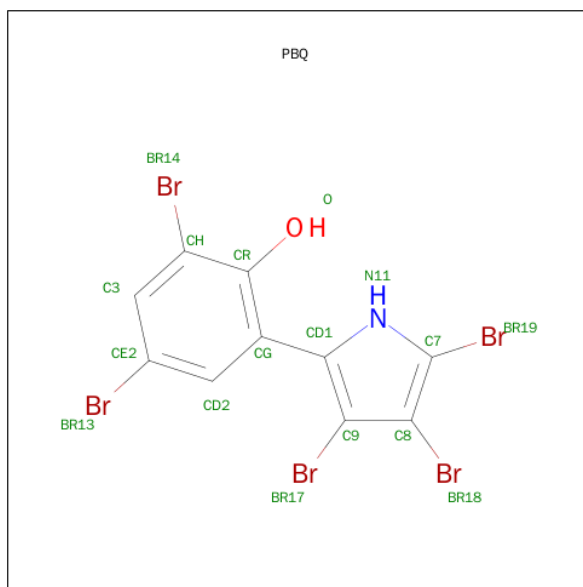


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	V	0	0
			31	10	5	13	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PENTABROMOPSEUDILIN (three-letter code: PBQ) (formula: $C_{10}H_4Br_5NO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	O	0	0
			17	5	10	1	1		

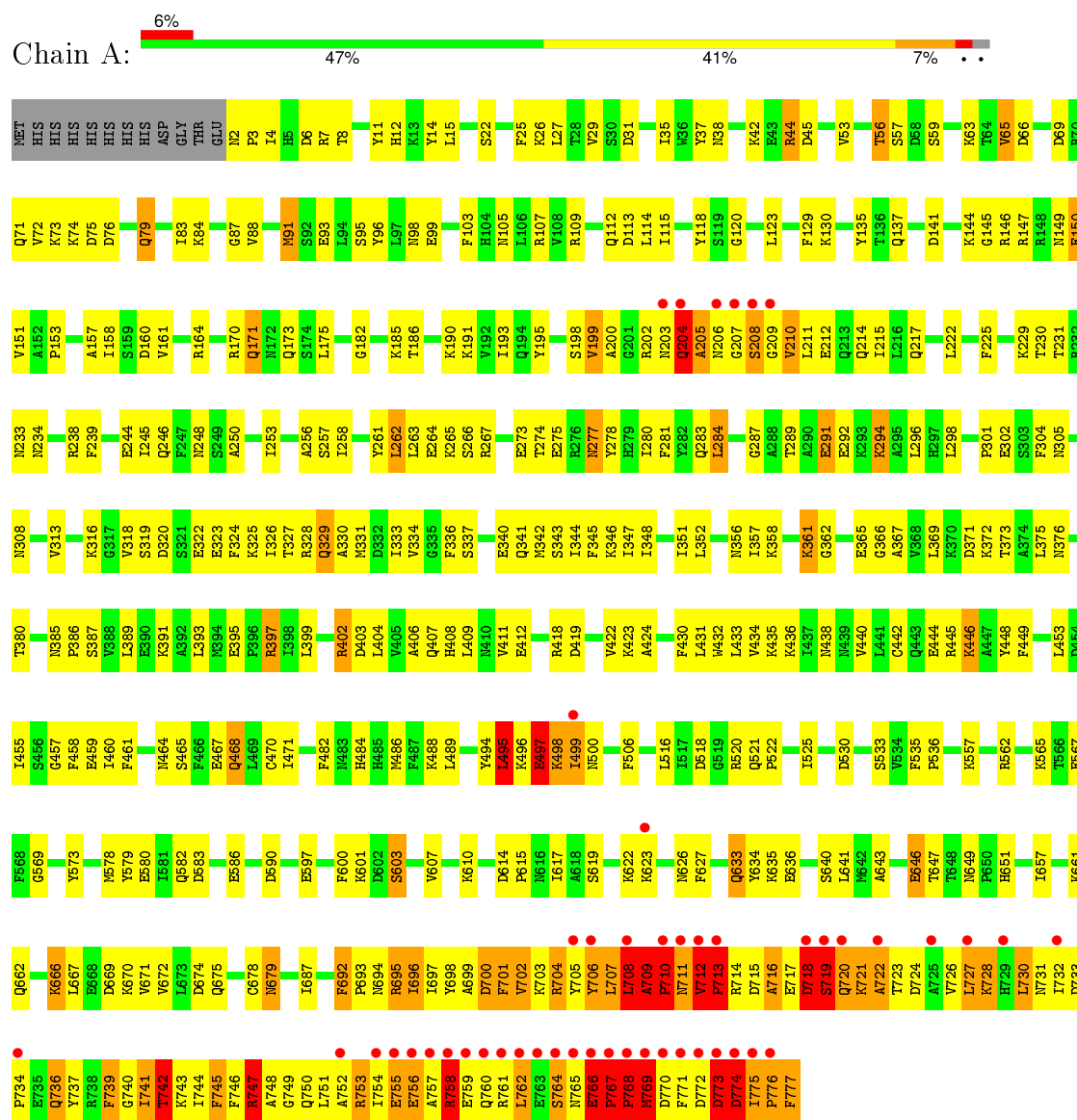
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	473	Total	O	0	0
			473	473		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYOSIN-2 HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.76 Å 150.46 Å 154.55 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 77.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 76.5 (77.08-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.20 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.265 0.222 , 0.256	Depositor DCC
R_{free} test set	1232 reflections (6.42%)	DCC
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 155.4	EDS
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 198675 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6761	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, PBQ, AD9

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	0.57	5/6364 (0.1%)	0.97	44/8590 (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	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	713	PRO	N-CD	19.30	1.74	1.47
1	A	747	ARG	C-N	-7.76	1.16	1.34
1	A	710	PRO	N-CD	7.02	1.57	1.47
1	A	767	PRO	N-CD	6.39	1.56	1.47
1	A	718	ASP	C-N	-5.10	1.22	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	CB-CA-C	-15.77	78.87	110.40
1	A	739	PHE	CB-CA-C	-15.21	79.97	110.40
1	A	708	LEU	CB-CA-C	14.16	137.10	110.20
1	A	757	ALA	CB-CA-C	13.91	130.97	110.10
1	A	722	ALA	CB-CA-C	-13.73	89.50	110.10
1	A	741	ILE	N-CA-C	13.59	147.70	111.00
1	A	711	ASN	N-CA-C	13.05	146.24	111.00
1	A	748	ALA	N-CA-CB	12.30	127.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	ILE	N-CA-CB	-12.20	82.75	110.80
1	A	741	ILE	CB-CA-C	-10.90	89.80	111.60
1	A	708	LEU	N-CA-C	-10.17	83.54	111.00
1	A	204	GLN	N-CA-C	10.06	138.18	111.00
1	A	747	ARG	CB-CA-C	-9.73	90.93	110.40
1	A	712	VAL	C-N-CD	-9.13	100.52	120.60
1	A	711	ASN	CB-CA-C	-9.04	92.32	110.40
1	A	713	PRO	CA-N-CD	-8.95	98.97	111.50
1	A	758	ARG	N-CA-CB	-8.59	95.14	110.60
1	A	718	ASP	CB-CA-C	8.44	127.27	110.40
1	A	495	LEU	N-CA-C	8.39	133.64	111.00
1	A	713	PRO	N-CA-CB	8.14	113.06	103.30
1	A	719	SER	N-CA-CB	8.06	122.58	110.50
1	A	742	THR	N-CA-C	-8.05	89.27	111.00
1	A	365	GLU	CB-CA-C	-7.94	94.52	110.40
1	A	208	SER	N-CA-CB	-7.55	99.17	110.50
1	A	747	ARG	O-C-N	-7.53	110.65	122.70
1	A	718	ASP	N-CA-C	-7.34	91.17	111.00
1	A	713	PRO	N-CA-C	-7.03	93.83	112.10
1	A	719	SER	N-CA-C	-6.90	92.38	111.00
1	A	718	ASP	O-C-N	-6.84	111.75	122.70
1	A	494	TYR	CB-CA-C	-6.63	97.14	110.40
1	A	742	THR	N-CA-CB	6.50	122.66	110.30
1	A	709	ALA	N-CA-CB	-6.05	101.63	110.10
1	A	365	GLU	N-CA-C	5.91	126.95	111.00
1	A	590	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	712	VAL	N-CA-C	-5.82	95.29	111.00
1	A	772	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	261	TYR	CB-CA-C	-5.75	98.90	110.40
1	A	262	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	709	ALA	CB-CA-C	5.40	118.19	110.10
1	A	709	ALA	N-CA-C	5.38	125.54	111.00
1	A	204	GLN	N-CA-CB	-5.37	100.93	110.60
1	A	205	ALA	CB-CA-C	5.09	117.74	110.10
1	A	773	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	774	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	711	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	712	VAL	Peptide
1	A	718	ASP	Mainchain
1	A	747	ARG	Mainchain
1	A	767	PRO	Peptide
1	A	768	PRO	Peptide
1	A	769	MET	Peptide
1	A	773	ASP	Peptide
1	A	775	ILE	Peptide
1	A	776	PRO	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	6239	0	6175	471	0
2	A	31	0	14	2	0
3	A	1	0	0	0	0
4	A	17	0	3	11	0
5	A	473	0	0	35	0
All	All	6761	0	6192	474	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 38.

All (474) 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:713:PRO:CD	1:A:713:PRO:N	1.74	1.44
1:A:431:LEU:HD13	4:A:1780:PBQ:BR18	1.95	1.20
1:A:773:ASP:H	1:A:775:ILE:HG22	1.10	1.16
1:A:496:LYS:O	1:A:498:LYS:HG2	1.47	1.12
1:A:739:PHE:HA	1:A:744:ILE:HG13	1.31	1.12
1:A:202:ARG:HB2	1:A:208:SER:HB3	1.34	1.09
1:A:424:ALA:HB2	4:A:1780:PBQ:BR14	2.07	1.09
1:A:767:PRO:HD2	1:A:768:PRO:CD	1.83	1.08
1:A:204:GLN:HA	1:A:209:GLY:HA3	1.25	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:PRO:HD2	1:A:768:PRO:HD2	1.03	1.02
1:A:204:GLN:CA	1:A:209:GLY:HA3	1.88	1.01
1:A:499:ILE:HD12	1:A:740:GLY:HA3	1.42	1.00
1:A:206:ASN:HA	1:A:210:VAL:HB	1.43	1.00
1:A:736:GLN:OE1	1:A:747:ARG:HB2	1.62	0.98
1:A:756:GLU:HA	1:A:759:GLU:HB3	1.41	0.97
1:A:766:GLU:H	1:A:767:PRO:HD3	1.30	0.94
1:A:767:PRO:CD	1:A:768:PRO:HD2	1.95	0.93
1:A:173:GLN:HE22	1:A:649:ASN:HD22	1.00	0.93
1:A:766:GLU:N	1:A:767:PRO:HD3	1.82	0.92
1:A:712:VAL:C	1:A:713:PRO:CD	2.38	0.92
1:A:204:GLN:HA	1:A:209:GLY:CA	1.99	0.92
1:A:277:ASN:HD22	1:A:278:TYR:H	1.18	0.92
1:A:740:GLY:O	1:A:743:LYS:O	1.90	0.90
1:A:366:GLY:HA3	1:A:408:HIS:ND1	1.89	0.87
1:A:366:GLY:HA3	1:A:408:HIS:CE1	2.09	0.86
1:A:712:VAL:CG1	1:A:712:VAL:O	2.25	0.85
1:A:773:ASP:N	1:A:775:ILE:HG22	1.92	0.85
1:A:712:VAL:N	1:A:713:PRO:HD3	1.91	0.85
1:A:741:ILE:HG23	1:A:741:ILE:O	1.77	0.84
1:A:325:LYS:O	1:A:329:GLN:HG2	1.78	0.84
1:A:610:LYS:HE3	1:A:614:ASP:HB2	1.59	0.83
1:A:262:LEU:HD11	1:A:470:CYS:HB3	1.60	0.83
1:A:712:VAL:CA	1:A:713:PRO:HD3	2.09	0.83
1:A:461:PHE:H	1:A:464:ASN:HD21	1.27	0.82
1:A:712:VAL:O	1:A:712:VAL:HG13	1.80	0.81
1:A:712:VAL:CA	1:A:713:PRO:CD	2.59	0.81
1:A:764:SER:HA	1:A:768:PRO:HD3	1.62	0.81
1:A:727:LEU:HD12	1:A:732:ILE:HD11	1.62	0.81
1:A:741:ILE:O	1:A:741:ILE:CG2	2.23	0.80
1:A:53:VAL:HG21	1:A:63:LYS:HG3	1.61	0.80
1:A:497:GLU:HG2	1:A:745:PHE:HE2	1.47	0.79
1:A:766:GLU:N	1:A:767:PRO:CD	2.46	0.79
1:A:697:ILE:H	1:A:697:ILE:HD12	1.47	0.79
1:A:750:GLN:HA	1:A:753:ARG:HH11	1.47	0.79
1:A:719:SER:O	1:A:723:THR:HG23	1.84	0.78
1:A:329:GLN:HA	1:A:329:GLN:HE21	1.49	0.78
1:A:707:LEU:O	1:A:708:LEU:C	2.22	0.77
1:A:173:GLN:HE22	1:A:649:ASN:ND2	1.80	0.77
1:A:746:PHE:HD2	1:A:751:LEU:HB2	1.51	0.76
1:A:760:GLN:HG3	5:A:2209:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:ARG:O	1:A:765:ASN:HB2	1.85	0.76
1:A:465:SER:H	1:A:468:GLN:NE2	1.82	0.76
1:A:239:PHE:HB3	1:A:263:LEU:HD12	1.68	0.75
1:A:695:ARG:HH11	1:A:695:ARG:HB3	1.51	0.75
1:A:424:ALA:HA	4:A:1780:PBQ:O	1.85	0.75
1:A:707:LEU:C	1:A:708:LEU:O	2.06	0.75
1:A:262:LEU:O	1:A:262:LEU:HD23	1.86	0.75
1:A:773:ASP:H	1:A:775:ILE:CG2	1.96	0.74
1:A:431:LEU:CD1	4:A:1780:PBQ:BR18	2.86	0.74
4:A:1780:PBQ:HD2	4:A:1780:PBQ:BR17	2.43	0.74
1:A:617:ILE:O	4:A:1780:PBQ:BR17	2.61	0.73
1:A:145:GLY:H	1:A:164:ARG:HH21	1.37	0.73
1:A:718:ASP:O	1:A:721:LYS:HE2	1.89	0.73
1:A:424:ALA:CB	4:A:1780:PBQ:BR14	2.91	0.72
1:A:693:PRO:HA	1:A:695:ARG:HH22	1.55	0.72
1:A:706:TYR:HD2	1:A:706:TYR:H	1.38	0.71
1:A:246:GLN:HG2	1:A:446:LYS:HB3	1.72	0.71
1:A:706:TYR:CD2	1:A:706:TYR:N	2.58	0.71
1:A:706:TYR:O	1:A:712:VAL:HG13	1.91	0.71
1:A:461:PHE:N	1:A:464:ASN:HD21	1.88	0.71
1:A:453:LEU:HD13	1:A:641:LEU:HD21	1.73	0.70
1:A:755:GLU:O	1:A:758:ARG:HG3	1.90	0.70
1:A:25:PHE:O	1:A:29:VAL:HG22	1.92	0.70
1:A:762:LEU:O	1:A:767:PRO:HG3	1.92	0.69
1:A:118:TYR:CD2	1:A:153:PRO:HG3	2.27	0.69
1:A:753:ARG:HA	1:A:756:GLU:OE1	1.92	0.69
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.73	0.69
1:A:186:THR:O	1:A:190:LYS:HG3	1.92	0.69
1:A:741:ILE:HG22	1:A:742:THR:N	2.02	0.69
1:A:305:ASN:H	1:A:356:ASN:HD21	1.41	0.69
1:A:736:GLN:OE1	1:A:750:GLN:HB2	1.92	0.68
1:A:695:ARG:HB2	1:A:743:LYS:HD2	1.75	0.68
1:A:347:ILE:O	1:A:351:ILE:HG13	1.93	0.68
1:A:291:GLU:O	1:A:294:LYS:HG3	1.93	0.68
1:A:499:ILE:HD12	1:A:740:GLY:CA	2.23	0.68
1:A:265:LYS:HD3	4:A:1780:PBQ:BR19	2.48	0.68
1:A:615:PRO:O	1:A:619:SER:HB2	1.93	0.68
1:A:727:LEU:HD23	1:A:728:LYS:N	2.09	0.68
1:A:395:GLU:HA	1:A:407:GLN:O	1.94	0.67
1:A:14:TYR:HA	5:A:2024:HOH:O	1.94	0.67
1:A:693:PRO:HA	1:A:695:ARG:NH2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:HG3	1:A:209:GLY:HA3	1.77	0.67
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.77	0.67
1:A:329:GLN:O	1:A:333:ILE:HD13	1.95	0.67
1:A:499:ILE:HD11	1:A:740:GLY:H	1.59	0.67
1:A:773:ASP:O	1:A:776:PRO:CG	2.43	0.67
1:A:775:ILE:HG23	1:A:776:PRO:CD	2.25	0.66
1:A:170:ARG:HH21	1:A:170:ARG:HG2	1.59	0.66
1:A:497:GLU:HG2	1:A:745:PHE:CE2	2.31	0.66
1:A:769:MET:HG2	1:A:770:ASP:OD1	1.94	0.66
1:A:773:ASP:HB2	1:A:775:ILE:H	1.60	0.66
1:A:775:ILE:HG23	1:A:776:PRO:HD3	1.78	0.66
1:A:767:PRO:CD	1:A:768:PRO:CD	2.65	0.65
1:A:206:ASN:CA	1:A:210:VAL:HB	2.23	0.65
1:A:773:ASP:O	1:A:776:PRO:HG2	1.97	0.65
1:A:764:SER:HA	1:A:768:PRO:CD	2.26	0.65
1:A:716:ALA:HB1	1:A:721:LYS:HE2	1.79	0.65
1:A:704:ARG:O	1:A:758:ARG:NH1	2.29	0.65
1:A:316:LYS:HB3	5:A:2200:HOH:O	1.97	0.65
1:A:736:GLN:CD	1:A:747:ARG:HB2	2.17	0.64
1:A:708:LEU:HD21	1:A:758:ARG:HD2	1.78	0.64
1:A:706:TYR:O	1:A:712:VAL:O	2.15	0.64
1:A:375:LEU:HD12	1:A:389:LEU:HD23	1.80	0.64
1:A:580:GLU:HG3	5:A:2394:HOH:O	1.98	0.64
1:A:257:SER:HB3	1:A:442:CYS:SG	2.38	0.63
2:A:1778:AD9:O2A	5:A:2472:HOH:O	2.16	0.63
1:A:144:LYS:HG3	1:A:199:VAL:HG22	1.81	0.63
1:A:465:SER:H	1:A:468:GLN:HE21	1.46	0.63
1:A:597:GLU:O	1:A:601:LYS:HG3	1.99	0.63
1:A:337:SER:HB2	1:A:340:GLU:HG3	1.81	0.62
1:A:323:GLU:OE1	1:A:326:ILE:HD12	1.98	0.62
1:A:761:ARG:HD2	1:A:761:ARG:O	1.99	0.62
1:A:145:GLY:N	1:A:164:ARG:HH21	1.97	0.62
1:A:697:ILE:N	1:A:697:ILE:HD12	2.14	0.62
1:A:144:LYS:HA	1:A:195:TYR:OH	2.00	0.61
1:A:727:LEU:HB2	1:A:732:ILE:HG12	1.83	0.61
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.80	0.61
1:A:202:ARG:HB3	5:A:2184:HOH:O	2.00	0.61
1:A:657:ILE:HG22	1:A:675:GLN:NE2	2.15	0.61
1:A:723:THR:O	1:A:727:LEU:HD22	2.00	0.61
1:A:496:LYS:O	1:A:498:LYS:CG	2.37	0.61
1:A:273:GLU:O	1:A:274:THR:OG1	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:LEU:HD23	1:A:728:LYS:H	1.64	0.61
1:A:724:ASP:HA	1:A:727:LEU:HD21	1.83	0.60
1:A:721:LYS:HG2	1:A:722:ALA:N	2.14	0.60
1:A:210:VAL:O	1:A:214:GLN:HG3	2.01	0.60
1:A:305:ASN:H	1:A:356:ASN:ND2	1.99	0.60
1:A:239:PHE:HB3	1:A:263:LEU:CD1	2.30	0.60
1:A:193:ILE:HD12	1:A:245:ILE:HD11	1.83	0.60
1:A:761:ARG:HH11	1:A:765:ASN:HA	1.66	0.60
1:A:412:GLU:HB2	5:A:2284:HOH:O	2.02	0.60
1:A:708:LEU:HD11	1:A:758:ARG:CB	2.32	0.59
1:A:211:LEU:O	1:A:215:ILE:HG13	2.00	0.59
1:A:4:ILE:HD12	1:A:146:ARG:NH2	2.17	0.59
2:A:1778:AD9:O1G	2:A:1778:AD9:VG	1.59	0.59
1:A:273:GLU:HG2	1:A:274:THR:HG23	1.84	0.59
1:A:246:GLN:HG2	1:A:446:LYS:HD2	1.85	0.59
1:A:329:GLN:CA	1:A:329:GLN:HE21	2.16	0.58
1:A:458:PHE:HE1	1:A:460:ILE:HD11	1.67	0.58
1:A:430:PHE:O	1:A:434:VAL:HG23	2.02	0.58
1:A:302:GLU:HA	1:A:308:ASN:HB3	1.85	0.58
1:A:696:ILE:HD11	1:A:746:PHE:CE2	2.39	0.58
1:A:45:ASP:OD1	1:A:670:LYS:HD2	2.02	0.58
1:A:202:ARG:HB2	1:A:208:SER:CB	2.22	0.58
1:A:438:ASN:O	1:A:442:CYS:HB2	2.03	0.58
1:A:565:LYS:HB2	1:A:565:LYS:NZ	2.19	0.58
1:A:361:LYS:HE3	1:A:362:GLY:O	2.04	0.58
1:A:499:ILE:CD1	1:A:740:GLY:HA3	2.27	0.57
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.69	0.57
1:A:170:ARG:NH2	1:A:170:ARG:HG2	2.16	0.57
1:A:93:GLU:HB3	5:A:2098:HOH:O	2.04	0.57
1:A:217:GLN:O	1:A:330:ALA:HB1	2.03	0.57
1:A:728:LYS:C	1:A:731:ASN:H	2.08	0.57
1:A:262:LEU:HD11	1:A:470:CYS:CB	2.34	0.57
1:A:753:ARG:HB2	5:A:2465:HOH:O	2.05	0.57
1:A:775:ILE:CG2	1:A:776:PRO:CD	2.81	0.57
1:A:766:GLU:HG3	1:A:766:GLU:O	2.04	0.57
1:A:720:GLN:HG3	1:A:720:GLN:O	2.05	0.57
1:A:375:LEU:CD1	1:A:389:LEU:HD23	2.35	0.57
1:A:708:LEU:HD11	1:A:758:ARG:HB3	1.86	0.56
1:A:761:ARG:HD2	1:A:765:ASN:HB2	1.88	0.56
1:A:496:LYS:C	1:A:498:LYS:N	2.56	0.56
1:A:281:PHE:CD1	1:A:352:LEU:HD21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:PHE:CE2	1:A:723:THR:HG22	2.41	0.56
1:A:736:GLN:O	1:A:747:ARG:HG3	2.06	0.56
1:A:761:ARG:O	1:A:765:ASN:CB	2.53	0.56
1:A:497:GLU:CD	1:A:742:THR:HG23	2.27	0.55
1:A:341:GLN:O	1:A:344:ILE:HB	2.06	0.55
1:A:495:LEU:N	1:A:495:LEU:CD1	2.67	0.55
1:A:231:THR:HG23	1:A:275:GLU:OE2	2.06	0.55
1:A:697:ILE:HG13	1:A:743:LYS:HB3	1.88	0.55
1:A:775:ILE:O	1:A:775:ILE:HG13	2.06	0.55
1:A:495:LEU:HD13	1:A:495:LEU:N	2.22	0.55
1:A:432:TRP:NE1	1:A:436:LYS:HD3	2.22	0.55
1:A:728:LYS:HA	5:A:2462:HOH:O	2.05	0.55
1:A:79:GLN:HG2	1:A:96:TYR:CE2	2.41	0.55
1:A:499:ILE:O	1:A:500:ASN:HB2	2.05	0.55
1:A:697:ILE:HG23	1:A:742:THR:O	2.06	0.55
1:A:173:GLN:NE2	1:A:649:ASN:HB3	2.21	0.55
1:A:135:TYR:CG	1:A:191:LYS:HD2	2.41	0.55
1:A:702:VAL:CG2	1:A:714:ARG:HG3	2.36	0.55
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.89	0.55
1:A:697:ILE:HG22	1:A:698:TYR:N	2.22	0.55
1:A:707:LEU:O	1:A:708:LEU:O	2.24	0.55
1:A:724:ASP:O	1:A:728:LYS:HB3	2.06	0.55
1:A:495:LEU:C	1:A:496:LYS:HE2	2.27	0.55
1:A:633:GLN:O	1:A:636:GLU:HB3	2.07	0.55
1:A:708:LEU:HD21	1:A:758:ARG:HB2	1.88	0.54
1:A:746:PHE:CD2	1:A:751:LEU:HB2	2.36	0.54
1:A:63:LYS:HG2	1:A:69:ASP:CG	2.28	0.54
1:A:230:THR:HA	1:A:275:GLU:CD	2.27	0.54
1:A:646:GLU:HA	1:A:646:GLU:OE1	2.06	0.54
1:A:497:GLU:OE2	1:A:742:THR:HG23	2.07	0.54
1:A:402:ARG:HH11	1:A:402:ARG:HG2	1.73	0.54
1:A:157:ALA:O	1:A:161:VAL:HG23	2.07	0.54
1:A:761:ARG:HB2	5:A:2466:HOH:O	2.07	0.54
1:A:701:PHE:CE2	1:A:723:THR:HA	2.43	0.54
1:A:758:ARG:C	1:A:758:ARG:HE	2.11	0.54
1:A:107:ARG:HD3	5:A:2109:HOH:O	2.07	0.54
1:A:324:PHE:HE2	1:A:328:ARG:HH21	1.56	0.54
1:A:766:GLU:H	1:A:767:PRO:CD	2.08	0.54
1:A:137:GLN:NE2	1:A:141:ASP:OD1	2.41	0.54
1:A:657:ILE:HG22	1:A:675:GLN:HE22	1.74	0.53
1:A:399:LEU:HA	1:A:403:ASP:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:CZ	1:A:662:GLN:HA	2.43	0.53
1:A:63:LYS:HG2	1:A:69:ASP:OD1	2.08	0.53
1:A:500:ASN:HB3	5:A:2324:HOH:O	2.06	0.53
1:A:118:TYR:CE2	1:A:153:PRO:HG3	2.43	0.53
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.39	0.53
1:A:455:ILE:HG12	5:A:2162:HOH:O	2.09	0.53
1:A:11:TYR:CD2	1:A:15:LEU:HD12	2.44	0.53
1:A:758:ARG:O	1:A:761:ARG:HB3	2.09	0.53
1:A:326:ILE:HG23	5:A:2247:HOH:O	2.08	0.53
1:A:371:ASP:OD2	1:A:373:THR:HG23	2.09	0.53
1:A:727:LEU:HA	1:A:730:LEU:CD1	2.39	0.53
1:A:6:ASP:OD1	1:A:8:THR:HB	2.09	0.53
1:A:262:LEU:CD1	1:A:470:CYS:HB3	2.36	0.52
1:A:204:GLN:HG3	1:A:209:GLY:CA	2.39	0.52
1:A:397:ARG:HB3	1:A:404:LEU:HD11	1.91	0.52
1:A:706:TYR:CD2	1:A:707:LEU:N	2.74	0.52
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.24	0.52
1:A:497:GLU:OE1	1:A:742:THR:HG23	2.09	0.52
1:A:484:HIS:CE1	1:A:489:LEU:HD21	2.44	0.52
1:A:112:GLN:O	1:A:113:ASP:HB2	2.10	0.52
1:A:694:ASN:CB	1:A:746:PHE:HB2	2.39	0.52
1:A:695:ARG:HH11	1:A:695:ARG:CB	2.22	0.52
1:A:225:PHE:CE2	1:A:280:ILE:HG12	2.44	0.52
1:A:419:ASP:O	1:A:423:LYS:HG3	2.10	0.52
1:A:200:ALA:O	1:A:253:ILE:HG12	2.09	0.52
1:A:714:ARG:HG2	1:A:714:ARG:O	2.10	0.52
1:A:367:ALA:HB2	1:A:411:VAL:N	2.25	0.52
1:A:635:LYS:HE2	5:A:2340:HOH:O	2.09	0.52
1:A:175:LEU:HD12	1:A:651:HIS:HB2	1.91	0.52
1:A:461:PHE:H	1:A:464:ASN:ND2	2.04	0.51
1:A:622:LYS:HA	1:A:627:PHE:HA	1.90	0.51
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.41	0.51
1:A:750:GLN:HG2	1:A:754:ILE:HD12	1.93	0.51
1:A:144:LYS:HG3	1:A:199:VAL:CG2	2.40	0.51
1:A:764:SER:C	1:A:767:PRO:HD2	2.31	0.51
1:A:715:ASP:O	1:A:716:ALA:HB2	2.09	0.51
1:A:291:GLU:O	1:A:294:LYS:HE2	2.11	0.51
1:A:330:ALA:O	1:A:334:VAL:HG23	2.11	0.51
1:A:699:ALA:O	1:A:702:VAL:HG13	2.11	0.51
1:A:674:ASP:HB2	5:A:2448:HOH:O	2.11	0.51
1:A:698:TYR:HE1	1:A:744:ILE:HB	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ASN:OD1	1:A:765:ASN:C	2.49	0.51
1:A:56:THR:O	1:A:74:LYS:HE3	2.11	0.51
1:A:289:THR:OG1	1:A:292:GLU:HG3	2.11	0.51
1:A:244:GLU:HG3	1:A:449:PHE:CD2	2.47	0.50
1:A:79:GLN:HG2	1:A:96:TYR:CZ	2.46	0.50
1:A:764:SER:O	1:A:768:PRO:HD2	2.12	0.50
1:A:506:PHE:CZ	1:A:687:ILE:HD13	2.47	0.50
1:A:727:LEU:HB2	1:A:732:ILE:CG1	2.41	0.50
1:A:751:LEU:O	1:A:755:GLU:HB2	2.11	0.50
1:A:773:ASP:C	1:A:776:PRO:HD2	2.32	0.50
1:A:135:TYR:CD1	1:A:191:LYS:HD2	2.47	0.50
1:A:8:THR:HA	5:A:2007:HOH:O	2.10	0.50
1:A:516:LEU:O	1:A:525:ILE:HG13	2.12	0.50
1:A:701:PHE:HE2	1:A:723:THR:HG22	1.76	0.50
1:A:773:ASP:CB	1:A:775:ILE:H	2.24	0.50
1:A:53:VAL:CG2	1:A:63:LYS:HG3	2.38	0.50
1:A:601:LYS:HD3	5:A:2414:HOH:O	2.11	0.50
1:A:280:ILE:HG13	1:A:348:ILE:HD13	1.92	0.50
1:A:499:ILE:HG23	1:A:499:ILE:O	2.10	0.50
1:A:535:PHE:HD2	1:A:536:PRO:HD2	1.77	0.50
1:A:369:LEU:HD23	1:A:375:LEU:HD22	1.94	0.49
1:A:245:ILE:O	1:A:449:PHE:HA	2.12	0.49
1:A:334:VAL:HG12	1:A:440:VAL:HG21	1.93	0.49
1:A:225:PHE:CE2	1:A:348:ILE:HD11	2.47	0.49
1:A:622:LYS:HG2	1:A:626:ASN:O	2.12	0.49
1:A:76:ASP:HB3	5:A:2082:HOH:O	2.12	0.49
1:A:697:ILE:H	1:A:697:ILE:CD1	2.20	0.49
1:A:700:ASP:HA	1:A:703:LYS:HG2	1.93	0.49
1:A:708:LEU:HD13	5:A:2469:HOH:O	2.13	0.49
1:A:701:PHE:HE2	1:A:723:THR:HA	1.78	0.49
1:A:718:ASP:HB3	1:A:721:LYS:HD3	1.93	0.49
1:A:323:GLU:HA	1:A:323:GLU:OE1	2.12	0.49
1:A:244:GLU:O	1:A:256:ALA:HA	2.12	0.49
1:A:720:GLN:O	1:A:723:THR:OG1	2.30	0.49
1:A:84:LYS:HG2	5:A:2095:HOH:O	2.13	0.49
1:A:120:GLY:HA3	5:A:2456:HOH:O	2.12	0.49
1:A:712:VAL:N	1:A:713:PRO:CD	2.72	0.49
1:A:173:GLN:NE2	1:A:649:ASN:HD22	1.85	0.49
1:A:482:PHE:CE1	1:A:486:MET:HG3	2.48	0.49
1:A:22:SER:O	1:A:26:LYS:HG2	2.13	0.49
1:A:774:ASP:O	1:A:776:PRO:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:SER:HB3	1:A:322:GLU:HB2	1.94	0.49
1:A:557:LYS:HE3	5:A:2336:HOH:O	2.13	0.49
1:A:147:ARG:HB2	1:A:150:GLU:CD	2.33	0.48
1:A:737:TYR:HB3	1:A:750:GLN:OE1	2.13	0.48
1:A:737:TYR:HB2	1:A:745:PHE:O	2.13	0.48
1:A:752:ALA:HA	1:A:755:GLU:HB2	1.94	0.48
1:A:770:ASP:O	1:A:773:ASP:OD1	2.31	0.48
1:A:567:GLU:HA	1:A:579:TYR:O	2.13	0.48
1:A:698:TYR:CE1	1:A:744:ILE:HB	2.47	0.48
1:A:482:PHE:CZ	1:A:486:MET:HG3	2.48	0.48
1:A:37:TYR:OH	1:A:65:VAL:HG22	2.13	0.48
1:A:44:ARG:NH1	1:A:99:GLU:OE2	2.47	0.48
1:A:692:PHE:HB2	1:A:745:PHE:HB3	1.94	0.48
1:A:518:ASP:HB2	1:A:635:LYS:HD2	1.95	0.48
1:A:277:ASN:ND2	1:A:278:TYR:H	1.99	0.48
1:A:432:TRP:CE2	1:A:436:LYS:HD3	2.49	0.48
1:A:569:GLY:HA3	1:A:578:MET:CE	2.44	0.48
1:A:732:ILE:O	1:A:732:ILE:HG13	2.14	0.48
1:A:204:GLN:HA	1:A:209:GLY:N	2.29	0.48
1:A:712:VAL:O	1:A:712:VAL:HG12	2.11	0.48
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.49	0.47
1:A:736:GLN:OE1	1:A:750:GLN:CB	2.61	0.47
1:A:728:LYS:O	1:A:731:ASN:ND2	2.47	0.47
1:A:206:ASN:O	1:A:206:ASN:OD1	2.32	0.47
1:A:222:LEU:HD11	1:A:258:ILE:HD13	1.96	0.47
1:A:246:GLN:HG2	1:A:446:LYS:CD	2.44	0.47
1:A:372:LYS:HB2	1:A:376:ASN:HD21	1.79	0.47
1:A:98:ASN:HB3	5:A:2100:HOH:O	2.14	0.47
1:A:698:TYR:HB3	1:A:719:SER:HB2	1.96	0.47
1:A:700:ASP:CA	1:A:703:LYS:HG2	2.44	0.47
1:A:724:ASP:HA	1:A:727:LEU:CD2	2.45	0.46
1:A:700:ASP:O	1:A:703:LYS:HG2	2.15	0.46
1:A:327:THR:HG22	1:A:331:MET:HE2	1.96	0.46
1:A:171:GLN:HE22	1:A:649:ASN:N	2.13	0.46
1:A:582:GLN:O	1:A:583:ASP:HB2	2.15	0.46
1:A:573:TYR:O	1:A:678:CYS:HB2	2.15	0.46
1:A:318:VAL:HG11	5:A:2083:HOH:O	2.15	0.46
1:A:736:GLN:CD	1:A:750:GLN:HB2	2.36	0.46
1:A:465:SER:N	1:A:468:GLN:HE21	2.11	0.46
1:A:160:ASP:OD1	5:A:2151:HOH:O	2.21	0.46
1:A:705:TYR:CZ	1:A:754:ILE:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:O	1:A:278:TYR:OH	2.29	0.46
1:A:366:GLY:CA	1:A:408:HIS:CE1	2.91	0.46
1:A:610:LYS:HE3	1:A:614:ASP:CB	2.38	0.46
1:A:397:ARG:HA	1:A:406:ALA:HA	1.97	0.46
1:A:225:PHE:CD2	1:A:280:ILE:HG12	2.51	0.46
1:A:248:ASN:HD21	1:A:250:ALA:HB3	1.81	0.46
1:A:385:ASN:HA	1:A:386:PRO:HD2	1.74	0.46
1:A:702:VAL:HG23	1:A:714:ARG:HG3	1.98	0.46
1:A:679:ASN:HD22	1:A:679:ASN:N	2.13	0.46
1:A:773:ASP:O	1:A:776:PRO:HD2	2.16	0.46
1:A:238:ARG:O	1:A:263:LEU:HD12	2.16	0.46
1:A:708:LEU:HD11	1:A:758:ARG:HB2	1.98	0.45
1:A:202:ARG:O	1:A:204:GLN:N	2.47	0.45
1:A:118:TYR:CE1	1:A:123:LEU:HD13	2.51	0.45
1:A:170:ARG:O	1:A:448:TYR:HE1	1.99	0.45
1:A:667:LEU:HD11	1:A:672:VAL:HG21	1.97	0.45
1:A:580:GLU:OE2	1:A:582:GLN:HB2	2.16	0.45
1:A:521:GLN:HA	1:A:522:PRO:HA	1.60	0.45
1:A:727:LEU:HB2	1:A:732:ILE:CD1	2.46	0.45
1:A:495:LEU:HA	1:A:495:LEU:HD12	1.62	0.45
1:A:496:LYS:C	1:A:498:LYS:H	2.20	0.45
1:A:709:ALA:HB3	1:A:712:VAL:HG11	1.97	0.45
1:A:301:PRO:HG2	1:A:302:GLU:OE1	2.16	0.45
1:A:773:ASP:HB2	1:A:775:ILE:HG22	1.98	0.45
1:A:458:PHE:CE1	1:A:460:ILE:HD11	2.50	0.45
1:A:26:LYS:NZ	5:A:2036:HOH:O	2.49	0.45
1:A:7:ARG:HA	1:A:12:HIS:CG	2.52	0.45
1:A:397:ARG:HG2	1:A:397:ARG:NH1	2.32	0.45
1:A:675:GLN:O	1:A:679:ASN:HB2	2.16	0.44
1:A:762:LEU:N	1:A:762:LEU:HD13	2.33	0.44
1:A:207:GLY:O	1:A:211:LEU:HB2	2.17	0.44
1:A:258:ILE:HB	1:A:438:ASN:HD21	1.81	0.44
1:A:115:ILE:O	5:A:2120:HOH:O	2.21	0.44
1:A:499:ILE:HD11	1:A:740:GLY:N	2.29	0.44
1:A:91:MET:CE	1:A:105:ASN:HB3	2.47	0.44
1:A:754:ILE:HG13	5:A:2465:HOH:O	2.18	0.44
1:A:343:SER:HB2	1:A:607:VAL:HG21	1.99	0.44
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.83	0.44
1:A:765:ASN:N	1:A:767:PRO:HD3	2.33	0.44
1:A:671:VAL:O	1:A:675:GLN:HG3	2.17	0.44
1:A:212:GLU:OE2	1:A:212:GLU:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:ALA:O	1:A:647:THR:HG23	2.17	0.44
1:A:283:GLN:HG2	1:A:320:ASP:O	2.18	0.44
1:A:745:PHE:CD2	1:A:745:PHE:N	2.86	0.43
1:A:468:GLN:NE2	1:A:468:GLN:H	2.16	0.43
1:A:207:GLY:O	1:A:211:LEU:CB	2.67	0.43
1:A:234:ASN:ND2	5:A:2201:HOH:O	2.50	0.43
1:A:562:ARG:NH1	5:A:2373:HOH:O	2.50	0.43
1:A:150:GLU:HG2	1:A:150:GLU:H	1.39	0.43
1:A:246:GLN:CG	1:A:446:LYS:HD2	2.47	0.43
1:A:393:LEU:O	1:A:409:LEU:HD12	2.18	0.43
1:A:600:PHE:O	1:A:603:SER:HB3	2.19	0.43
1:A:391:LYS:HA	1:A:391:LYS:HD2	1.72	0.43
1:A:764:SER:C	1:A:768:PRO:HD2	2.39	0.43
1:A:773:ASP:O	1:A:776:PRO:CD	2.67	0.43
1:A:291:GLU:HA	1:A:294:LYS:HZ3	1.84	0.43
1:A:336:PHE:CE2	1:A:433:LEU:HD23	2.54	0.43
1:A:705:TYR:OH	1:A:755:GLU:HA	2.18	0.43
1:A:728:LYS:O	1:A:731:ASN:N	2.48	0.43
1:A:741:ILE:CG2	1:A:742:THR:HG22	2.46	0.43
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.33	0.43
1:A:56:THR:HG23	1:A:59:SER:OG	2.19	0.43
1:A:640:SER:O	1:A:643:ALA:HB3	2.19	0.43
1:A:262:LEU:HD12	1:A:634:TYR:CG	2.54	0.43
1:A:702:VAL:HG23	1:A:702:VAL:O	2.18	0.43
1:A:296:LEU:HB2	1:A:298:LEU:HG	2.00	0.43
1:A:776:PRO:O	1:A:777:PHE:C	2.57	0.43
1:A:750:GLN:HG2	1:A:754:ILE:CD1	2.49	0.42
1:A:149:ASN:N	1:A:149:ASN:OD1	2.40	0.42
1:A:284:LEU:HD13	1:A:345:PHE:HB3	2.00	0.42
1:A:732:ILE:HD12	1:A:754:ILE:CD1	2.49	0.42
1:A:431:LEU:HD22	4:A:1780:PBQ:BR18	2.74	0.42
1:A:775:ILE:N	1:A:776:PRO:HD2	2.33	0.42
1:A:171:GLN:NE2	1:A:649:ASN:HB2	2.33	0.42
1:A:173:GLN:HE21	1:A:173:GLN:HB3	1.68	0.42
1:A:704:ARG:HB3	5:A:2460:HOH:O	2.18	0.42
1:A:305:ASN:HA	1:A:308:ASN:OD1	2.19	0.42
1:A:661:LYS:NZ	1:A:666:LYS:NZ	2.68	0.42
1:A:267:ARG:HB3	1:A:278:TYR:CE2	2.55	0.42
1:A:657:ILE:O	1:A:675:GLN:NE2	2.50	0.42
1:A:717:GLU:O	1:A:718:ASP:HB2	2.20	0.42
1:A:431:LEU:HD22	4:A:1780:PBQ:BR17	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:GLU:OE2	1:A:468:GLN:HG3	2.19	0.42
1:A:147:ARG:NH1	1:A:759:GLU:OE2	2.52	0.42
1:A:266:SER:HA	1:A:423:LYS:HD2	2.02	0.42
1:A:56:THR:OG1	1:A:57:SER:N	2.52	0.42
1:A:376:ASN:O	1:A:380:THR:OG1	2.30	0.42
1:A:705:TYR:HE2	1:A:758:ARG:HD3	1.85	0.42
1:A:291:GLU:HB3	5:A:2229:HOH:O	2.20	0.42
1:A:258:ILE:N	1:A:438:ASN:OD1	2.47	0.42
1:A:280:ILE:HG23	1:A:281:PHE:N	2.34	0.42
1:A:713:PRO:HB2	1:A:715:ASP:H	1.85	0.42
1:A:623:LYS:N	1:A:626:ASN:O	2.52	0.42
1:A:182:GLY:HA2	1:A:233:ASN:ND2	2.35	0.42
1:A:695:ARG:HB2	1:A:743:LYS:CD	2.47	0.41
1:A:697:ILE:HA	1:A:743:LYS:CB	2.50	0.41
1:A:265:LYS:HE2	4:A:1780:PBQ:H11	1.84	0.41
1:A:495:LEU:HB3	1:A:496:LYS:CE	2.50	0.41
1:A:422:VAL:HG12	1:A:423:LYS:N	2.34	0.41
1:A:586:GLU:HB3	5:A:2399:HOH:O	2.19	0.41
1:A:565:LYS:HB2	1:A:565:LYS:HZ2	1.85	0.41
1:A:727:LEU:O	1:A:731:ASN:N	2.53	0.41
1:A:773:ASP:N	1:A:776:PRO:HD2	2.35	0.41
1:A:210:VAL:HG12	1:A:211:LEU:N	2.35	0.41
1:A:614:ASP:HA	1:A:615:PRO:HD3	1.91	0.41
1:A:319:SER:O	1:A:323:GLU:HG2	2.19	0.41
1:A:137:GLN:HE21	1:A:141:ASP:CG	2.24	0.41
1:A:72:VAL:HG22	1:A:73:LYS:O	2.18	0.41
1:A:313:VAL:HG12	1:A:313:VAL:O	2.21	0.41
1:A:752:ALA:O	1:A:755:GLU:N	2.53	0.41
1:A:497:GLU:OE1	1:A:497:GLU:HA	2.21	0.41
1:A:109:ARG:O	1:A:114:LEU:HB2	2.20	0.41
1:A:749:GLY:O	1:A:753:ARG:HD2	2.21	0.41
1:A:205:ALA:O	1:A:208:SER:N	2.52	0.41
1:A:289:THR:O	1:A:292:GLU:N	2.54	0.41
1:A:499:ILE:CD1	1:A:740:GLY:H	2.32	0.41
1:A:755:GLU:O	1:A:759:GLU:N	2.46	0.41
1:A:225:PHE:HE2	1:A:348:ILE:HD11	1.84	0.41
1:A:229:LYS:O	1:A:275:GLU:HB3	2.21	0.41
1:A:283:GLN:HB3	1:A:324:PHE:HB2	2.03	0.41
1:A:530:ASP:O	1:A:533:SER:HB2	2.20	0.41
1:A:2:ASN:HA	1:A:3:PRO:HD3	1.84	0.41
1:A:732:ILE:O	1:A:733:ASP:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ILE:HG22	1:A:742:THR:CA	2.50	0.41
1:A:775:ILE:CG2	1:A:776:PRO:HD2	2.51	0.41
1:A:496:LYS:O	1:A:498:LYS:N	2.54	0.41
1:A:727:LEU:HG	1:A:732:ILE:HG12	2.03	0.40
1:A:753:ARG:O	1:A:756:GLU:HG2	2.21	0.40
1:A:766:GLU:CG	1:A:766:GLU:O	2.69	0.40
1:A:467:GLU:O	1:A:471:ILE:HG13	2.21	0.40
1:A:103:PHE:CE2	1:A:669:ASP:HB3	2.57	0.40
1:A:185:LYS:NZ	1:A:457:GLY:HA3	2.36	0.40
1:A:499:ILE:CD1	1:A:740:GLY:N	2.84	0.40
1:A:716:ALA:HB1	1:A:721:LYS:CE	2.50	0.40
1:A:484:HIS:CD2	1:A:488:LYS:HB3	2.57	0.40
1:A:569:GLY:HA3	1:A:578:MET:HE2	2.04	0.40
1:A:87:GLY:O	1:A:88:VAL:C	2.60	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	774/788 (98%)	692 (89%)	72 (9%)	10 (1%)	15	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLU
1	A	713	PRO
1	A	709	ALA
1	A	710	PRO
1	A	766	GLU
1	A	287	GLY
1	A	708	LEU

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Mol	Chain	Res	Type
1	A	712	VAL
1	A	716	ALA
1	A	768	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	680/691 (98%)	597 (88%)	83 (12%)	6	18

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	31	ASP
1	A	35	ILE
1	A	38	ASN
1	A	42	LYS
1	A	44	ARG
1	A	56	THR
1	A	65	VAL
1	A	66	ASP
1	A	71	GLN
1	A	75	ASP
1	A	79	GLN
1	A	83	ILE
1	A	91	MET
1	A	95	SER
1	A	130	LYS
1	A	150	GLU
1	A	151	VAL
1	A	158	ILE
1	A	171	GLN
1	A	198	SER
1	A	199	VAL
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	210	VAL
1	A	277	ASN
1	A	284	LEU
1	A	291	GLU
1	A	294	LYS
1	A	329	GLN
1	A	358	LYS
1	A	361	LYS
1	A	387	SER
1	A	397	ARG
1	A	402	ARG
1	A	435	LYS
1	A	444	GLU
1	A	445	ARG
1	A	446	LYS
1	A	468	GLN
1	A	495	LEU
1	A	497	GLU
1	A	498	LYS
1	A	499	ILE
1	A	520	ARG
1	A	603	SER
1	A	633	GLN
1	A	646	GLU
1	A	666	LYS
1	A	679	ASN
1	A	692	PHE
1	A	695	ARG
1	A	696	ILE
1	A	700	ASP
1	A	701	PHE
1	A	702	VAL
1	A	704	ARG
1	A	706	TYR
1	A	707	LEU
1	A	708	LEU
1	A	710	PRO
1	A	719	SER
1	A	720	GLN
1	A	721	LYS
1	A	726	VAL
1	A	727	LEU

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Mol	Chain	Res	Type
1	A	728	LYS
1	A	730	LEU
1	A	736	GLN
1	A	742	THR
1	A	745	PHE
1	A	753	ARG
1	A	755	GLU
1	A	756	GLU
1	A	758	ARG
1	A	762	LEU
1	A	764	SER
1	A	766	GLU
1	A	767	PRO
1	A	769	MET
1	A	771	PHE
1	A	773	ASP
1	A	774	ASP
1	A	777	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	137	GLN
1	A	171	GLN
1	A	173	GLN
1	A	206	ASN
1	A	234	ASN
1	A	271	GLN
1	A	277	ASN
1	A	329	GLN
1	A	356	ASN
1	A	376	ASN
1	A	407	GLN
1	A	408	HIS
1	A	443	GLN
1	A	464	ASN
1	A	468	GLN
1	A	484	HIS
1	A	500	ASN
1	A	613	ASN
1	A	616	ASN

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Mol	Chain	Res	Type
1	A	633	GLN
1	A	679	ASN
1	A	731	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	AD9	A	1778	3	24,33,33	3.37	9 (37%)	30,52,52	1.77	7 (23%)
4	PBQ	A	1780	-	17,18,18	0.72	0	19,27,27	1.32	1 (5%)

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	AD9	A	1778	3	-	0/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PBQ	A	1780	-	-	0/2/4/4	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1778	AD9	C4-N3	2.22	1.38	1.35
2	A	1778	AD9	C2-N3	2.23	1.36	1.32
2	A	1778	AD9	PA-O1A	2.49	1.55	1.48
2	A	1778	AD9	PB-O2B	3.51	1.56	1.48
2	A	1778	AD9	PB-O3A	4.06	1.68	1.60
2	A	1778	AD9	PA-O3A	4.14	1.68	1.60
2	A	1778	AD9	O4'-C1'	4.98	1.47	1.41
2	A	1778	AD9	PB-O1B	8.65	1.70	1.48
2	A	1778	AD9	PA-O2A	9.93	1.71	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1778	AD9	O3A-PB-O1B	-4.20	98.72	108.79
2	A	1778	AD9	N3-C2-N1	-3.62	126.12	128.89
2	A	1778	AD9	O2A-PA-O3A	-2.94	100.77	108.79
2	A	1778	AD9	PA-O5'-C5'	2.59	129.17	120.25
2	A	1778	AD9	O3B-PB-O3A	2.90	106.22	100.46
2	A	1778	AD9	O3A-PA-O1A	3.20	116.47	108.79
2	A	1778	AD9	O2B-PB-O3B	3.25	117.60	108.80
4	A	1780	PBQ	C7-C8-C9	3.76	107.59	104.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1778	AD9	2	0
4	A	1780	PBQ	11	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	776/788 (98%)	-0.11	48 (6%) 24 15	8, 35, 92, 96	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	ASN	10.7
1	A	769	MET	8.7
1	A	719	SER	7.0
1	A	762	LEU	6.8
1	A	767	PRO	6.4
1	A	771	PHE	6.3
1	A	761	ARG	5.9
1	A	718	ASP	5.9
1	A	764	SER	5.8
1	A	763	GLU	5.8
1	A	754	ILE	5.4
1	A	734	PRO	5.3
1	A	770	ASP	5.3
1	A	207	GLY	5.2
1	A	729	HIS	4.8
1	A	711	ASN	4.8
1	A	768	PRO	4.7
1	A	208	SER	4.7
1	A	757	ALA	4.4
1	A	732	ILE	4.4
1	A	706	TYR	4.4
1	A	708	LEU	4.3
1	A	752	ALA	4.3
1	A	206	ASN	4.3
1	A	710	PRO	4.2
1	A	722	ALA	4.2
1	A	758	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	776	PRO	4.0
1	A	755	GLU	3.8
1	A	727	LEU	3.8
1	A	712	VAL	3.8
1	A	774	ASP	3.6
1	A	623	LYS	3.6
1	A	204	GLN	3.4
1	A	773	ASP	3.3
1	A	766	GLU	3.2
1	A	705	TYR	3.1
1	A	720	GLN	3.1
1	A	759	GLU	3.0
1	A	775	ILE	2.9
1	A	209	GLY	2.9
1	A	760	GLN	2.9
1	A	772	ASP	2.7
1	A	499	ILE	2.3
1	A	203	ASN	2.2
1	A	713	PRO	2.2
1	A	725	ALA	2.1
1	A	756	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	PBQ	A	1780	17/17	0.67	0.62	9.51	31,35,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	AD9	A	1778	31/31	0.96	0.17	0.61	13,28,36,40	0
3	MG	A	1779	1/1	0.51	0.21	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.