



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:21 PM EDT

PDB ID : 3IKJ / pdb_00003ikj
Title : Structural characterization for the nucleotide binding ability of subunit A mutant S238A of the A1AO ATP synthase
Authors : Kumar, A.; Manimekali, M.S.S.; Balakrishna, A.M.; Jeyakanthan, J.; Gruber, G.
Deposited on : 2009-08-06
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

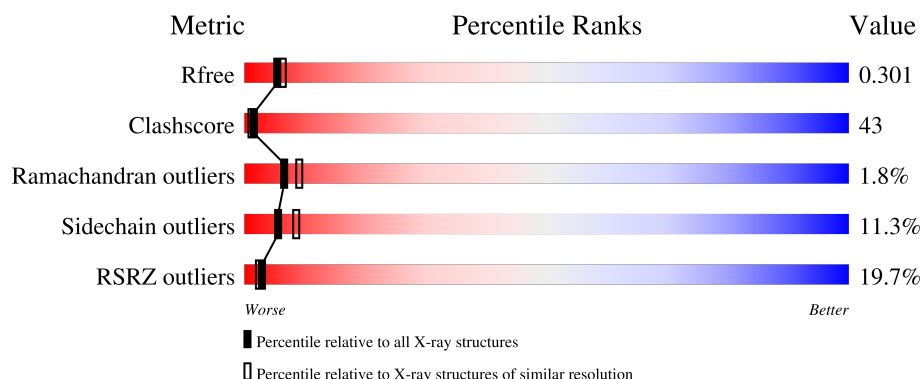
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	588	

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
2	MPD	A	589	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	591	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4353 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.

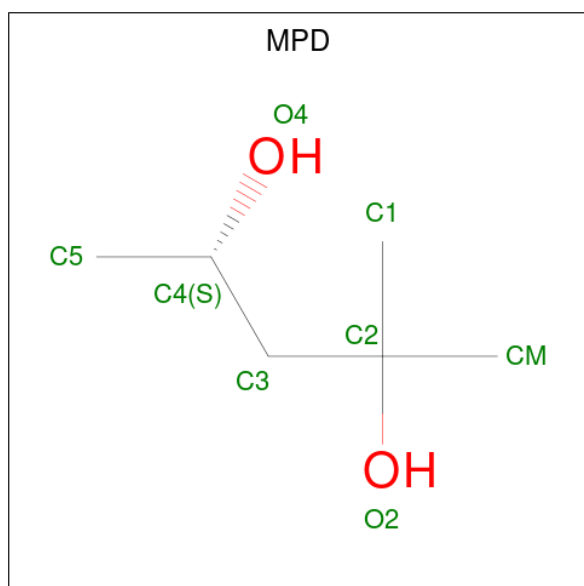
- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	4055	2595	693	751	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ARG	GLY	engineered mutation	UNP O57728
A	238	ALA	SER	engineered mutation	UNP O57728

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



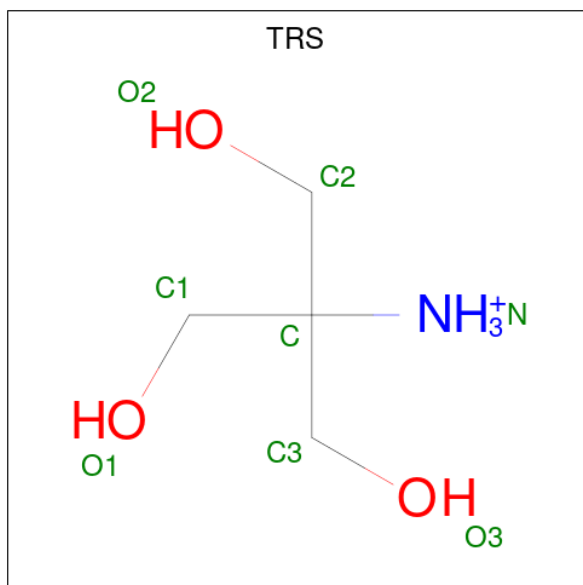
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

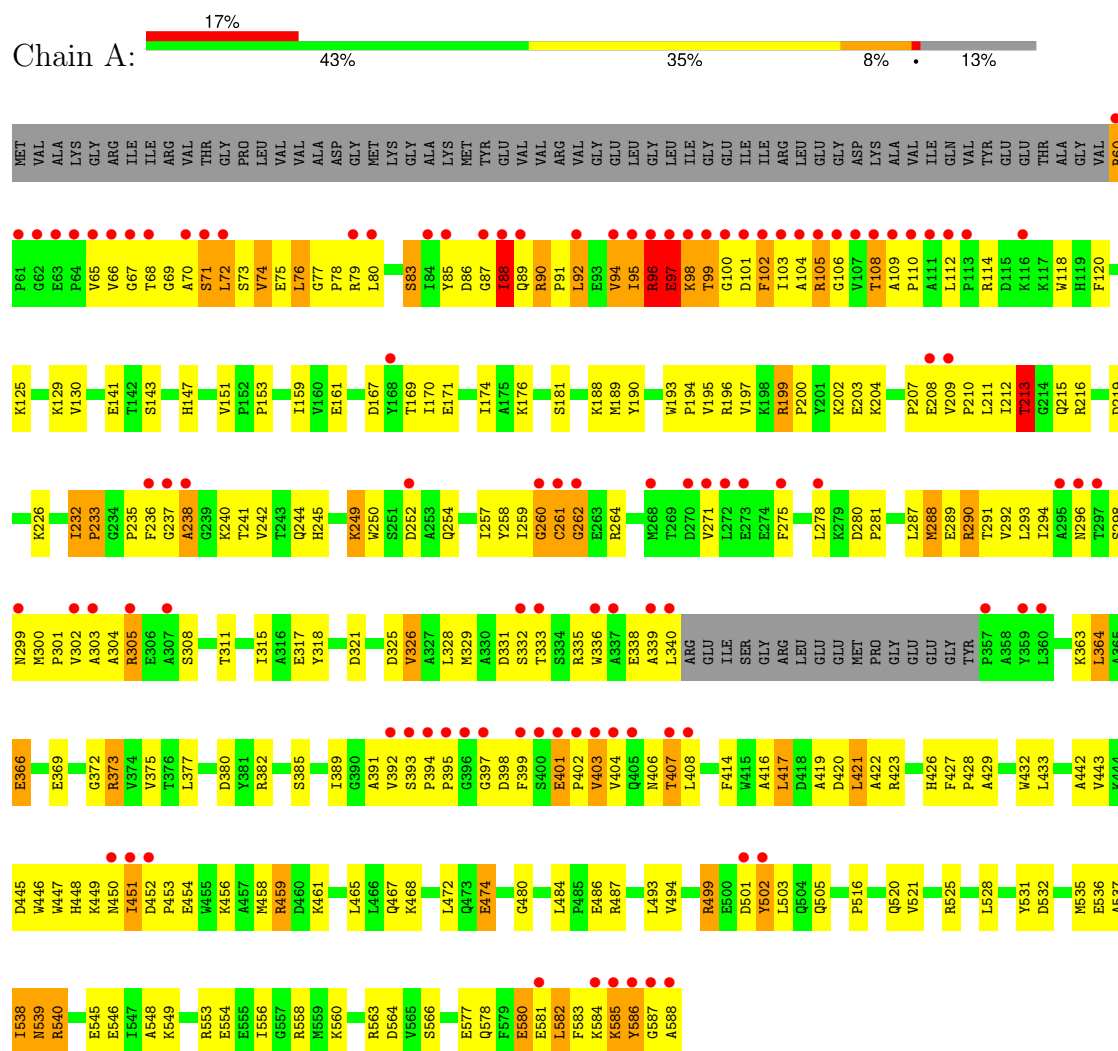
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	266	Total	O	0	0
			266	266		

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: V-type ATP synthase alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.21 Å 128.21 Å 105.83 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 2.40 29.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.84-2.40) 99.8 (29.84-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.239 , 0.304 0.251 , 0.301	Depositor DCC
R_{free} test set	1752 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4353	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: TRS, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.21	5/4144 (0.1%)	1.29	32/5614 (0.6%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	THR	CA-CB	7.48	1.62	1.53
1	A	326	VAL	CA-CB	7.20	1.65	1.54
1	A	516	PRO	CA-C	5.55	1.54	1.51
1	A	76	LEU	C-O	-5.33	1.18	1.24
1	A	108	THR	CA-CB	5.31	1.60	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	PHE	N-CA-C	10.35	122.64	111.36
1	A	407	THR	N-CA-C	9.28	121.16	111.14
1	A	585	LYS	N-CA-C	-9.05	96.88	110.28
1	A	480	GLY	CA-C-N	8.31	129.36	120.47
1	A	480	GLY	C-N-CA	8.31	129.36	120.47
1	A	459	ARG	N-CA-CB	7.35	120.93	110.12
1	A	151	VAL	CA-C-N	7.15	124.88	119.66
1	A	151	VAL	C-N-CA	7.15	124.88	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	VAL	CB-CA-C	-6.59	99.87	110.28
1	A	108	THR	N-CA-C	6.53	116.89	108.34
1	A	199	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	A	582	LEU	N-CA-C	-6.38	106.03	113.88
1	A	213	THR	N-CA-C	-6.25	105.78	113.41
1	A	199	ARG	NE-CZ-NH2	6.23	124.80	119.20
1	A	459	ARG	CG-CD-NE	6.20	125.63	112.00
1	A	373	ARG	NE-CZ-NH2	-6.05	113.76	119.20
1	A	213	THR	N-CA-CB	-6.04	101.65	110.47
1	A	364	LEU	N-CA-C	-5.92	105.72	113.12
1	A	96	ARG	N-CA-C	5.84	118.42	108.90
1	A	97	GLU	N-CA-C	5.73	118.58	110.50
1	A	537	ALA	N-CA-C	-5.42	105.03	111.69
1	A	535	MET	N-CA-C	-5.38	105.45	112.23
1	A	125	LYS	N-CA-C	5.28	117.70	109.52
1	A	373	ARG	CG-CD-NE	-5.28	100.40	112.00
1	A	502	TYR	N-CA-C	5.25	119.66	112.68
1	A	499	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	A	238	ALA	N-CA-C	5.20	116.78	108.41
1	A	459	ARG	CA-CB-CG	5.15	124.40	114.10
1	A	465	LEU	CB-CG-CD2	-5.11	95.36	110.70
1	A	375	VAL	N-CA-C	-5.08	102.19	108.89
1	A	280	ASP	CA-C-N	5.08	124.74	119.56
1	A	280	ASP	C-N-CA	5.08	124.74	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	GLY	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	4055	0	4112	348	0
2	A	24	0	42	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	12	1	0
4	A	266	0	0	42	0
All	All	4353	0	4166	353	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 43.

All (353) 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:261:CYS:SG	1:A:332:SER:HB2	1.41	1.56
1:A:233:PRO:HG3	1:A:414:PHE:CE1	1.55	1.38
1:A:245:HIS:NE2	2:A:589:MPD:H52	1.41	1.33
1:A:233:PRO:CG	1:A:414:PHE:CE1	2.15	1.27
1:A:97:GLU:HB2	1:A:105:ARG:O	1.27	1.25
1:A:261:CYS:SG	1:A:332:SER:CB	2.31	1.18
2:A:591:MPD:H53	4:A:690:HOH:O	1.39	1.18
1:A:83:SER:OG	1:A:85:TYR:CE2	2.00	1.15
1:A:79:ARG:HG2	4:A:818:HOH:O	0.97	1.14
1:A:79:ARG:HB2	1:A:118:TRP:CZ2	1.84	1.13
1:A:258:TYR:CE2	1:A:260:GLY:HA3	1.83	1.13
1:A:97:GLU:CB	1:A:105:ARG:O	1.98	1.12
1:A:96:ARG:HG3	1:A:301:PRO:HD2	1.22	1.11
1:A:90:ARG:NH2	1:A:96:ARG:HA	1.67	1.10
1:A:99:THR:HG22	1:A:100:GLY:H	1.15	1.10
1:A:88:ILE:HG22	1:A:89:GLN:H	1.05	1.08
1:A:245:HIS:CD2	1:A:249:LYS:HD3	1.89	1.08
1:A:233:PRO:HB3	1:A:392:VAL:HG23	1.37	1.07
1:A:79:ARG:O	1:A:79:ARG:HD3	1.54	1.06
1:A:233:PRO:CD	1:A:414:PHE:CE1	2.40	1.05
1:A:96:ARG:CG	1:A:301:PRO:HD2	1.87	1.04
1:A:389:ILE:HB	4:A:838:HOH:O	1.55	1.03
1:A:458:MET:HE1	1:A:525:ARG:HG2	1.36	1.03
1:A:233:PRO:CG	1:A:414:PHE:CZ	2.42	1.02
1:A:88:ILE:CG2	1:A:89:GLN:H	1.72	1.02
1:A:90:ARG:HH12	1:A:96:ARG:HE	1.07	1.01
1:A:79:ARG:HB2	1:A:118:TRP:HZ2	1.13	1.01
1:A:99:THR:CG2	1:A:100:GLY:H	1.73	1.01
1:A:233:PRO:CG	1:A:414:PHE:HE1	1.59	1.00
1:A:233:PRO:HG3	1:A:414:PHE:HE1	0.90	1.00
1:A:80:LEU:O	1:A:83:SER:HB3	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLU:HG2	1:A:402:PRO:HD3	1.46	0.98
1:A:445:ASP:HB2	4:A:689:HOH:O	1.62	0.97
1:A:448:HIS:HA	1:A:452:ASP:O	1.65	0.97
1:A:245:HIS:CD2	2:A:589:MPD:H31	2.00	0.97
1:A:88:ILE:HG22	1:A:89:GLN:N	1.67	0.96
1:A:258:TYR:CE2	1:A:260:GLY:CA	2.48	0.96
1:A:75:GLU:H	1:A:89:GLN:HE22	1.03	0.94
1:A:245:HIS:CD2	2:A:589:MPD:H52	2.02	0.93
1:A:208:GLU:O	1:A:443:VAL:HG12	1.68	0.93
1:A:96:ARG:HG3	1:A:301:PRO:CD	1.99	0.93
1:A:261:CYS:HG	1:A:332:SER:HB2	1.28	0.92
1:A:213:THR:HG22	1:A:215:GLN:H	1.35	0.91
1:A:249:LYS:HE2	2:A:589:MPD:H53	1.50	0.91
1:A:216:ARG:H	1:A:505:GLN:HE22	1.17	0.90
1:A:232:ILE:HD13	1:A:391:ALA:HA	1.51	0.90
1:A:90:ARG:HH22	1:A:96:ARG:HA	1.33	0.90
1:A:102:PHE:C	1:A:103:ILE:HD12	1.98	0.89
1:A:546:GLU:HG3	1:A:582:LEU:HD11	1.53	0.89
1:A:112:LEU:HG	4:A:831:HOH:O	1.72	0.88
1:A:90:ARG:HH12	1:A:96:ARG:NE	1.71	0.88
1:A:258:TYR:HE2	1:A:260:GLY:HA3	1.35	0.87
1:A:120:PHE:HB2	4:A:756:HOH:O	1.73	0.86
1:A:96:ARG:HB2	1:A:301:PRO:HG2	1.56	0.86
1:A:233:PRO:HG3	1:A:414:PHE:CZ	2.08	0.86
1:A:233:PRO:HD3	1:A:414:PHE:CE1	2.10	0.85
1:A:458:MET:CE	1:A:525:ARG:HG2	2.07	0.84
1:A:216:ARG:HD2	1:A:502:TYR:CE1	2.13	0.84
1:A:233:PRO:HG2	1:A:414:PHE:CZ	2.12	0.84
1:A:96:ARG:CB	1:A:301:PRO:HD2	2.09	0.83
1:A:102:PHE:HB2	1:A:103:ILE:HD12	1.61	0.83
1:A:99:THR:HG22	1:A:100:GLY:N	1.93	0.83
1:A:91:PRO:O	1:A:94:VAL:HG22	1.78	0.83
1:A:108:THR:HG22	1:A:109:ALA:H	1.42	0.82
1:A:245:HIS:HD2	1:A:249:LYS:HD3	1.42	0.82
1:A:92:LEU:HD13	4:A:726:HOH:O	1.78	0.82
1:A:249:LYS:NZ	1:A:281:PRO:HG3	1.96	0.81
1:A:467:GLN:HG3	4:A:701:HOH:O	1.80	0.81
1:A:238:ALA:HB3	1:A:422:ALA:HB1	1.63	0.80
1:A:245:HIS:HD2	2:A:589:MPD:H31	1.43	0.80
1:A:96:ARG:HB2	1:A:301:PRO:HD2	1.64	0.80
1:A:249:LYS:CE	2:A:589:MPD:H53	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:HB3	1:A:502:TYR:CE2	2.19	0.78
1:A:86:ASP:O	1:A:88:ILE:O	2.00	0.78
1:A:79:ARG:O	1:A:79:ARG:CD	2.30	0.77
1:A:96:ARG:HB2	1:A:301:PRO:CG	2.15	0.77
1:A:74:VAL:HG23	1:A:195:VAL:CG1	2.15	0.76
1:A:245:HIS:NE2	2:A:589:MPD:C5	2.37	0.76
1:A:199:ARG:NH1	1:A:321:ASP:OD2	2.18	0.76
1:A:339:ALA:HA	4:A:824:HOH:O	1.84	0.76
1:A:580:GLU:O	1:A:584:LYS:HG3	1.86	0.76
1:A:96:ARG:HD3	1:A:300:MET:HG2	1.68	0.76
1:A:103:ILE:HG22	1:A:104:ALA:N	2.01	0.76
1:A:153:PRO:HG2	1:A:193:TRP:CZ3	2.21	0.76
1:A:88:ILE:CG2	1:A:89:GLN:N	2.35	0.75
1:A:78:PRO:O	4:A:831:HOH:O	2.03	0.75
1:A:454:GLU:HG3	4:A:830:HOH:O	1.86	0.75
1:A:261:CYS:HB3	1:A:296:ASN:H	1.51	0.74
2:A:589:MPD:HM1	2:A:589:MPD:O4	1.88	0.74
1:A:69:GLY:HA2	1:A:103:ILE:HA	1.71	0.73
1:A:108:THR:HG22	1:A:109:ALA:N	2.03	0.73
1:A:109:ALA:HB1	1:A:110:PRO:HD2	1.69	0.73
1:A:235:PRO:HG3	1:A:419:ALA:HB2	1.69	0.73
1:A:90:ARG:CZ	1:A:95:ILE:O	2.36	0.72
1:A:216:ARG:H	1:A:505:GLN:NE2	1.86	0.72
1:A:87:GLY:HA2	1:A:308:SER:HB3	1.70	0.72
1:A:96:ARG:HB2	1:A:301:PRO:CD	2.19	0.72
1:A:103:ILE:CG2	1:A:104:ALA:N	2.52	0.72
1:A:448:HIS:HE1	1:A:456:LYS:H	1.35	0.72
1:A:249:LYS:CD	2:A:589:MPD:H53	2.19	0.72
1:A:458:MET:HE1	1:A:525:ARG:CG	2.16	0.71
1:A:97:GLU:HB3	1:A:106:GLY:HA2	1.72	0.71
1:A:254:GLN:HE22	1:A:325:ASP:H	1.37	0.71
1:A:447:TRP:CZ3	1:A:451:ILE:HG21	2.25	0.71
1:A:311:THR:O	1:A:315:ILE:HG13	1.91	0.71
1:A:264:ARG:HD2	4:A:815:HOH:O	1.91	0.71
1:A:427:PHE:HA	1:A:428:PRO:C	2.16	0.70
1:A:258:TYR:CD2	1:A:260:GLY:HA3	2.26	0.70
1:A:402:PRO:O	1:A:403:VAL:HG12	1.92	0.70
1:A:216:ARG:HD2	1:A:502:TYR:CD1	2.27	0.69
1:A:233:PRO:HG2	1:A:414:PHE:HZ	1.56	0.69
1:A:86:ASP:O	1:A:87:GLY:C	2.35	0.69
1:A:90:ARG:NH1	1:A:96:ARG:HE	1.87	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLU:N	1:A:366:GLU:OE2	2.25	0.69
1:A:452:ASP:OD1	1:A:453:PRO:N	2.25	0.69
1:A:75:GLU:N	1:A:89:GLN:HE22	1.86	0.69
1:A:69:GLY:HA2	1:A:103:ILE:HG13	1.75	0.69
1:A:97:GLU:C	1:A:97:GLU:OE1	2.35	0.68
1:A:143:SER:OG	1:A:289:GLU:OE2	2.11	0.68
1:A:521:VAL:O	1:A:525:ARG:HG3	1.94	0.68
1:A:90:ARG:HB2	1:A:94:VAL:HG21	1.76	0.68
1:A:563:ARG:HD3	4:A:762:HOH:O	1.94	0.68
1:A:259:ILE:O	1:A:261:CYS:SG	2.52	0.67
1:A:401:GLU:CG	1:A:402:PRO:HD3	2.24	0.67
1:A:91:PRO:O	1:A:94:VAL:CG2	2.43	0.67
1:A:211:LEU:HD12	1:A:252:ASP:OD1	1.94	0.66
1:A:329:MET:HG2	4:A:838:HOH:O	1.95	0.66
1:A:83:SER:OG	1:A:85:TYR:CZ	2.37	0.66
1:A:461:LYS:HZ3	2:A:591:MPD:HM1	1.58	0.66
1:A:536:GLU:O	1:A:540:ARG:HG3	1.94	0.65
1:A:369:GLU:HB3	4:A:725:HOH:O	1.96	0.65
1:A:245:HIS:O	1:A:249:LYS:HG2	1.95	0.65
1:A:447:TRP:CE3	1:A:451:ILE:HG21	2.31	0.65
1:A:66:VAL:HG12	1:A:67:GLY:N	2.11	0.65
1:A:249:LYS:CD	2:A:589:MPD:C5	2.75	0.64
1:A:97:GLU:HB3	1:A:105:ARG:O	1.96	0.64
1:A:461:LYS:NZ	2:A:591:MPD:HM1	2.10	0.64
1:A:254:GLN:NE2	1:A:325:ASP:H	1.95	0.64
1:A:102:PHE:O	1:A:103:ILE:HD12	1.95	0.64
1:A:87:GLY:N	1:A:96:ARG:HH22	1.96	0.64
1:A:101:ASP:OD1	1:A:102:PHE:N	2.31	0.64
1:A:261:CYS:CB	1:A:332:SER:HB2	2.25	0.64
1:A:487:ARG:HD2	4:A:670:HOH:O	1.98	0.63
1:A:233:PRO:HB3	1:A:392:VAL:CG2	2.22	0.63
1:A:585:LYS:O	1:A:586:TYR:HB2	1.98	0.63
1:A:99:THR:CG2	1:A:100:GLY:N	2.49	0.63
1:A:401:GLU:HG2	1:A:402:PRO:CD	2.26	0.63
1:A:458:MET:SD	1:A:525:ARG:HG2	2.39	0.63
1:A:528:LEU:HB3	2:A:591:MPD:HM2	1.81	0.62
1:A:80:LEU:HD21	1:A:89:GLN:OE1	1.99	0.62
1:A:102:PHE:O	1:A:103:ILE:CD1	2.47	0.62
1:A:102:PHE:O	1:A:103:ILE:HG13	1.99	0.62
1:A:96:ARG:CG	1:A:301:PRO:CD	2.68	0.61
1:A:200:PRO:HG2	1:A:377:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:NH2	1:A:304:ALA:HB1	2.15	0.61
1:A:258:TYR:CE2	1:A:260:GLY:HA2	2.34	0.60
1:A:329:MET:HA	4:A:838:HOH:O	2.01	0.60
1:A:394:PRO:HD2	4:A:766:HOH:O	2.01	0.60
1:A:494:VAL:HG11	1:A:531:TYR:HB2	1.83	0.60
1:A:86:ASP:HB2	1:A:96:ARG:CZ	2.31	0.60
1:A:109:ALA:HB1	1:A:110:PRO:CD	2.31	0.60
1:A:249:LYS:HZ2	1:A:281:PRO:HG3	1.65	0.59
1:A:259:ILE:C	1:A:261:CYS:SG	2.85	0.59
1:A:448:HIS:CA	1:A:452:ASP:O	2.47	0.59
1:A:86:ASP:O	1:A:88:ILE:N	2.35	0.59
1:A:67:GLY:CA	4:A:717:HOH:O	2.50	0.59
1:A:540:ARG:NH2	1:A:588:ALA:OXT	2.36	0.59
1:A:232:ILE:O	1:A:232:ILE:HG12	1.99	0.58
1:A:189:MET:SD	4:A:756:HOH:O	2.57	0.58
1:A:233:PRO:CB	1:A:392:VAL:HG23	2.24	0.58
1:A:394:PRO:HB2	1:A:398:ASP:HB3	1.85	0.58
1:A:502:TYR:OH	1:A:520:GLN:HB3	2.02	0.58
1:A:532:ASP:OD2	2:A:591:MPD:HM3	2.04	0.58
1:A:102:PHE:O	1:A:103:ILE:CG1	2.51	0.58
1:A:90:ARG:NH2	1:A:95:ILE:O	2.37	0.58
1:A:290:ARG:CZ	4:A:804:HOH:O	2.52	0.58
1:A:199:ARG:NH1	1:A:318:TYR:HA	2.18	0.58
1:A:245:HIS:CD2	2:A:589:MPD:C3	2.83	0.57
1:A:197:VAL:HA	4:A:652:HOH:O	2.05	0.57
1:A:90:ARG:HH22	1:A:96:ARG:CA	2.14	0.57
1:A:103:ILE:CG2	1:A:104:ALA:H	2.17	0.57
1:A:554:GLU:OE2	1:A:558:ARG:NH2	2.32	0.57
1:A:364:LEU:HD21	1:A:407:THR:OG1	2.05	0.57
1:A:118:TRP:HH2	4:A:818:HOH:O	1.86	0.56
1:A:331:ASP:HA	1:A:391:ALA:HB3	1.88	0.56
1:A:587:GLY:O	1:A:588:ALA:HB3	2.04	0.56
1:A:288:MET:HE1	1:A:293:LEU:HD11	1.86	0.55
1:A:203:GLU:OE2	4:A:696:HOH:O	2.17	0.55
1:A:250:TRP:CH2	1:A:281:PRO:HB2	2.40	0.55
1:A:245:HIS:CD2	2:A:589:MPD:C5	2.86	0.55
1:A:451:ILE:HG22	1:A:521:VAL:HG11	1.89	0.55
1:A:65:VAL:HG12	1:A:66:VAL:O	2.07	0.55
1:A:245:HIS:HE1	1:A:278:LEU:HD13	1.71	0.55
1:A:75:GLU:HB2	1:A:112:LEU:HD13	1.89	0.55
1:A:448:HIS:CE1	1:A:456:LYS:H	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:HB	1:A:219:ASP:OD1	2.06	0.54
1:A:110:PRO:HG2	4:A:819:HOH:O	2.05	0.54
1:A:577:GLU:HB3	4:A:793:HOH:O	2.08	0.54
1:A:226:LYS:NZ	1:A:252:ASP:OD2	2.21	0.54
1:A:108:THR:CG2	1:A:109:ALA:H	2.16	0.54
1:A:153:PRO:HG2	1:A:193:TRP:HZ3	1.72	0.53
1:A:421:LEU:HD13	2:A:590:MPD:O4	2.09	0.53
1:A:249:LYS:NZ	1:A:249:LYS:HB2	2.24	0.53
1:A:261:CYS:HB2	1:A:332:SER:OG	2.09	0.53
1:A:417:LEU:HA	1:A:429:ALA:O	2.08	0.52
1:A:474:GLU:OE2	1:A:474:GLU:HA	2.08	0.52
1:A:170:ILE:HG12	4:A:657:HOH:O	2.09	0.52
1:A:258:TYR:HE2	1:A:260:GLY:CA	2.05	0.52
1:A:249:LYS:HB2	1:A:249:LYS:HZ3	1.75	0.52
1:A:96:ARG:O	1:A:301:PRO:HG2	2.10	0.52
1:A:249:LYS:HD3	2:A:589:MPD:C5	2.40	0.52
1:A:538:ILE:C	1:A:540:ARG:H	2.17	0.52
1:A:232:ILE:O	1:A:232:ILE:CG1	2.59	0.51
1:A:458:MET:HE2	2:A:591:MPD:H11	1.93	0.51
1:A:86:ASP:OD2	1:A:90:ARG:O	2.29	0.51
1:A:90:ARG:HD3	1:A:108:THR:HG23	1.92	0.51
1:A:108:THR:CG2	1:A:109:ALA:N	2.74	0.51
1:A:501:ASP:O	1:A:560:LYS:HE2	2.11	0.51
1:A:452:ASP:OD2	1:A:525:ARG:NH1	2.44	0.51
1:A:86:ASP:OD1	1:A:96:ARG:NH2	2.44	0.51
1:A:96:ARG:CB	1:A:301:PRO:CD	2.83	0.51
1:A:202:LYS:NZ	4:A:835:HOH:O	2.20	0.51
1:A:447:TRP:HZ3	1:A:451:ILE:HG21	1.75	0.50
1:A:585:LYS:O	1:A:586:TYR:CB	2.59	0.50
1:A:468:LYS:HE3	1:A:472:LEU:HG	1.93	0.50
1:A:66:VAL:CG1	1:A:67:GLY:N	2.74	0.50
1:A:199:ARG:HG3	1:A:317:GLU:OE1	2.11	0.50
1:A:90:ARG:HH11	1:A:90:ARG:HG3	1.76	0.50
1:A:373:ARG:HG3	1:A:385:SER:HB3	1.93	0.50
1:A:236:PHE:CE1	1:A:240:LYS:HE2	2.46	0.50
1:A:288:MET:HE1	1:A:293:LEU:CD1	2.41	0.49
1:A:97:GLU:C	1:A:97:GLU:CD	2.80	0.49
1:A:79:ARG:CG	4:A:818:HOH:O	1.85	0.49
1:A:249:LYS:CE	2:A:589:MPD:H32	2.42	0.49
1:A:75:GLU:HB2	1:A:112:LEU:CD1	2.42	0.49
1:A:97:GLU:OE1	1:A:97:GLU:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:HG22	1:A:446:TRP:CD1	2.47	0.49
1:A:451:ILE:HD13	1:A:451:ILE:N	2.27	0.49
1:A:79:ARG:CB	1:A:118:TRP:HZ2	2.04	0.49
1:A:249:LYS:HD3	2:A:589:MPD:H52	1.93	0.49
1:A:452:ASP:OD1	1:A:453:PRO:CD	2.60	0.49
1:A:88:ILE:N	1:A:88:ILE:CD1	2.75	0.49
1:A:582:LEU:O	1:A:585:LYS:O	2.31	0.49
1:A:71:SER:C	4:A:808:HOH:O	2.55	0.48
1:A:97:GLU:OE1	1:A:98:LYS:O	2.31	0.48
1:A:536:GLU:O	1:A:539:ASN:ND2	2.47	0.48
1:A:74:VAL:HG23	1:A:195:VAL:HG11	1.93	0.48
1:A:147:HIS:HE1	1:A:318:TYR:OH	1.96	0.48
1:A:290:ARG:NH2	4:A:804:HOH:O	2.45	0.48
1:A:258:TYR:N	4:A:851:HOH:O	2.36	0.48
1:A:288:MET:CE	1:A:293:LEU:CD1	2.92	0.48
1:A:207:PRO:O	1:A:442:ALA:HB1	2.13	0.48
1:A:102:PHE:CB	1:A:103:ILE:HD12	2.39	0.48
1:A:241:THR:OG1	1:A:264:ARG:NH2	2.47	0.48
1:A:114:ARG:HD3	1:A:170:ILE:HD11	1.96	0.48
1:A:176:LYS:HE2	4:A:857:HOH:O	2.14	0.47
1:A:102:PHE:C	1:A:103:ILE:CD1	2.78	0.47
1:A:102:PHE:HB2	1:A:103:ILE:CD1	2.39	0.47
1:A:67:GLY:HA2	4:A:717:HOH:O	2.13	0.47
1:A:209:VAL:HG13	1:A:210:PRO:HD2	1.97	0.47
1:A:66:VAL:HG12	1:A:67:GLY:H	1.78	0.47
1:A:258:TYR:HB3	1:A:293:LEU:HD23	1.96	0.47
1:A:499:ARG:HA	1:A:503:LEU:HB2	1.95	0.47
1:A:90:ARG:HD2	1:A:94:VAL:HB	1.96	0.47
1:A:364:LEU:CD2	1:A:407:THR:OG1	2.62	0.47
1:A:578:GLN:HA	1:A:581:GLU:HG2	1.96	0.47
1:A:393:SER:HB3	4:A:813:HOH:O	2.13	0.47
1:A:380:ASP:OD2	1:A:382:ARG:HD3	2.15	0.47
1:A:103:ILE:HG23	1:A:104:ALA:H	1.80	0.47
1:A:261:CYS:HB3	1:A:296:ASN:N	2.25	0.47
2:A:589:MPD:O4	2:A:589:MPD:CM	2.62	0.47
1:A:452:ASP:OD1	1:A:453:PRO:HD2	2.15	0.47
1:A:249:LYS:HE2	2:A:589:MPD:H32	1.96	0.46
1:A:301:PRO:O	1:A:302:VAL:C	2.57	0.46
1:A:458:MET:HE2	2:A:591:MPD:C1	2.45	0.46
1:A:545:GLU:O	1:A:549:LYS:HG2	2.15	0.46
1:A:216:ARG:HD2	1:A:502:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASP:OD1	1:A:566:SER:OG	2.30	0.46
1:A:414:PHE:CE2	1:A:416:ALA:HB2	2.51	0.46
1:A:449:LYS:HE2	4:A:840:HOH:O	2.16	0.46
1:A:399:PHE:O	1:A:399:PHE:CD2	2.69	0.46
1:A:86:ASP:C	1:A:88:ILE:N	2.71	0.46
1:A:257:ILE:HB	1:A:328:LEU:HD12	1.98	0.46
1:A:79:ARG:CB	1:A:118:TRP:CZ2	2.77	0.45
1:A:302:VAL:HG21	1:A:338:GLU:OE2	2.16	0.45
1:A:141:GLU:OE1	1:A:147:HIS:HD2	1.98	0.45
1:A:88:ILE:H	1:A:96:ARG:NH2	2.14	0.45
1:A:97:GLU:O	1:A:303:ALA:HB3	2.16	0.45
1:A:233:PRO:HA	1:A:392:VAL:O	2.17	0.45
1:A:97:GLU:O	1:A:303:ALA:CB	2.65	0.45
1:A:501:ASP:OD2	1:A:556:ILE:HG22	2.17	0.45
1:A:262:GLY:O	1:A:335:ARG:NE	2.48	0.45
1:A:83:SER:OG	1:A:85:TYR:HE2	1.87	0.44
1:A:432:TRP:CH2	2:A:590:MPD:HM3	2.52	0.44
1:A:233:PRO:CD	1:A:414:PHE:HE1	2.01	0.44
1:A:336:TRP:CH2	1:A:364:LEU:HD13	2.52	0.44
1:A:245:HIS:NE2	1:A:249:LYS:HD3	2.27	0.44
1:A:240:LYS:HE3	1:A:240:LYS:HB3	1.79	0.44
1:A:287:LEU:O	1:A:291:THR:OG1	2.25	0.44
1:A:79:ARG:HA	4:A:802:HOH:O	2.17	0.44
1:A:583:PHE:HB3	1:A:588:ALA:O	2.18	0.44
2:A:590:MPD:O4	2:A:590:MPD:CM	2.65	0.44
1:A:66:VAL:CG1	1:A:67:GLY:H	2.31	0.44
1:A:331:ASP:OD1	1:A:331:ASP:O	2.36	0.44
1:A:587:GLY:O	1:A:588:ALA:CB	2.67	0.43
1:A:60:ARG:HG3	1:A:108:THR:HG21	2.00	0.43
1:A:94:VAL:O	1:A:96:ARG:HD2	2.18	0.43
1:A:77:GLY:H	1:A:80:LEU:HD12	1.82	0.43
1:A:420:ASP:OD1	1:A:423:ARG:NH1	2.52	0.43
1:A:261:CYS:HB2	1:A:296:ASN:HB2	2.00	0.43
1:A:366:GLU:HA	1:A:369:GLU:HB2	2.01	0.43
1:A:249:LYS:HZ3	1:A:249:LYS:CB	2.32	0.43
1:A:74:VAL:HG23	1:A:195:VAL:HG12	1.98	0.43
1:A:72:LEU:HD12	1:A:196:ARG:HH12	1.84	0.42
1:A:76:LEU:HA	1:A:80:LEU:HD11	2.01	0.42
1:A:536:GLU:O	1:A:540:ARG:CG	2.66	0.42
1:A:130:VAL:HG11	1:A:159:ILE:HD11	2.01	0.42
1:A:171:GLU:O	1:A:188:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ILE:HD13	1:A:212:ILE:HA	1.89	0.42
1:A:244:GLN:HE22	1:A:391:ALA:HB2	1.84	0.42
1:A:338:GLU:CG	1:A:339:ALA:N	2.82	0.42
1:A:92:LEU:HD23	1:A:92:LEU:O	2.18	0.42
1:A:204:LYS:HD2	1:A:372:GLY:HA3	2.02	0.42
3:A:592:TRS:H31	4:A:856:HOH:O	2.18	0.42
1:A:161:GLU:OE1	1:A:176:LYS:HE3	2.20	0.42
1:A:118:TRP:O	1:A:167:ASP:HA	2.20	0.42
1:A:216:ARG:N	1:A:505:GLN:HE22	2.00	0.42
1:A:548:ALA:O	1:A:553:ARG:NH1	2.51	0.42
1:A:78:PRO:O	1:A:79:ARG:CB	2.67	0.42
1:A:291:THR:CG2	4:A:851:HOH:O	2.68	0.42
1:A:315:ILE:HD13	1:A:315:ILE:HG21	1.86	0.41
1:A:525:ARG:HB3	4:A:841:HOH:O	2.20	0.41
1:A:584:LYS:HB2	1:A:584:LYS:HE2	1.86	0.41
1:A:70:ALA:O	1:A:71:SER:CB	2.68	0.41
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.88	0.41
1:A:304:ALA:O	1:A:305:ARG:C	2.62	0.41
1:A:577:GLU:HG3	4:A:791:HOH:O	2.20	0.41
1:A:426:HIS:HD2	4:A:677:HOH:O	2.02	0.41
1:A:271:VAL:HA	1:A:275:PHE:HD1	1.86	0.41
1:A:447:TRP:CE3	1:A:451:ILE:HG13	2.56	0.41
1:A:546:GLU:CG	1:A:582:LEU:HD11	2.39	0.41
1:A:73:SER:HB2	1:A:193:TRP:O	2.20	0.41
1:A:88:ILE:H	1:A:96:ARG:HH22	1.69	0.41
1:A:261:CYS:CB	1:A:332:SER:CB	2.93	0.41
1:A:114:ARG:NH1	1:A:190:TYR:CZ	2.78	0.41
1:A:108:THR:HG22	1:A:109:ALA:O	2.21	0.40
1:A:69:GLY:CA	1:A:103:ILE:HG13	2.47	0.40
1:A:87:GLY:HA2	1:A:308:SER:CB	2.45	0.40
1:A:486:GLU:HB3	1:A:538:ILE:HD13	2.03	0.40
1:A:249:LYS:CD	2:A:589:MPD:H52	2.49	0.40
1:A:114:ARG:O	1:A:169:THR:HB	2.22	0.40
1:A:193:TRP:CD2	1:A:194:PRO:HD2	2.57	0.40
1:A:394:PRO:HA	1:A:395:PRO:HD3	1.85	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	509/588 (87%)	465 (91%)	35 (7%)	9 (2%)	6 9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	237	GLY
1	A	262	GLY
1	A	233	PRO
1	A	397	GLY
1	A	401	GLU
1	A	586	TYR
1	A	403	VAL
1	A	88	ILE

5.3.2 Protein sidechains [i](#)

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	434/492 (88%)	385 (89%)	49 (11%)	5 8

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	68	THR

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	74	VAL
1	A	83	SER
1	A	88	ILE
1	A	90	ARG
1	A	92	LEU
1	A	94	VAL
1	A	95	ILE
1	A	96	ARG
1	A	97	GLU
1	A	98	LYS
1	A	105	ARG
1	A	129	LYS
1	A	174	ILE
1	A	181	SER
1	A	213	THR
1	A	232	ILE
1	A	242	VAL
1	A	249	LYS
1	A	261	CYS
1	A	288	MET
1	A	290	ARG
1	A	294	ILE
1	A	298	SER
1	A	299	ASN
1	A	305	ARG
1	A	326	VAL
1	A	333	THR
1	A	340	LEU
1	A	363	LYS
1	A	366	GLU
1	A	404	VAL
1	A	406	ASN
1	A	408	LEU
1	A	417	LEU
1	A	421	LEU
1	A	433	LEU
1	A	450	ASN
1	A	451	ILE
1	A	459	ARG
1	A	474	GLU
1	A	484	LEU

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Mol	Chain	Res	Type
1	A	493	LEU
1	A	538	ILE
1	A	539	ASN
1	A	540	ARG
1	A	580	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	147	HIS
1	A	245	HIS
1	A	254	GLN
1	A	266	ASN
1	A	299	ASN
1	A	426	HIS
1	A	448	HIS
1	A	504	GLN
1	A	505	GLN
1	A	529	ASN

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](#)

4 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	MPD	A	590	-	7,7,7	1.30	2 (28%)	9,10,10	0.31	0
3	TRS	A	592	-	7,7,7	0.32	0	9,9,9	0.61	0
2	MPD	A	591	-	7,7,7	1.31	2 (28%)	9,10,10	1.10	1 (11%)
2	MPD	A	589	-	7,7,7	1.31	2 (28%)	9,10,10	0.21	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	MPD	A	590	-	-	3/5/5/5	-
3	TRS	A	592	-	-	2/9/9/9	-
2	MPD	A	591	-	-	3/5/5/5	-
2	MPD	A	589	-	-	0/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	591	MPD	O4-C4	2.47	1.53	1.43
2	A	590	MPD	O4-C4	2.47	1.53	1.43
2	A	589	MPD	O4-C4	2.42	1.53	1.43
2	A	589	MPD	C5-C4	-2.42	1.41	1.51
2	A	590	MPD	C5-C4	-2.34	1.41	1.51
2	A	591	MPD	C5-C4	-2.28	1.41	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	591	MPD	CM-C2-C1	-2.21	105.67	110.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	590	MPD	CM-C2-C3-C4
2	A	591	MPD	C1-C2-C3-C4
3	A	592	TRS	C2-C-C3-O3
3	A	592	TRS	N-C-C3-O3
2	A	590	MPD	O2-C2-C3-C4
2	A	591	MPD	O2-C2-C3-C4
2	A	590	MPD	C1-C2-C3-C4
2	A	591	MPD	CM-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	590	MPD	3	0
3	A	592	TRS	1	0
2	A	591	MPD	7	0
2	A	589	MPD	18	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	513/588 (87%)	1.01	101 (19%) 3 2	26, 52, 104, 123	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ARG	9.7
1	A	99	THR	8.9
1	A	340	LEU	7.3
1	A	100	GLY	7.1
1	A	107	VAL	6.8
1	A	395	PRO	6.8
1	A	60	ARG	6.8
1	A	98	LYS	6.5
1	A	336	TRP	6.4
1	A	70	ALA	6.4
1	A	337	ALA	6.3
1	A	396	GLY	5.9
1	A	85	TYR	5.7
1	A	452	ASP	5.7
1	A	95	ILE	5.7
1	A	66	VAL	5.6
1	A	103	ILE	5.5
1	A	94	VAL	5.5
1	A	408	LEU	5.3
1	A	584	LYS	5.2
1	A	502	TYR	5.1
1	A	64	PRO	5.0
1	A	208	GLU	4.9
1	A	588	ALA	4.9
1	A	62	GLY	4.9
1	A	451	ILE	4.9
1	A	65	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	104	ALA	4.8
1	A	108	THR	4.7
1	A	275	PHE	4.5
1	A	106	GLY	4.3
1	A	63	GLU	4.3
1	A	299	ASN	4.2
1	A	260	GLY	4.2
1	A	102	PHE	4.2
1	A	399	PHE	4.1
1	A	360	LEU	4.1
1	A	97	GLU	4.1
1	A	271	VAL	4.1
1	A	238	ALA	4.0
1	A	587	GLY	4.0
1	A	268	MET	4.0
1	A	80	LEU	4.0
1	A	339	ALA	3.8
1	A	359	TYR	3.8
1	A	92	LEU	3.8
1	A	405	GLN	3.7
1	A	88	ILE	3.7
1	A	252	ASP	3.7
1	A	404	VAL	3.6
1	A	392	VAL	3.6
1	A	68	THR	3.6
1	A	450	ASN	3.6
1	A	261	CYS	3.5
1	A	61	PRO	3.5
1	A	67	GLY	3.5
1	A	101	ASP	3.4
1	A	357	PRO	3.4
1	A	297	THR	3.3
1	A	407	THR	3.3
1	A	84	ILE	3.3
1	A	105	ARG	3.1
1	A	209	VAL	3.1
1	A	236	PHE	3.0
1	A	111	ALA	2.9
1	A	401	GLU	2.9
1	A	403	VAL	2.9
1	A	237	GLY	2.9
1	A	87	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	2.7
1	A	400	SER	2.6
1	A	303	ALA	2.6
1	A	333	THR	2.6
1	A	295	ALA	2.5
1	A	332	SER	2.5
1	A	272	LEU	2.5
1	A	397	GLY	2.5
1	A	168	TYR	2.5
1	A	296	ASN	2.4
1	A	394	PRO	2.4
1	A	581	GLU	2.4
1	A	262	GLY	2.4
1	A	393	SER	2.3
1	A	302	VAL	2.3
1	A	89	GLN	2.3
1	A	270	ASP	2.3
1	A	586	TYR	2.3
1	A	307	ALA	2.2
1	A	278	LEU	2.2
1	A	110	PRO	2.2
1	A	305	ARG	2.1
1	A	79	ARG	2.1
1	A	273	GLU	2.1
1	A	71	SER	2.1
1	A	116	LYS	2.1
1	A	585	LYS	2.1
1	A	501	ASP	2.1
1	A	109	ALA	2.0
1	A	113	PRO	2.0
1	A	402	PRO	2.0
1	A	112	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	MPD	A	591	8/8	0.75	0.22	74,76,77,78	0
2	MPD	A	589	8/8	0.78	0.27	61,63,64,67	0
2	MPD	A	590	8/8	0.83	0.28	76,79,80,80	0
3	TRS	A	592	8/8	0.84	0.21	93,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.