



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:29 AM UTC

PDB ID : 7X20 / pdb_00007x20
Title : Crystal structure of non gastric H,K-ATPase alpha2 in (K⁺)E2-AlF state
Authors : Nakanishi, H.; Abe, K.
Deposited on : 2022-02-25
Resolution : 3.30 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

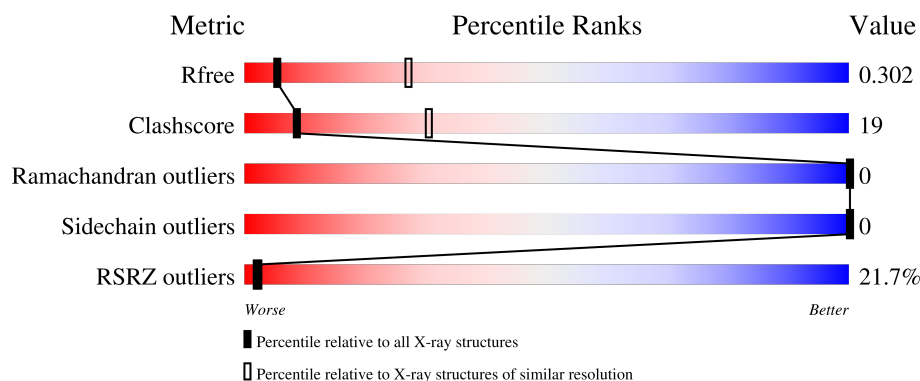
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	986	22% 63% 37%
2	B	324	19% 57% 32% 11%

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
3	ALF	A	1101	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10041 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 Potassium-transporting ATPase alpha chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	986	Total	C	N	O	S	0	0	0
			7666	4914	1281	1434	37			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP P54708
A	52	MET	-	expression tag	UNP P54708
A	315	GLY	ASP	conflict	UNP P54708

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	288	Total	C	N	O	S	0	0	0
			2353	1524	385	432	12			

There are 20 discrepancies between the modelled and reference sequences:

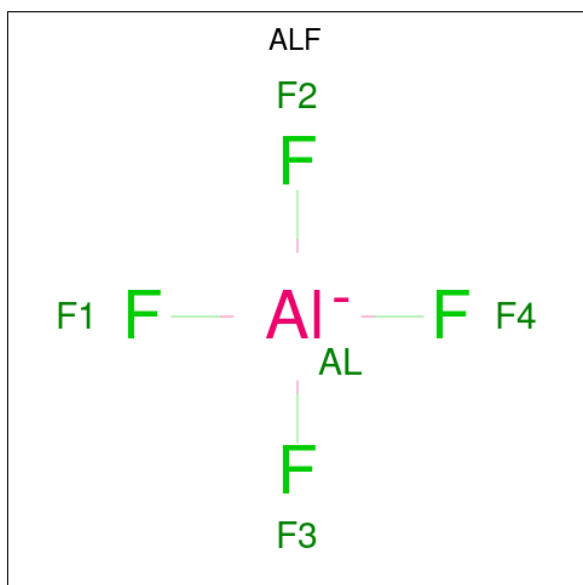
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P07340
B	-18	GLY	-	expression tag	UNP P07340
B	-17	ASP	-	expression tag	UNP P07340
B	-16	TYR	-	expression tag	UNP P07340
B	-15	LYS	-	expression tag	UNP P07340
B	-14	ASP	-	expression tag	UNP P07340
B	-13	ASP	-	expression tag	UNP P07340
B	-12	ASP	-	expression tag	UNP P07340
B	-11	ASP	-	expression tag	UNP P07340
B	-10	LYS	-	expression tag	UNP P07340
B	-9	SER	-	expression tag	UNP P07340
B	-8	SER	-	expression tag	UNP P07340
B	-7	GLY	-	expression tag	UNP P07340

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLU	-	expression tag	UNP P07340
B	-5	ASN	-	expression tag	UNP P07340
B	-4	LEU	-	expression tag	UNP P07340
B	-3	TYR	-	expression tag	UNP P07340
B	-2	PHE	-	expression tag	UNP P07340
B	-1	GLN	-	expression tag	UNP P07340
B	0	GLY	-	expression tag	UNP P07340

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

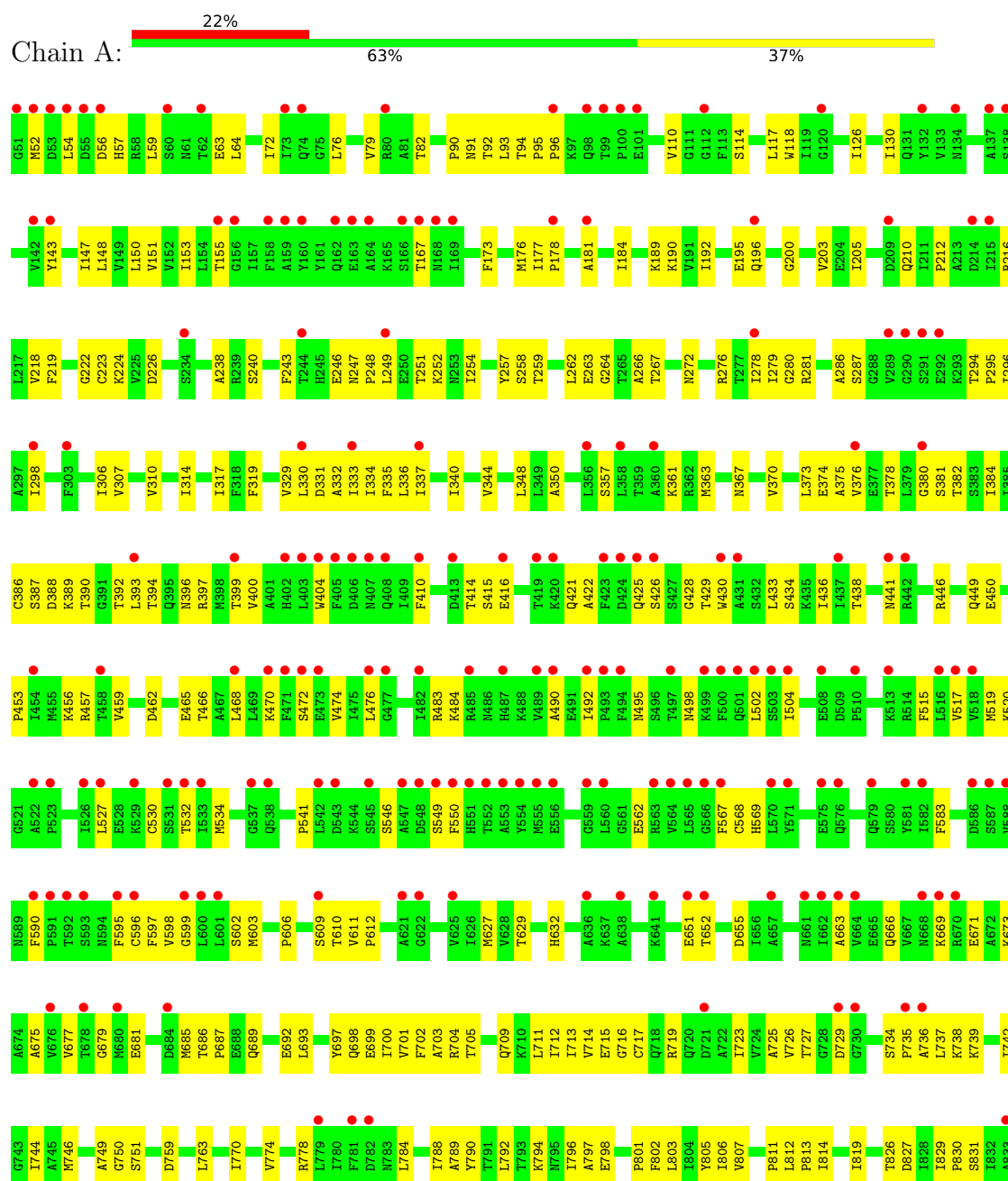
- Molecule 6 is water.

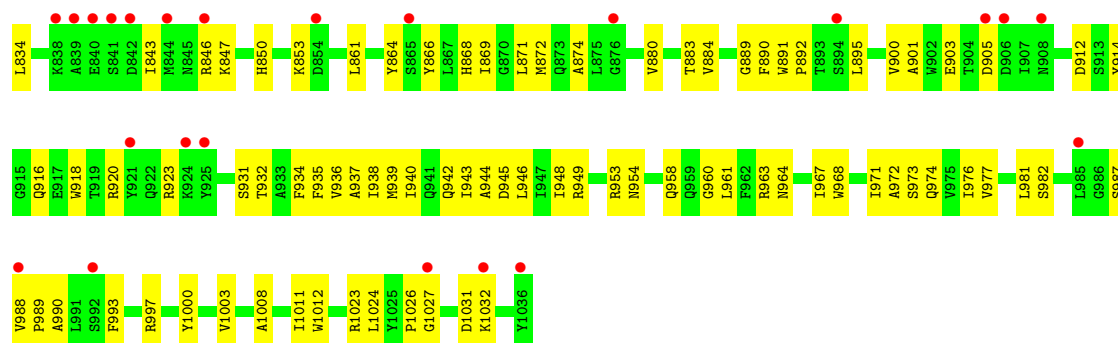
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

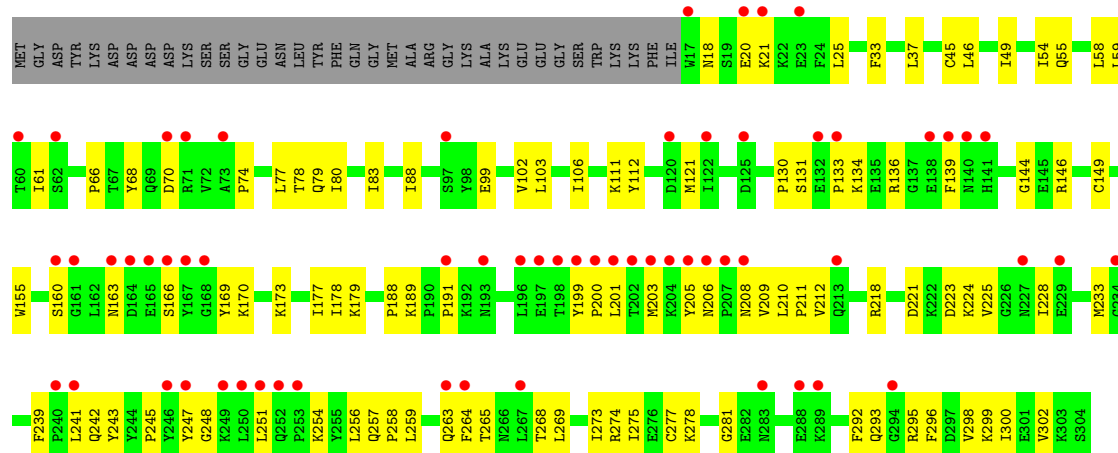
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Potassium-transporting ATPase alpha chain 2





• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.97Å 109.06Å 267.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 3.30 48.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	72.6 (48.06-3.30) 72.6 (48.06-3.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.265 , 0.316 (Not available) , 0.302	Depositor DCC
R_{free} test set	1276 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 16.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	10041	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, K, ALF

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	0.52	0/7809	0.80	0/10598
2	B	0.54	0/2414	0.82	1/3253 (0.0%)
All	All	0.53	0/10223	0.81	1/13851 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	248	GLY	CA-C-O	-5.13	118.13	122.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7666	0	7811	300	1
2	B	2353	0	2335	85	0
3	A	5	0	0	2	0
4	A	2	0	0	0	0
5	B	14	0	13	0	0
6	A	1	0	0	1	0
All	All	10041	0	10159	379	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (379) 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:59:LEU:HD13	1:A:64:LEU:HB3	1.44	0.97
1:A:226:ASP:HB2	1:A:262:LEU:HD21	1.49	0.94
1:A:686:THR:HG22	1:A:689:GLN:HG2	1.59	0.83
1:A:814:ILE:HG23	1:A:934:PHE:HB3	1.61	0.83
1:A:59:LEU:CD1	1:A:64:LEU:HB3	2.08	0.82
1:A:987:SER:HB2	1:A:993:PHE:HB3	1.59	0.82
1:A:490:ALA:HB3	1:A:504:ILE:HB	1.63	0.81
1:A:872:MET:HG2	2:B:46:LEU:HD11	1.64	0.80
2:B:173:LYS:HB3	2:B:265:THR:HA	1.62	0.80
1:A:943:ILE:HD12	1:A:971:ILE:HG23	1.63	0.78
2:B:88:ILE:HB	2:B:300:ILE:HG22	1.65	0.76
1:A:72:ILE:HD11	1:A:218:VAL:HG21	1.66	0.76
1:A:502:LEU:HD12	1:A:519:MET:HB2	1.68	0.76
1:A:729:ASP:O	1:A:751:SER:N	2.15	0.75
1:A:91:ASN:HB3	1:A:195:GLU:HA	1.68	0.74
1:A:981:LEU:O	1:A:987:SER:HB3	1.87	0.73
1:A:178:PRO:HB3	1:A:210:GLN:HB2	1.71	0.73
1:A:715:GLU:HG2	1:A:739:LYS:HE2	1.69	0.73
2:B:218:ARG:HB2	2:B:221:ASP:HB3	1.71	0.73
1:A:79:VAL:O	1:A:82:THR:OG1	2.05	0.73
2:B:191:PRO:HD3	2:B:281:GLY:HA2	1.72	0.72
1:A:905:ASP:HB3	1:A:920:ARG:HH11	1.56	0.71
1:A:205:ILE:HG22	1:A:266:ALA:O	1.92	0.70
1:A:450:GLU:N	1:A:450:GLU:OE1	2.25	0.69
1:A:663:ALA:HB3	1:A:666:GLN:HG2	1.75	0.69
1:A:689:GLN:HA	1:A:692:GLU:HB3	1.74	0.68
1:A:436:ILE:HD13	1:A:567:PHE:HB3	1.74	0.68
1:A:247:ASN:OD1	1:A:249:LEU:HB2	1.94	0.67
1:A:278:ILE:HD12	1:A:279:ILE:N	2.09	0.67
1:A:56:ASP:HB2	1:A:59:LEU:HD21	1.77	0.67
1:A:803:LEU:O	1:A:807:VAL:HG22	1.94	0.67
1:A:892:PRO:HG3	2:B:58:LEU:HD11	1.77	0.67
1:A:367:ASN:HA	1:A:763:LEU:HD12	1.78	0.66
1:A:388:ASP:OD2	3:A:1101:ALF:F1	2.04	0.66
1:A:834:LEU:HD11	1:A:949:ARG:HB3	1.78	0.65
1:A:380:GLY:HA2	1:A:774:VAL:HG13	1.79	0.65
1:A:686:THR:HG22	1:A:689:GLN:CG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HG21	1:A:330:LEU:HD13	1.79	0.65
1:A:504:ILE:HG13	1:A:517:VAL:HG23	1.78	0.65
2:B:77:LEU:HB3	2:B:296:PHE:HE1	1.62	0.65
1:A:982:SER:O	1:A:987:SER:OG	2.09	0.64
1:A:727:THR:HA	1:A:744:ILE:O	1.97	0.64
1:A:382:THR:HA	1:A:723:ILE:HB	1.78	0.64
1:A:54:LEU:HD12	1:A:54:LEU:O	1.97	0.64
1:A:295:PRO:HA	1:A:298:ILE:HG12	1.80	0.64
1:A:415:SER:OG	1:A:609:SER:OG	2.13	0.64
1:A:920:ARG:HD2	1:A:923:ARG:HH21	1.63	0.63
1:A:492:ILE:HD12	1:A:502:LEU:HB3	1.79	0.63
1:A:778:ARG:HB3	1:A:843:ILE:HG21	1.80	0.63
1:A:258:SER:OG	1:A:279:ILE:HD13	1.99	0.63
1:A:964:ASN:ND2	1:A:967:ILE:HG23	2.13	0.63
1:A:562:GLU:HB3	1:A:602:SER:HB2	1.80	0.63
1:A:1008:ALA:HA	1:A:1011:ILE:HG22	1.81	0.63
1:A:390:THR:HA	1:A:394:THR:HB	1.81	0.62
2:B:80:ILE:HB	2:B:177:ILE:HB	1.81	0.62
1:A:370:VAL:HG13	1:A:375:ALA:HB3	1.82	0.62
1:A:687:PRO:HB3	1:A:719:ARG:HH12	1.64	0.62
1:A:997:ARG:HH21	2:B:68:TYR:HD2	1.48	0.62
1:A:294:THR:O	1:A:298:ILE:HG23	2.00	0.61
1:A:827:ASP:O	1:A:831:SER:HB3	2.00	0.61
1:A:744:ILE:HD13	1:A:770:ILE:HD12	1.82	0.61
1:A:357:SER:HB3	1:A:373:LEU:HD21	1.81	0.61
1:A:224:LYS:HA	1:A:238:ALA:HA	1.81	0.61
1:A:363:MET:HE2	1:A:376:VAL:HG12	1.81	0.61
1:A:671:GLU:OE1	1:A:671:GLU:N	2.32	0.61
2:B:239:PHE:HD1	2:B:258:PRO:HB2	1.65	0.61
2:B:144:GLY:O	2:B:146:ARG:NH1	2.33	0.60
1:A:400:VAL:HG12	1:A:603:MET:HG2	1.83	0.60
1:A:797:ALA:HA	1:A:874:ALA:HB2	1.82	0.60
2:B:160:SER:HA	2:B:166:SER:OG	2.01	0.60
1:A:143:TYR:O	1:A:147:ILE:HG13	2.02	0.60
1:A:627:MET:HB3	1:A:701:VAL:HG12	1.84	0.60
1:A:711:LEU:HA	1:A:714:VAL:HG12	1.84	0.60
1:A:742:ILE:HG13	1:A:759:ASP:HB2	1.84	0.60
2:B:112:TYR:CZ	2:B:259:LEU:HD11	2.37	0.60
1:A:155:THR:HG22	1:A:350:ALA:HB2	1.84	0.59
1:A:889:GLY:HA2	1:A:914:TYR:CE2	2.36	0.59
1:A:932:THR:O	1:A:936:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:HIS:HB3	1:A:853:LYS:HB2	1.83	0.59
2:B:33:PHE:CZ	2:B:37:LEU:HD12	2.37	0.59
1:A:296:ILE:HG21	1:A:374:GLU:HB3	1.84	0.58
1:A:1027:GLY:H	1:A:1031:ASP:CB	2.16	0.58
1:A:453:PRO:O	1:A:457:ARG:HG3	2.03	0.58
1:A:770:ILE:O	1:A:774:VAL:HG23	2.03	0.58
2:B:224:LYS:HB3	2:B:268:THR:OG1	2.04	0.58
1:A:798:GLU:HB3	1:A:819:ILE:HD12	1.85	0.58
1:A:397:ARG:O	1:A:399:THR:HG23	2.03	0.57
1:A:960:GLY:HA3	1:A:963:ARG:HG2	1.85	0.57
1:A:726:VAL:HG23	1:A:737:LEU:HD23	1.85	0.57
1:A:203:VAL:HG11	1:A:212:PRO:HG2	1.85	0.57
1:A:880:VAL:O	1:A:884:VAL:HG12	2.03	0.57
1:A:59:LEU:HD13	1:A:64:LEU:CB	2.27	0.57
1:A:517:VAL:HG13	1:A:595:PHE:HE2	1.70	0.57
1:A:734:SER:OG	1:A:735:PRO:HD3	2.05	0.57
1:A:441:ASN:HB2	1:A:483:ARG:NH2	2.20	0.56
1:A:632:HIS:CD2	1:A:704:ARG:HD2	2.40	0.56
1:A:774:VAL:HG12	1:A:778:ARG:HD2	1.87	0.56
2:B:77:LEU:HB3	2:B:296:PHE:CE1	2.40	0.56
1:A:679:GLY:N	1:A:703:ALA:O	2.36	0.56
1:A:96:PRO:HB3	1:A:287:SER:HB2	1.88	0.56
1:A:669:LYS:HB3	1:A:697:TYR:OH	2.06	0.56
2:B:55:GLN:O	2:B:59:LEU:HG	2.04	0.56
1:A:796:ILE:HG21	1:A:871:LEU:HD12	1.86	0.56
1:A:891:TRP:HB3	1:A:892:PRO:HD2	1.87	0.55
1:A:410:PHE:HE2	1:A:425:GLN:HG3	1.70	0.55
2:B:79:GLN:HE22	2:B:292:PHE:HE2	1.54	0.55
1:A:441:ASN:HD21	1:A:468:LEU:HB2	1.71	0.55
1:A:532:THR:O	1:A:596:CYS:HA	2.06	0.55
1:A:725:ALA:HA	1:A:742:ILE:O	2.07	0.55
1:A:334:ILE:HD12	1:A:337:ILE:HD12	1.88	0.55
1:A:416:GLU:HG2	1:A:456:LYS:HE3	1.89	0.55
1:A:433:LEU:HD12	1:A:599:GLY:HA3	1.88	0.55
1:A:629:THR:O	1:A:705:THR:HG22	2.07	0.55
2:B:160:SER:HB2	2:B:169:TYR:HE1	1.72	0.54
1:A:415:SER:OG	1:A:416:GLU:N	2.40	0.54
1:A:889:GLY:HA2	1:A:914:TYR:HE2	1.73	0.54
1:A:331:ASP:O	1:A:334:ILE:HG22	2.07	0.54
2:B:33:PHE:CE1	2:B:37:LEU:HD12	2.43	0.54
2:B:179:LYS:HD2	2:B:257:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG21	1:A:866:TYR:HE2	1.73	0.53
1:A:726:VAL:HG21	1:A:736:ALA:O	2.08	0.53
1:A:248:PRO:O	1:A:254:ILE:HD11	2.08	0.53
1:A:306:ILE:HG13	1:A:307:VAL:N	2.23	0.53
1:A:651:GLU:HB3	1:A:655:ASP:HB2	1.90	0.53
2:B:254:LYS:O	2:B:256:LEU:HD22	2.09	0.53
2:B:274:ARG:HG2	2:B:299:LYS:HG2	1.89	0.53
1:A:381:SER:O	1:A:723:ILE:HD13	2.08	0.53
1:A:801:PRO:HB3	1:A:813:PRO:HB2	1.91	0.53
1:A:1027:GLY:H	1:A:1031:ASP:HB3	1.72	0.53
1:A:184:ILE:HG12	1:A:189:LYS:HD3	1.91	0.53
1:A:386:CYS:HB2	1:A:726:VAL:HG12	1.90	0.53
1:A:961:LEU:HD12	1:A:968:TRP:HZ2	1.74	0.53
1:A:446:ARG:O	1:A:449:GLN:HG3	2.10	0.52
1:A:964:ASN:HB3	1:A:967:ILE:HG12	1.91	0.52
1:A:332:ALA:HA	1:A:335:PHE:HD2	1.74	0.52
1:A:709:GLN:HA	1:A:712:ILE:HB	1.92	0.52
1:A:990:ALA:O	1:A:993:PHE:HB2	2.10	0.52
1:A:465:GLU:HG3	1:A:520:LYS:NZ	2.25	0.52
1:A:517:VAL:HG13	1:A:595:PHE:CE2	2.45	0.52
1:A:546:SER:HA	1:A:549:SER:HB2	1.92	0.51
2:B:112:TYR:CZ	2:B:256:LEU:HD12	2.45	0.51
1:A:685:MET:HG3	1:A:689:GLN:HG3	1.92	0.51
1:A:59:LEU:CD1	1:A:64:LEU:HD23	2.40	0.51
1:A:389:LYS:O	1:A:393:LEU:N	2.42	0.51
1:A:723:ILE:H	1:A:723:ILE:HD12	1.76	0.51
2:B:298:VAL:HG12	2:B:300:ILE:HG23	1.92	0.51
1:A:794:LYS:HE3	6:A:1201:HOH:O	2.11	0.51
2:B:205:TYR:HE2	2:B:208:ASN:HB2	1.76	0.51
1:A:310:VAL:O	1:A:314:ILE:HG12	2.11	0.51
1:A:954:ASN:ND2	1:A:958:GLN:HG3	2.26	0.51
1:A:697:TYR:O	1:A:700:ILE:HD11	2.10	0.51
1:A:988:VAL:HB	1:A:989:PRO:CD	2.41	0.51
1:A:880:VAL:O	1:A:883:THR:HG22	2.11	0.50
2:B:74:PRO:HB2	2:B:293:GLN:HG3	1.93	0.50
1:A:222:GLY:O	1:A:264:GLY:HA3	2.11	0.50
2:B:218:ARG:O	2:B:221:ASP:HB3	2.12	0.50
1:A:380:GLY:O	1:A:381:SER:OG	2.29	0.50
1:A:729:ASP:HB2	1:A:750:GLY:HA2	1.93	0.50
1:A:677:VAL:HG13	1:A:681:GLU:HG3	1.94	0.50
1:A:686:THR:CG2	1:A:689:GLN:HG2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:HIS:O	1:A:596:CYS:HB3	2.11	0.50
1:A:944:ALA:O	1:A:948:ILE:HG23	2.11	0.50
2:B:209:VAL:O	2:B:211:PRO:HD3	2.11	0.50
1:A:57:HIS:CE1	1:A:246:GLU:O	2.65	0.50
1:A:380:GLY:C	1:A:382:THR:H	2.20	0.50
1:A:421:GLN:HG2	1:A:422:ALA:N	2.27	0.50
1:A:652:THR:HG23	1:A:655:ASP:H	1.77	0.50
1:A:389:LYS:HG3	1:A:390:THR:N	2.27	0.49
1:A:843:ILE:HG23	1:A:846:ARG:HH21	1.77	0.49
2:B:223:ASP:C	2:B:225:VAL:H	2.21	0.49
1:A:117:LEU:CD1	1:A:344:VAL:HG11	2.42	0.49
1:A:240:SER:N	1:A:252:LYS:O	2.46	0.49
1:A:778:ARG:HE	1:A:843:ILE:HG22	1.77	0.49
2:B:37:LEU:HD23	2:B:37:LEU:O	2.13	0.49
1:A:173:PHE:O	1:A:177:ILE:HG12	2.13	0.49
1:A:262:LEU:N	1:A:262:LEU:HD22	2.28	0.49
1:A:392:THR:HA	1:A:746:MET:HE3	1.93	0.49
1:A:438:THR:O	1:A:483:ARG:NE	2.46	0.49
2:B:277:CYS:H	2:B:296:PHE:HB2	1.77	0.49
1:A:890:PHE:HE2	1:A:918:TRP:CE2	2.31	0.49
2:B:78:THR:HG23	2:B:179:LYS:HE2	1.93	0.49
2:B:160:SER:HB2	2:B:169:TYR:CE1	2.48	0.49
1:A:223:CYS:HA	1:A:263:GLU:O	2.12	0.48
1:A:459:VAL:HG21	1:A:470:LYS:HE3	1.94	0.48
1:A:716:GLY:O	1:A:719:ARG:HG2	2.14	0.48
1:A:802:PHE:O	1:A:806:ILE:HG22	2.13	0.48
1:A:569:HIS:ND1	1:A:598:VAL:HG22	2.28	0.48
2:B:83:ILE:HG21	2:B:88:ILE:HG12	1.95	0.48
2:B:131:SER:HB3	2:B:242:GLN:HB3	1.94	0.48
1:A:388:ASP:O	1:A:392:THR:OG1	2.28	0.48
1:A:390:THR:O	3:A:1101:ALF:F1	2.21	0.48
1:A:226:ASP:O	1:A:259:THR:HB	2.14	0.48
1:A:248:PRO:HA	1:A:251:THR:OG1	2.13	0.48
1:A:789:ALA:HB1	1:A:949:ARG:HH21	1.79	0.48
1:A:126:ILE:O	1:A:130:ILE:HG12	2.13	0.48
1:A:900:VAL:HG13	1:A:901:ALA:H	1.79	0.48
2:B:45:CYS:O	2:B:49:ILE:HG13	2.13	0.47
1:A:410:PHE:CE2	1:A:425:GLN:HG3	2.49	0.47
1:A:789:ALA:HB2	1:A:861:LEU:HD21	1.97	0.47
1:A:939:MET:HA	1:A:942:GLN:HB2	1.97	0.47
1:A:997:ARG:HH22	2:B:70:ASP:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:TRP:HA	1:A:433:LEU:HB3	1.97	0.47
1:A:429:THR:HA	1:A:534:MET:HE3	1.96	0.47
1:A:438:THR:HG22	1:A:472:SER:HB2	1.95	0.47
1:A:52:MET:HG2	1:A:272:ASN:HD21	1.80	0.47
1:A:1027:GLY:O	1:A:1032:LYS:HE3	2.15	0.47
2:B:264:PHE:CZ	2:B:275:ILE:HD12	2.50	0.47
1:A:257:TYR:HB3	1:A:279:ILE:HG12	1.96	0.47
1:A:811:PRO:HD2	1:A:895:LEU:HD22	1.97	0.47
1:A:276:ARG:O	1:A:281:ARG:NH2	2.47	0.47
1:A:426:SER:C	1:A:428:GLY:H	2.23	0.47
2:B:99:GLU:O	2:B:103:LEU:HD23	2.14	0.47
2:B:112:TYR:CE1	2:B:256:LEU:HD12	2.50	0.47
1:A:465:GLU:HG3	1:A:520:LYS:HZ1	1.79	0.47
1:A:880:VAL:HG21	1:A:937:ALA:HB2	1.96	0.47
1:A:387:SER:OG	1:A:393:LEU:HD13	2.14	0.46
1:A:610:THR:C	1:A:612:PRO:HD2	2.40	0.46
2:B:112:TYR:CE1	2:B:259:LEU:HD11	2.50	0.46
2:B:201:LEU:O	2:B:203:MET:HG2	2.15	0.46
1:A:76:LEU:HD22	1:A:200:GLY:O	2.15	0.46
1:A:286:ALA:O	1:A:738:LYS:HG3	2.15	0.46
1:A:936:VAL:O	1:A:940:ILE:HG12	2.15	0.46
1:A:788:ILE:O	1:A:792:LEU:HG	2.15	0.46
1:A:829:ILE:HD13	1:A:973:SER:HB2	1.97	0.46
2:B:233:MET:HE1	2:B:242:GLN:NE2	2.30	0.46
1:A:110:VAL:HG12	1:A:110:VAL:O	2.16	0.46
1:A:834:LEU:HA	1:A:834:LEU:HD23	1.65	0.46
1:A:987:SER:CB	1:A:993:PHE:HB3	2.39	0.46
1:A:310:VAL:HG21	1:A:866:TYR:CE2	2.51	0.46
1:A:778:ARG:CB	1:A:843:ILE:HG21	2.44	0.46
2:B:54:ILE:HD12	2:B:54:ILE:HG23	1.67	0.46
1:A:348:LEU:HD21	1:A:788:ILE:HG12	1.98	0.46
1:A:296:ILE:CG2	1:A:374:GLU:HB3	2.45	0.46
2:B:178:ILE:HG21	2:B:212:VAL:HG11	1.97	0.46
1:A:118:TRP:CE3	1:A:118:TRP:HA	2.51	0.45
1:A:192:ILE:HD12	1:A:196:GLN:HB3	1.98	0.45
1:A:370:VAL:CG1	1:A:375:ALA:HB3	2.46	0.45
1:A:796:ILE:HD13	1:A:796:ILE:HA	1.74	0.45
1:A:1008:ALA:HA	1:A:1011:ILE:CG2	2.44	0.45
2:B:179:LYS:HD2	2:B:257:GLN:HE22	1.81	0.45
1:A:330:LEU:O	1:A:333:ILE:HG13	2.16	0.45
1:A:972:ALA:O	1:A:976:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LEU:O	2:B:61:ILE:HG13	2.16	0.45
1:A:370:VAL:HG11	1:A:376:VAL:HG13	1.97	0.45
1:A:492:ILE:CD1	1:A:502:LEU:HB3	2.46	0.45
1:A:912:ASP:OD1	1:A:916:GLN:HB2	2.16	0.45
1:A:973:SER:HA	1:A:976:ILE:HD11	1.97	0.45
2:B:239:PHE:CD1	2:B:258:PRO:HB2	2.48	0.45
1:A:826:THR:HA	1:A:977:VAL:HG11	1.98	0.45
1:A:434:SER:HB2	1:A:476:LEU:HD11	1.98	0.45
2:B:189:LYS:HA	2:B:189:LYS:HD2	1.69	0.45
2:B:218:ARG:HB2	2:B:221:ASP:CB	2.43	0.45
1:A:90:PRO:HB2	1:A:92:THR:HG22	1.99	0.45
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.72	0.45
1:A:150:LEU:O	1:A:153:ILE:HG22	2.16	0.45
1:A:317:ILE:HD13	1:A:317:ILE:HA	1.72	0.45
2:B:18:ASN:C	2:B:20:GLU:H	2.25	0.45
2:B:134:LYS:O	2:B:245:PRO:HD3	2.17	0.45
1:A:686:THR:HG22	1:A:689:GLN:CD	2.42	0.45
1:A:147:ILE:O	1:A:151:VAL:HG13	2.17	0.44
1:A:681:GLU:O	1:A:685:MET:HE3	2.17	0.44
1:A:864:TYR:O	1:A:868:HIS:HB2	2.18	0.44
1:A:942:GLN:HB3	1:A:974:GLN:HE22	1.82	0.44
1:A:114:SER:O	1:A:118:TRP:CD1	2.70	0.44
1:A:404:TRP:CH2	1:A:550:PHE:HA	2.52	0.44
1:A:462:ASP:O	1:A:466:THR:HG23	2.16	0.44
1:A:568:CYS:HA	1:A:598:VAL:HG23	1.98	0.44
1:A:190:LYS:HD3	1:A:190:LYS:HA	1.76	0.44
1:A:813:PRO:O	1:A:931:SER:HA	2.17	0.44
1:A:1024:LEU:O	1:A:1026:PRO:HD3	2.18	0.44
2:B:133:PRO:HG3	2:B:241:LEU:HB3	1.99	0.44
2:B:136:ARG:NH2	2:B:149:CYS:SG	2.91	0.44
1:A:953:ARG:HH12	1:A:1023:ARG:HA	1.80	0.44
1:A:76:LEU:HA	1:A:76:LEU:HD12	1.60	0.44
1:A:117:LEU:HD11	1:A:344:VAL:HG11	2.00	0.44
1:A:181:ALA:HB2	1:A:212:PRO:HB3	2.00	0.44
1:A:184:ILE:HD11	1:A:189:LYS:HE2	1.99	0.44
1:A:530:CYS:SG	1:A:597:PHE:N	2.91	0.44
2:B:170:LYS:HE2	2:B:263:GLN:HG3	1.99	0.44
1:A:57:HIS:ND1	1:A:243:PHE:HE1	2.16	0.44
1:A:1011:ILE:HG23	1:A:1012:TRP:H	1.83	0.44
2:B:201:LEU:C	2:B:203:MET:HG2	2.43	0.44
1:A:414:THR:HB	1:A:606:PRO:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ALA:HB3	1:A:700:ILE:HG23	1.99	0.44
2:B:102:VAL:O	2:B:106:ILE:HG13	2.18	0.43
1:A:386:CYS:O	1:A:726:VAL:HA	2.17	0.43
1:A:802:PHE:CD1	1:A:812:LEU:HD11	2.52	0.43
1:A:1011:ILE:HG23	1:A:1012:TRP:N	2.33	0.43
1:A:997:ARG:HE	2:B:68:TYR:HE2	1.61	0.43
1:A:219:PHE:HB2	1:A:267:THR:HB	2.00	0.43
2:B:170:LYS:NZ	2:B:263:GLN:HB2	2.33	0.43
1:A:319:PHE:HD2	1:A:336:LEU:HD13	1.82	0.43
1:A:935:PHE:O	1:A:938:ILE:HG13	2.18	0.43
2:B:221:ASP:C	2:B:223:ASP:H	2.26	0.43
2:B:269:LEU:HD12	2:B:302:VAL:HB	2.01	0.43
1:A:702:PHE:CD2	1:A:713:ILE:HD12	2.54	0.43
1:A:530:CYS:SG	1:A:597:PHE:HB2	2.59	0.43
2:B:130:PRO:HB2	2:B:205:TYR:CE2	2.53	0.43
2:B:170:LYS:HE2	2:B:263:GLN:CG	2.49	0.43
1:A:94:THR:HA	1:A:95:PRO:HD3	1.88	0.43
1:A:673:LYS:HE3	1:A:698:GLN:NE2	2.34	0.43
1:A:702:PHE:CE1	1:A:713:ILE:HD11	2.53	0.43
1:A:216:ARG:HA	1:A:254:ILE:HG22	2.01	0.43
1:A:361:LYS:HD3	1:A:361:LYS:HA	1.75	0.43
1:A:429:THR:HG23	1:A:534:MET:HE3	2.01	0.42
1:A:905:ASP:HB3	1:A:920:ARG:NH1	2.29	0.42
1:A:192:ILE:HD12	1:A:196:GLN:OE1	2.19	0.42
1:A:433:LEU:HA	1:A:436:ILE:HG22	2.01	0.42
1:A:698:GLN:HG2	1:A:699:GLU:HG3	1.99	0.42
1:A:830:PRO:HB3	1:A:946:LEU:HD22	2.02	0.42
2:B:54:ILE:HD13	2:B:54:ILE:HA	1.87	0.42
2:B:155:TRP:CH2	2:B:233:MET:HE2	2.54	0.42
2:B:223:ASP:C	2:B:225:VAL:N	2.77	0.42
1:A:332:ALA:O	1:A:335:PHE:HB2	2.19	0.42
1:A:340:ILE:HD13	1:A:340:ILE:HG21	1.74	0.42
2:B:111:LYS:HG2	2:B:256:LEU:HD11	2.01	0.42
1:A:459:VAL:HG11	1:A:466:THR:HG22	2.01	0.42
1:A:52:MET:HB2	1:A:54:LEU:HG	2.02	0.42
1:A:389:LYS:NZ	1:A:390:THR:HG23	2.34	0.42
1:A:400:VAL:HG12	1:A:603:MET:CG	2.49	0.42
1:A:295:PRO:CG	1:A:378:THR:HG23	2.49	0.42
1:A:449:GLN:N	1:A:450:GLU:OE1	2.52	0.42
2:B:243:TYR:CD1	2:B:258:PRO:HG3	2.55	0.42
1:A:176:MET:HE3	1:A:176:MET:HB2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:TYR:CE1	1:A:942:GLN:NE2	2.88	0.42
1:A:93:LEU:HD23	1:A:280:GLY:HA2	2.01	0.42
2:B:163:ASN:N	2:B:166:SER:HB2	2.34	0.42
2:B:273:ILE:O	2:B:299:LYS:HA	2.20	0.42
1:A:329:VAL:O	1:A:333:ILE:HG23	2.20	0.42
1:A:453:PRO:HG2	1:A:456:LYS:HD2	2.02	0.42
2:B:121:MET:HE2	2:B:121:MET:HB3	1.89	0.42
1:A:257:TYR:CG	1:A:279:ILE:HD11	2.55	0.41
1:A:393:LEU:HG	1:A:611:VAL:HG21	2.01	0.41
2:B:80:ILE:HD13	2:B:80:ILE:HA	1.84	0.41
2:B:228:ILE:HG22	2:B:264:PHE:HD1	1.85	0.41
1:A:515:PHE:HD1	1:A:515:PHE:HA	1.74	0.41
1:A:814:ILE:CG2	1:A:934:PHE:HB3	2.41	0.41
2:B:163:ASN:O	2:B:166:SER:HB2	2.19	0.41
1:A:495:ASN:HB3	1:A:498:ASN:HB2	2.01	0.41
1:A:693:LEU:HD12	1:A:700:ILE:HD13	2.02	0.41
1:A:869:ILE:HG13	1:A:949:ARG:HH12	1.85	0.41
1:A:389:LYS:HG3	1:A:390:THR:HG23	2.02	0.41
1:A:847:LYS:HD2	1:A:847:LYS:N	2.36	0.41
1:A:916:GLN:OE1	2:B:66:PRO:HG3	2.21	0.41
2:B:139:PHE:HE1	2:B:247:TYR:HA	1.86	0.41
2:B:191:PRO:O	2:B:206:ASN:OD1	2.39	0.41
1:A:59:LEU:HB2	1:A:63:GLU:HB3	2.02	0.41
1:A:148:LEU:HA	1:A:148:LEU:HD23	1.73	0.41
1:A:294:THR:OG1	1:A:296:ILE:HG22	2.20	0.41
1:A:532:THR:HA	1:A:541:PRO:HA	2.01	0.41
1:A:583:PHE:HB3	1:A:590:PHE:HD2	1.84	0.41
2:B:188:PRO:CB	2:B:210:LEU:HD11	2.51	0.41
1:A:205:ILE:CG2	1:A:266:ALA:HB3	2.51	0.41
1:A:827:ASP:O	1:A:831:SER:CB	2.66	0.41
2:B:228:ILE:HG22	2:B:264:PHE:CD1	2.56	0.41
1:A:126:ILE:HD13	1:A:126:ILE:HA	1.78	0.41
1:A:397:ARG:HD3	1:A:470:LYS:HZ3	1.86	0.41
1:A:470:LYS:O	1:A:474:VAL:HG22	2.21	0.41
1:A:942:GLN:HA	1:A:945:ASP:HB3	2.03	0.41
1:A:389:LYS:CD	1:A:629:THR:HG21	2.51	0.41
1:A:394:THR:HG22	1:A:396:ASN:H	1.86	0.41
1:A:685:MET:HE3	1:A:685:MET:HB2	1.83	0.41
1:A:726:VAL:CG2	1:A:737:LEU:HA	2.51	0.41
1:A:900:VAL:HG13	1:A:901:ALA:N	2.36	0.41
2:B:199:TYR:O	2:B:200:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:LYS:HG2	2:B:295:ARG:HG2	2.03	0.41
1:A:389:LYS:HG2	1:A:629:THR:HG21	2.02	0.40
1:A:527:LEU:HD23	1:A:527:LEU:HA	1.93	0.40
1:A:1000:TYR:HA	1:A:1003:VAL:HG23	2.03	0.40
1:A:224:LYS:O	1:A:262:LEU:HB2	2.21	0.40
1:A:805:TYR:OH	1:A:903:GLU:OE2	2.34	0.40
1:A:167:THR:O	1:A:167:THR:HG22	2.22	0.40
1:A:307:VAL:HA	1:A:310:VAL:HG22	2.04	0.40
1:A:729:ASP:HB2	1:A:749:ALA:O	2.22	0.40
2:B:21:LYS:HD2	2:B:21:LYS:HA	1.84	0.40
2:B:251:LEU:HD23	2:B:251:LEU:HA	1.92	0.40
1:A:330:LEU:H	1:A:330:LEU:HG	1.71	0.40
1:A:384:ILE:HD12	1:A:717:CYS:HB3	2.04	0.40
2:B:25:LEU:HD12	2:B:25:LEU:HA	1.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LYS:NZ	1:A:671:GLU:OE2[3_554]	2.13	0.07

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	984/986 (100%)	920 (94%)	64 (6%)	0	100	100
2	B	286/324 (88%)	248 (87%)	38 (13%)	0	100	100
All	All	1270/1310 (97%)	1168 (92%)	102 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	841/841 (100%)	841 (100%)	0	100	100
2	B	257/286 (90%)	257 (100%)	0	100	100
All	All	1098/1127 (97%)	1098 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	272	ASN
1	A	395	GLN
1	A	441	ASN
1	A	501	GLN
1	A	551	HIS
1	A	698	GLN
1	A	720	GLN
1	A	795	ASN
1	A	958	GLN
2	B	79	GLN
2	B	93	ASN
2	B	104	ASN
2	B	208	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 [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	$\# Z > 2$
3	ALF	A	1101	-	4,4,4	1.43	0	-		
5	NAG	B	401	2	14,14,15	0.96	1 (7%)	17,19,21	0.80	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
5	NAG	B	401	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	NAG	O5-C1	3.31	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	NAG	C1-O5-C5	2.53	115.58	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	ALF	2	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	986/986 (100%)	1.21	215 (21%) 2 2	13, 34, 96, 119	0
2	B	288/324 (88%)	1.49	62 (21%) 2 2	20, 45, 86, 114	0
All	All	1274/1310 (97%)	1.27	277 (21%) 2 2	13, 38, 95, 119	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	164	ASP	13.3
2	B	23	GLU	11.2
1	A	404	TRP	10.6
2	B	202	THR	10.4
2	B	20	GLU	9.8
2	B	165	GLU	7.1
2	B	253	PRO	7.0
1	A	600	LEU	6.8
1	A	841	SER	6.3
1	A	661	ASN	5.6
1	A	554	TYR	5.4
1	A	424	ASP	5.3
2	B	263	GLN	5.3
1	A	167	THR	5.3
1	A	552	THR	5.1
1	A	556	GLU	5.0
1	A	844	MET	5.0
1	A	292	GLU	4.8
1	A	555	MET	4.7
2	B	120	ASP	4.7
1	A	599	GLY	4.7
1	A	403	LEU	4.6
1	A	100	PRO	4.6
1	A	425	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	267	LEU	4.6
2	B	247	TYR	4.5
2	B	21	LYS	4.5
1	A	501	GLN	4.5
1	A	601	LEU	4.5
2	B	251	LEU	4.5
1	A	405	PHE	4.5
1	A	542	LEU	4.4
1	A	560	LEU	4.4
1	A	55	ASP	4.4
1	A	668	ASN	4.4
1	A	551	HIS	4.4
1	A	854	ASP	4.3
2	B	246	TYR	4.2
1	A	426	SER	4.2
1	A	454	ILE	4.1
1	A	249	LEU	4.0
2	B	168	GLY	4.0
1	A	621	ALA	3.9
2	B	283	ASN	3.9
1	A	215	ILE	3.9
2	B	249	LYS	3.9
1	A	559	GLY	3.9
1	A	590	PHE	3.9
1	A	684	ASP	3.8
1	A	420	LYS	3.8
2	B	200	PRO	3.8
1	A	564	VAL	3.8
1	A	156	GLY	3.8
1	A	163	GLU	3.8
2	B	197	GLU	3.8
2	B	208	ASN	3.7
1	A	410	PHE	3.7
1	A	472	SER	3.7
1	A	652	THR	3.7
1	A	839	ALA	3.6
1	A	408	GLN	3.6
1	A	470	LYS	3.6
1	A	565	LEU	3.6
2	B	138	GLU	3.6
1	A	168	ASN	3.5
2	B	60	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	161	GLY	3.5
2	B	140	ASN	3.5
2	B	196	LEU	3.5
1	A	537	GLY	3.5
2	B	250	LEU	3.5
2	B	201	LEU	3.5
2	B	139	PHE	3.4
1	A	430	TRP	3.4
2	B	70	ASP	3.4
1	A	158	PHE	3.4
1	A	591	PRO	3.4
2	B	62	SER	3.4
1	A	52	MET	3.4
2	B	198	THR	3.4
1	A	290	GLY	3.4
1	A	54	LEU	3.3
1	A	575	GLU	3.3
2	B	199	TYR	3.3
1	A	567	PHE	3.3
1	A	358	LEU	3.3
1	A	169	ILE	3.3
1	A	588	VAL	3.3
1	A	73	ILE	3.3
2	B	71	ARG	3.3
1	A	278	ILE	3.3
1	A	865	SER	3.2
1	A	407	ASN	3.2
2	B	229	GLU	3.2
2	B	167	TYR	3.2
1	A	523	PRO	3.2
2	B	289	LYS	3.2
1	A	423	PHE	3.2
1	A	586	ASP	3.2
1	A	494	PHE	3.2
1	A	664	VAL	3.1
1	A	676	VAL	3.1
1	A	159	ALA	3.1
1	A	894	SER	3.1
1	A	337	ILE	3.1
1	A	437	ILE	3.1
1	A	101	GLU	3.0
1	A	566	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	518	VAL	3.0
2	B	133	PRO	3.0
1	A	508	GLU	3.0
2	B	141	HIS	3.0
1	A	517	VAL	3.0
2	B	125	ASP	3.0
2	B	252	GLN	3.0
1	A	840	GLU	2.9
1	A	581	TYR	2.9
1	A	487	HIS	2.9
1	A	550	PHE	2.9
1	A	99	THR	2.9
1	A	587	SER	2.9
1	A	593	SER	2.9
2	B	234	GLY	2.9
1	A	510	PRO	2.9
1	A	490	ALA	2.9
1	A	545	SER	2.9
1	A	402	HIS	2.9
1	A	570	LEU	2.9
1	A	678	THR	2.9
1	A	393	LEU	2.9
1	A	516	LEU	2.9
2	B	17	TRP	2.8
2	B	206	ASN	2.8
1	A	563	ARG	2.8
2	B	241	LEU	2.8
1	A	680	MET	2.8
1	A	905	ASP	2.8
1	A	468	LEU	2.8
1	A	779	LEU	2.8
2	B	203	MET	2.8
1	A	132	TYR	2.8
1	A	181	ALA	2.8
1	A	209	ASP	2.8
1	A	729	ASP	2.8
1	A	657	ALA	2.8
1	A	493	PRO	2.8
1	A	62	THR	2.8
1	A	782	ASP	2.7
1	A	527	LEU	2.7
1	A	985	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	419	THR	2.7
2	B	163	ASN	2.7
2	B	204	LYS	2.7
1	A	376	VAL	2.7
1	A	166	SER	2.7
1	A	992	SER	2.7
2	B	73	ALA	2.7
1	A	538	GLN	2.7
1	A	214	ASP	2.7
2	B	213	GLN	2.7
1	A	120	GLY	2.7
1	A	499	LYS	2.7
1	A	155	THR	2.7
1	A	663	ALA	2.6
1	A	571	TYR	2.6
1	A	921	TYR	2.6
1	A	846	ARG	2.6
2	B	227	ASN	2.6
1	A	730	GLY	2.6
1	A	234	SER	2.6
2	B	166	SER	2.6
1	A	781	PHE	2.6
1	A	56	ASP	2.6
2	B	160	SER	2.6
1	A	96	PRO	2.6
1	A	244	THR	2.6
1	A	330	LEU	2.6
1	A	532	THR	2.6
1	A	504	ILE	2.5
1	A	138	SER	2.5
1	A	291	SER	2.5
1	A	609	SER	2.5
1	A	543	ASP	2.5
1	A	80	ARG	2.5
1	A	513	LYS	2.5
1	A	74	GLN	2.5
1	A	53	ASP	2.5
1	A	1032	LYS	2.5
2	B	205	TYR	2.5
1	A	51	GLY	2.5
1	A	576	GLN	2.5
1	A	533	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	641	LYS	2.5
1	A	162	GLN	2.5
1	A	298	ILE	2.4
1	A	582	ILE	2.4
1	A	651	GLU	2.4
1	A	497	THR	2.4
1	A	502	LEU	2.4
1	A	592	THR	2.4
1	A	1036	TYR	2.4
1	A	289	VAL	2.4
1	A	380	GLY	2.4
1	A	833	ALA	2.4
1	A	492	ILE	2.4
1	A	442	ARG	2.4
1	A	413	ASP	2.4
1	A	547	ALA	2.4
1	A	98	GLN	2.4
1	A	60	SER	2.4
1	A	531	SER	2.4
1	A	548	ASP	2.4
1	A	160	TYR	2.4
1	A	925	TYR	2.4
1	A	736	ALA	2.4
1	A	595	PHE	2.4
1	A	178	PRO	2.4
1	A	441	ASN	2.4
1	A	477	GLY	2.4
1	A	908	ASN	2.3
2	B	132	GLU	2.3
1	A	669	LYS	2.3
2	B	294	GLY	2.3
1	A	522	ALA	2.3
1	A	134	ASN	2.3
1	A	471	PHE	2.3
1	A	842	ASP	2.3
1	A	196	GLN	2.3
1	A	579	GLN	2.3
1	A	360	ALA	2.3
1	A	553	ALA	2.3
2	B	193	ASN	2.3
1	A	924	LYS	2.3
2	B	288	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	876	GLY	2.3
2	B	207	PRO	2.2
1	A	529	LYS	2.2
1	A	625	VAL	2.2
1	A	526	ILE	2.2
1	A	596	CYS	2.2
1	A	622	GLY	2.2
1	A	638	ALA	2.2
1	A	670	ARG	2.2
1	A	333	ILE	2.2
1	A	503	SER	2.2
1	A	662	ILE	2.2
2	B	122	ILE	2.2
1	A	476	LEU	2.2
1	A	636	ALA	2.2
2	B	240	PRO	2.2
1	A	356	LEU	2.1
1	A	431	ALA	2.1
1	A	489	VAL	2.1
1	A	473	GLU	2.1
1	A	906	ASP	2.1
1	A	458	THR	2.1
1	A	164	ALA	2.1
2	B	191	PRO	2.1
1	A	549	SER	2.1
2	B	264	PHE	2.1
1	A	988	VAL	2.1
1	A	406	ASP	2.1
1	A	838	LYS	2.1
1	A	482	ILE	2.1
1	A	485	ARG	2.1
1	A	143	TYR	2.1
1	A	721	ASP	2.1
1	A	137	ALA	2.1
1	A	303	PHE	2.1
1	A	142	VAL	2.0
2	B	97	SER	2.0
1	A	399	THR	2.0
1	A	500	PHE	2.0
1	A	1027	GLY	2.0
1	A	416	GLU	2.0
1	A	112	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	735	PRO	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](#)

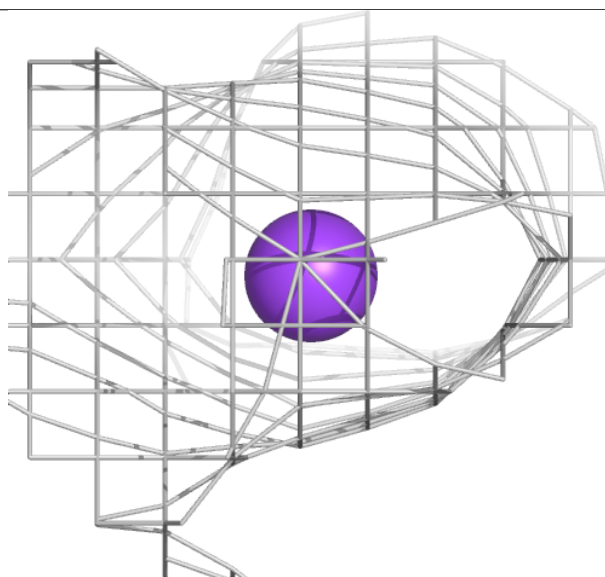
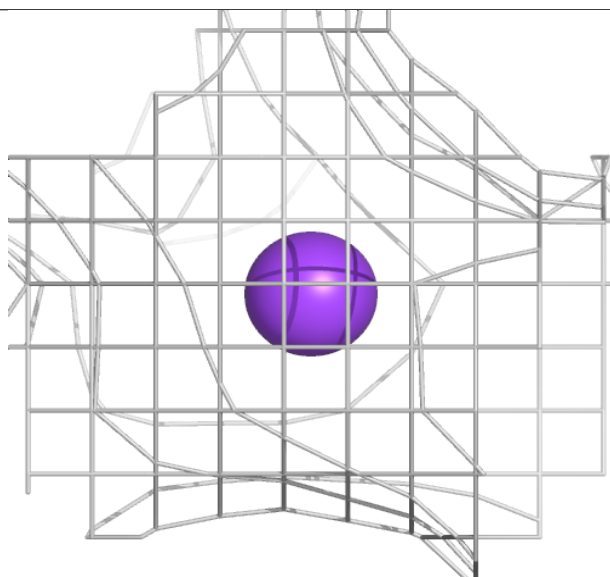
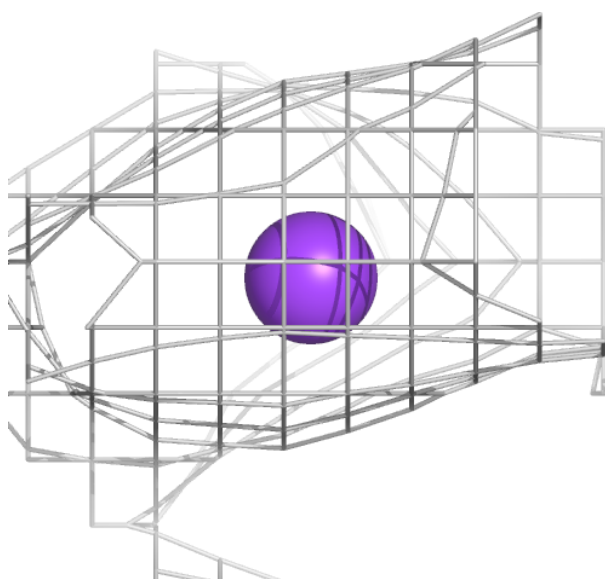
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

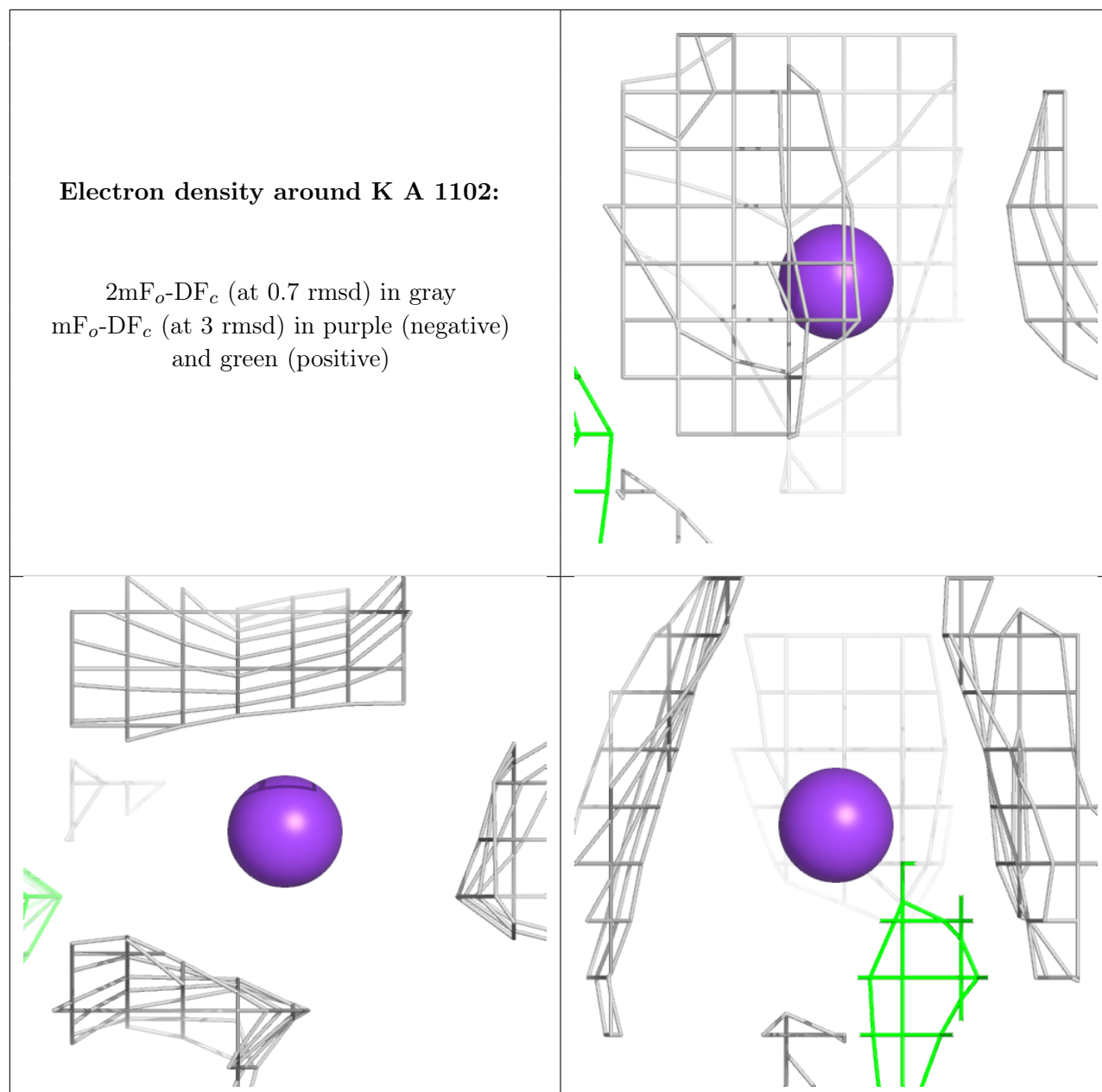
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	401	14/15	0.57	0.20	74,85,93,94	0
3	ALF	A	1101	5/5	0.91	0.14	19,21,25,26	0
4	K	A	1103	1/1	0.93	0.07	24,24,24,24	0
4	K	A	1102	1/1	0.95	0.06	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around K A 1103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.