



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:45 am BST

PDB ID : 3BA6
Title : Structure of the Ca₂E1P phosphoenzyme intermediate of the SERCA Ca²⁺-ATPase
Authors : Picard, M.; Winther, A.M.L.; Olesen, C.; Gyrupe, C.; Morth, J.P.; Oxvig, C.; Moller, J.V.; Nissen, P.
Deposited on : 2007-11-07
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

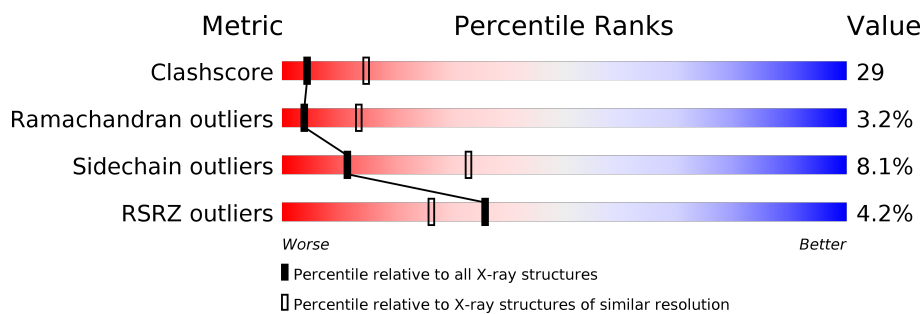
1 Overall quality at a glance

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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	994	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7714 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	P	S	0	0	0
			7674	4876	1287	1453	1	57			

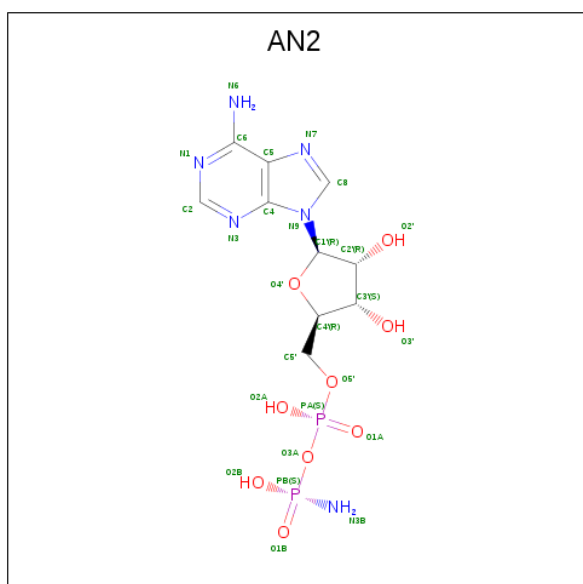
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

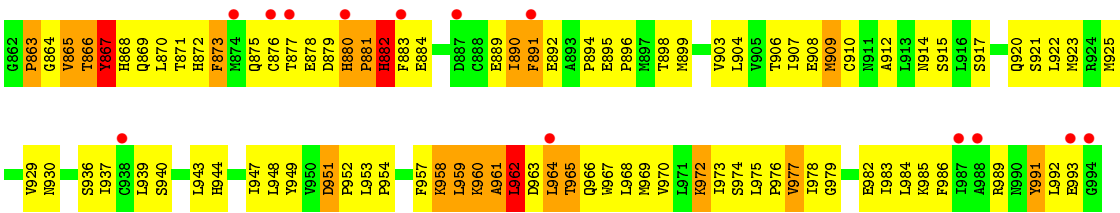
- Molecule 4 is AMP PHOSPHORAMIDATE (three-letter code: AN2) (formula: C₁₀H₁₆N₆O₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	6	9	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.51Å 75.97Å 152.41Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 44.09 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.0 (10.00-2.80) 84.9 (44.09-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.288 0.250 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.896	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7714	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: K, CA, AN2, PHD

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	0.46	0/7802	0.63	0/10578

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7674	0	7765	445	0
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	27	0	14	7	0
5	A	9	0	0	0	0
All	All	7714	0	7779	446	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 29.

All (446) 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:60:LEU:H	1:A:60:LEU:HD23	1.21	1.06
1:A:894:PRO:HB2	1:A:959:LEU:HB2	1.40	1.04
1:A:788:ILE:HG12	1:A:789:PRO:HD2	1.44	0.97
1:A:866:THR:HG22	1:A:867:TYR:H	1.34	0.91
1:A:909:MET:HG2	1:A:937:ILE:HG23	1.55	0.87
1:A:342:LEU:HD13	1:A:716:ILE:HG13	1.54	0.87
1:A:230:THR:HG22	1:A:232:ILE:H	1.42	0.84
1:A:944:HIS:O	1:A:947:ILE:HG22	1.79	0.83
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.14	0.82
1:A:716:ILE:N	1:A:716:ILE:HD13	1.95	0.82
1:A:624:ILE:O	1:A:684:LYS:HE2	1.79	0.81
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.63	0.81
1:A:866:THR:HG22	1:A:867:TYR:N	1.95	0.81
1:A:962:LEU:HA	1:A:966:GLN:HB2	1.63	0.80
1:A:341:THR:HG22	1:A:716:ILE:HD12	1.64	0.80
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.11	0.79
1:A:958:LYS:HE3	1:A:958:LYS:HA	1.65	0.78
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.64	0.78
1:A:361:MET:HE2	1:A:560:ARG:HD3	1.65	0.78
1:A:921:SER:H	1:A:989:ARG:HH22	1.28	0.78
1:A:716:ILE:H	1:A:716:ILE:HD13	1.50	0.77
1:A:865:VAL:O	1:A:866:THR:O	2.01	0.77
1:A:795:VAL:HG11	1:A:904:LEU:HD23	1.67	0.77
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.68	0.76
1:A:60:LEU:H	1:A:60:LEU:CD2	1.95	0.75
1:A:807:LEU:HD12	1:A:810:ASN:HD21	1.51	0.75
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.69	0.75
1:A:762:ARG:HA	1:A:837:TYR:HE1	1.52	0.75
1:A:704:GLY:O	1:A:707:ASP:HB2	1.87	0.74
1:A:957:PHE:O	1:A:958:LYS:NZ	2.12	0.74
1:A:558:THR:HG21	1:A:635:ILE:HG13	1.69	0.74
1:A:326:MET:HE2	1:A:329:LYS:HD2	1.69	0.74
1:A:794:TRP:CE2	1:A:947:ILE:HD12	2.23	0.74
1:A:629:LYS:HD2	1:A:654:THR:CG2	2.18	0.74
1:A:342:LEU:HG	1:A:747:VAL:HG12	1.70	0.73
1:A:308:PRO:HB3	1:A:764:LEU:HD12	1.69	0.73
1:A:865:VAL:HG13	1:A:870:LEU:HG	1.71	0.73
1:A:909:MET:CG	1:A:937:ILE:HG23	2.18	0.73
1:A:960:LYS:O	1:A:961:ALA:HB2	1.89	0.73
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.70	0.72
1:A:441:THR:HG23	1:A:560:ARG:HH12	1.54	0.71
1:A:948:LEU:HB3	1:A:949:TYR:CE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:VAL:HG22	1:A:940:SER:HB3	1.73	0.70
1:A:947:ILE:HA	1:A:953:LEU:HD23	1.74	0.70
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.72	0.70
1:A:866:THR:CG2	1:A:867:TYR:H	2.05	0.70
1:A:459:VAL:HA	1:A:462:LEU:HD12	1.73	0.70
1:A:171:THR:HG23	1:A:486:GLU:OE2	1.92	0.69
1:A:869:GLN:HG2	1:A:869:GLN:O	1.91	0.69
1:A:868:HIS:O	1:A:869:GLN:HB3	1.92	0.69
1:A:441:THR:CG2	1:A:560:ARG:HH12	2.06	0.69
1:A:847:ALA:HB1	1:A:973:ILE:HG22	1.73	0.69
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.75	0.69
1:A:894:PRO:O	1:A:898:THR:HG23	1.93	0.69
1:A:762:ARG:HA	1:A:837:TYR:CE1	2.28	0.68
1:A:964:LEU:O	1:A:966:GLN:N	2.26	0.68
1:A:529:ARG:NH2	1:A:592:THR:HG21	2.09	0.68
1:A:769:VAL:O	1:A:773:VAL:HG23	1.93	0.68
1:A:607:VAL:O	1:A:611:ILE:HG12	1.94	0.67
1:A:95:LEU:O	1:A:99:ILE:HG12	1.94	0.67
1:A:198:ARG:HD3	1:A:199:ALA:N	2.10	0.67
1:A:626:GLY:HA3	4:A:1001:AN2:O1A	1.95	0.67
1:A:871:THR:HG22	1:A:872:HIS:CE1	2.30	0.66
1:A:478:LEU:HD23	1:A:479:MET:HG2	1.76	0.66
1:A:340:GLU:HG2	1:A:341:THR:N	2.10	0.66
4:A:1001:AN2:O2B	4:A:1001:AN2:H5'2	1.95	0.66
1:A:126:MET:HE1	1:A:141:LYS:HA	1.78	0.66
1:A:119:LEU:HD13	1:A:332:ILE:HG13	1.77	0.65
1:A:170:SER:CB	1:A:486:GLU:HG2	2.27	0.65
1:A:115:ALA:O	1:A:118:ALA:HB3	1.95	0.65
1:A:354:GLY:HA2	1:A:359:ASN:HB2	1.77	0.65
1:A:81:GLY:O	1:A:84:THR:HG23	1.97	0.65
1:A:921:SER:OG	1:A:923:MET:HG2	1.96	0.65
1:A:54:ILE:O	1:A:56:GLN:N	2.28	0.64
1:A:629:LYS:HD2	1:A:654:THR:HG23	1.79	0.64
1:A:71:ILE:HD11	1:A:300:VAL:HG11	1.80	0.64
1:A:951:ASP:O	1:A:954:PRO:HD2	1.98	0.64
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.80	0.64
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.80	0.64
1:A:744:VAL:O	1:A:747:VAL:HG22	1.98	0.63
1:A:49:LEU:HB2	1:A:52:LEU:HD23	1.80	0.63
1:A:13:LEU:HD11	1:A:20:GLU:HB2	1.80	0.63
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:HB3	1:A:583:ARG:HE	1.63	0.62
1:A:13:LEU:CD1	1:A:20:GLU:HB2	2.29	0.62
1:A:230:THR:CG2	1:A:232:ILE:HG22	2.29	0.62
1:A:777:LEU:O	1:A:781:LEU:HB2	2.00	0.62
1:A:948:LEU:HB3	1:A:949:TYR:CD2	2.33	0.62
1:A:499:SER:HB2	1:A:500:PRO:HD2	1.81	0.62
1:A:533:THR:HG22	1:A:534:ARG:N	2.15	0.61
1:A:991:TYR:O	1:A:991:TYR:CG	2.53	0.61
1:A:737:ASP:OD1	1:A:739:ASN:HB2	1.99	0.61
1:A:2:GLU:HG3	1:A:16:PHE:CE1	2.36	0.61
1:A:274:ILE:HD12	1:A:776:PHE:CE1	2.35	0.61
1:A:414:ALA:HB2	1:A:452:MET:CE	2.31	0.61
1:A:847:ALA:HB1	1:A:973:ILE:CG2	2.31	0.61
1:A:195:PRO:O	1:A:197:PRO:HD3	2.00	0.61
1:A:791:GLN:NE2	1:A:958:LYS:HG3	2.16	0.61
1:A:414:ALA:HB2	1:A:452:MET:HE2	1.82	0.60
1:A:119:LEU:HD11	1:A:330:ASN:C	2.20	0.60
1:A:155:VAL:HG22	1:A:217:GLY:N	2.16	0.60
1:A:53:VAL:HG12	1:A:106:VAL:HG22	1.83	0.60
1:A:351:PHD:OP2	1:A:353:THR:N	2.33	0.60
1:A:891:PHE:N	1:A:891:PHE:HD2	1.99	0.60
1:A:90:GLU:HB2	1:A:91:PRO:HD3	1.84	0.60
1:A:762:ARG:NH1	1:A:836:ARG:HH21	1.99	0.60
1:A:891:PHE:N	1:A:891:PHE:CD2	2.69	0.60
1:A:333:VAL:HG13	1:A:338:SER:OG	2.01	0.60
1:A:276:ILE:O	1:A:279:PHE:HB2	2.02	0.60
1:A:361:MET:CE	1:A:560:ARG:HD3	2.31	0.59
1:A:305:ALA:HA	1:A:796:ASN:OD1	2.01	0.59
1:A:580:ASP:OD2	1:A:582:SER:HB3	2.02	0.59
1:A:489:ARG:NH1	4:A:1001:AN2:O2A	2.33	0.59
1:A:770:GLY:HA2	1:A:841:GLY:O	2.02	0.59
1:A:321:LEU:HD21	1:A:325:ARG:CZ	2.32	0.59
1:A:871:THR:HG22	1:A:872:HIS:NE2	2.18	0.59
1:A:155:VAL:HG22	1:A:217:GLY:H	1.66	0.59
1:A:558:THR:HG21	1:A:635:ILE:CG1	2.32	0.59
1:A:826:GLU:OE1	1:A:827:PRO:HD2	2.03	0.59
1:A:624:ILE:HG22	1:A:684:LYS:HG2	1.85	0.58
1:A:230:THR:HG21	1:A:232:ILE:HG22	1.85	0.58
1:A:243:GLU:O	1:A:244:GLN:O	2.21	0.58
1:A:442:GLU:O	1:A:445:LEU:HB2	2.04	0.58
1:A:743:ILE:O	1:A:747:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:O	1:A:451:LYS:HE2	2.04	0.58
1:A:836:ARG:HG3	1:A:984:LEU:HD23	1.86	0.58
1:A:275:ASN:C	1:A:277:GLY:H	2.08	0.57
1:A:97:ILE:HD11	1:A:800:ASP:O	2.04	0.57
1:A:501:ALA:C	1:A:503:SER:H	2.08	0.57
1:A:815:ASP:HB2	1:A:819:ARG:NH2	2.19	0.57
1:A:24:LEU:HD13	1:A:149:ASP:HA	1.87	0.57
1:A:678:ARG:NH2	4:A:1001:AN2:O3'	2.38	0.57
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.35	0.56
1:A:921:SER:H	1:A:989:ARG:NH2	2.02	0.56
1:A:170:SER:HB2	1:A:486:GLU:HG2	1.88	0.56
1:A:415:THR:HA	1:A:475:ILE:HD13	1.87	0.56
1:A:25:THR:O	1:A:28:GLN:N	2.39	0.56
1:A:843:TYR:OH	1:A:976:PRO:HB2	2.06	0.56
1:A:768:ASN:HA	1:A:771:GLU:HG3	1.87	0.56
1:A:275:ASN:O	1:A:276:ILE:HG22	2.06	0.56
1:A:873:PHE:O	1:A:873:PHE:CG	2.56	0.56
1:A:90:GLU:HG2	1:A:790:VAL:HG22	1.86	0.56
1:A:196:ASP:OD1	1:A:198:ARG:HD2	2.06	0.55
1:A:228:VAL:C	1:A:230:THR:H	2.10	0.55
1:A:352:LYS:HD2	1:A:635:ILE:HD12	1.88	0.55
1:A:142:ALA:O	1:A:145:ILE:HG23	2.05	0.55
1:A:873:PHE:HA	1:A:891:PHE:HE1	1.71	0.55
1:A:158:LYS:HE3	1:A:211:GLY:HA2	1.88	0.55
1:A:875:GLN:HA	1:A:880:HIS:HB3	1.87	0.55
1:A:501:ALA:O	1:A:503:SER:N	2.39	0.55
1:A:60:LEU:HG	1:A:61:LEU:H	1.72	0.55
1:A:279:PHE:CZ	1:A:288:TRP:C	2.80	0.55
1:A:279:PHE:HZ	1:A:288:TRP:C	2.09	0.55
1:A:177:GLN:HB3	1:A:212:THR:HG21	1.88	0.55
1:A:441:THR:HG23	1:A:560:ARG:NH1	2.21	0.55
1:A:794:TRP:CD2	1:A:947:ILE:HD12	2.41	0.55
1:A:496:VAL:O	1:A:512:MET:HA	2.06	0.55
1:A:530:VAL:O	1:A:533:THR:HB	2.07	0.55
1:A:868:HIS:O	1:A:871:THR:N	2.40	0.55
1:A:979:GLY:O	1:A:983:ILE:HG12	2.07	0.55
1:A:626:GLY:O	1:A:678:ARG:HA	2.06	0.55
1:A:965:THR:H	1:A:968:LEU:HD12	1.71	0.55
1:A:341:THR:CG2	1:A:716:ILE:HD12	2.35	0.54
1:A:515:LYS:HE3	4:A:1001:AN2:C2	2.37	0.54
1:A:788:ILE:CG1	1:A:789:PRO:HD2	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:GLN:HA	1:A:989:ARG:HH21	1.71	0.54
1:A:308:PRO:CB	1:A:764:LEU:HD12	2.36	0.54
1:A:533:THR:CG2	1:A:534:ARG:N	2.70	0.54
1:A:171:THR:HG21	1:A:584:PHE:CZ	2.42	0.54
1:A:515:LYS:HE3	4:A:1001:AN2:N1	2.23	0.54
1:A:58:GLU:HG3	1:A:63:ARG:NH2	2.22	0.54
1:A:962:LEU:HB2	1:A:967:TRP:CD1	2.42	0.54
1:A:55:GLU:N	1:A:55:GLU:OE2	2.41	0.54
1:A:54:ILE:C	1:A:56:GLN:H	2.10	0.54
1:A:351:PHD:HB2	1:A:355:THR:HB	1.90	0.54
1:A:32:HIS:O	1:A:36:TYR:HB2	2.08	0.54
1:A:627:ASP:N	4:A:1001:AN2:O2B	2.42	0.54
1:A:59:ASP:HB3	1:A:60:LEU:HD23	1.89	0.54
1:A:909:MET:HE2	1:A:909:MET:HA	1.90	0.54
1:A:823:SER:HB3	1:A:826:GLU:HG2	1.90	0.53
1:A:794:TRP:CZ2	1:A:947:ILE:HD12	2.43	0.53
1:A:920:GLN:HA	1:A:989:ARG:NH2	2.24	0.53
1:A:230:THR:O	1:A:234:LYS:HG3	2.08	0.53
1:A:873:PHE:C	1:A:873:PHE:CD2	2.78	0.53
1:A:302:LEU:O	1:A:305:ALA:HB3	2.08	0.53
1:A:19:SER:HB2	1:A:22:THR:OG1	2.07	0.53
1:A:230:THR:HG22	1:A:232:ILE:N	2.19	0.53
1:A:407:PHE:O	1:A:411:VAL:HG23	2.08	0.53
1:A:898:THR:HG21	1:A:959:LEU:O	2.09	0.53
1:A:495:SER:HB3	1:A:588:GLU:OE2	2.09	0.53
1:A:788:ILE:HG22	1:A:791:GLN:HG3	1.91	0.52
1:A:904:LEU:O	1:A:908:GLU:HG3	2.08	0.52
1:A:906:THR:HG22	1:A:974:SER:CB	2.39	0.52
1:A:487:PHE:HB2	1:A:494:MET:HB2	1.89	0.52
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.09	0.52
1:A:279:PHE:CE2	1:A:288:TRP:HA	2.44	0.52
1:A:338:SER:HB3	1:A:732:GLU:HB3	1.91	0.52
1:A:345:THR:O	1:A:619:ILE:HG12	2.09	0.52
1:A:247:THR:H	1:A:250:GLN:NE2	2.08	0.52
1:A:471:CYS:O	1:A:474:VAL:HB	2.10	0.52
1:A:773:VAL:HB	1:A:845:GLY:HA3	1.91	0.52
1:A:716:ILE:N	1:A:716:ILE:CD1	2.67	0.52
1:A:778:THR:HG22	1:A:849:VAL:HG13	1.91	0.52
1:A:102:ALA:O	1:A:106:VAL:HG23	2.09	0.51
1:A:969:MET:O	1:A:973:ILE:HG13	2.09	0.51
1:A:355:THR:HG23	1:A:720:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:HA	1:A:192:GLU:OE1	2.10	0.51
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.46	0.51
1:A:894:PRO:CB	1:A:959:LEU:HB2	2.28	0.51
1:A:170:SER:HB3	1:A:486:GLU:HG2	1.92	0.51
1:A:247:THR:H	1:A:250:GLN:HE21	1.58	0.51
1:A:459:VAL:HA	1:A:462:LEU:CD1	2.41	0.51
1:A:86:THR:HG22	1:A:790:VAL:HG21	1.92	0.51
1:A:321:LEU:O	1:A:325:ARG:HG3	2.09	0.51
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.41	0.51
1:A:865:VAL:O	1:A:865:VAL:HG12	2.10	0.51
1:A:287:SER:HB3	1:A:290:ARG:HB2	1.93	0.50
1:A:491:ARG:NH1	1:A:588:GLU:OE2	2.45	0.50
1:A:774:CYS:HB2	1:A:848:THR:HG21	1.93	0.50
1:A:960:LYS:O	1:A:961:ALA:CB	2.55	0.50
1:A:124:PRO:HB2	1:A:126:MET:CE	2.42	0.50
1:A:879:ASP:HB3	1:A:882:HIS:CD2	2.47	0.50
1:A:271:VAL:HG22	1:A:776:PHE:HE1	1.76	0.50
1:A:395:VAL:O	1:A:396:LEU:HD23	2.12	0.50
1:A:330:ASN:HB2	1:A:737:ASP:HB2	1.94	0.50
1:A:357:THR:HG22	1:A:603:PRO:HA	1.93	0.50
1:A:864:GLY:C	1:A:866:THR:H	2.15	0.50
1:A:65:LEU:HD22	1:A:309:GLU:HG3	1.93	0.50
1:A:294:TYR:OH	1:A:788:ILE:HG13	2.11	0.50
1:A:90:GLU:CG	1:A:790:VAL:HG22	2.41	0.50
1:A:92:PHE:O	1:A:96:LEU:HB2	2.12	0.50
1:A:315:ILE:HG12	1:A:757:MET:HE1	1.94	0.49
1:A:108:GLN:HG2	1:A:317:THR:HG23	1.95	0.49
1:A:379:LEU:CD2	1:A:544:LYS:HD2	2.42	0.49
1:A:868:HIS:C	1:A:871:THR:H	2.16	0.49
1:A:929:VAL:HG23	1:A:930:ASN:N	2.26	0.49
1:A:921:SER:N	1:A:989:ARG:HH22	2.02	0.49
1:A:331:ALA:HB2	1:A:742:THR:HG21	1.94	0.49
1:A:866:THR:HG22	1:A:867:TYR:CG	2.47	0.49
1:A:560:ARG:O	1:A:599:MET:HB2	2.13	0.49
1:A:159:VAL:HG12	1:A:210:SER:HA	1.95	0.48
1:A:64:ILE:HG21	1:A:307:ILE:HD12	1.96	0.48
1:A:413:LEU:HD12	1:A:452:MET:CE	2.43	0.48
1:A:2:GLU:HG3	1:A:16:PHE:CZ	2.48	0.48
1:A:326:MET:HB3	1:A:331:ALA:HB3	1.94	0.48
1:A:866:THR:HG22	1:A:867:TYR:CD1	2.48	0.48
1:A:992:LEU:HD12	1:A:993:GLU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ARG:HD2	1:A:823:SER:O	2.13	0.48
1:A:880:HIS:O	1:A:881:PRO:C	2.52	0.48
1:A:936:SER:O	1:A:939:LEU:HB3	2.13	0.48
1:A:258:GLU:O	1:A:261:SER:HB3	2.12	0.48
1:A:294:TYR:O	1:A:297:LYS:HB2	2.12	0.48
1:A:326:MET:HA	1:A:326:MET:HE2	1.96	0.48
1:A:662:PRO:HD2	1:A:665:GLU:HB2	1.95	0.48
1:A:50:TRP:O	1:A:54:ILE:HG12	2.13	0.48
1:A:59:ASP:O	1:A:63:ARG:HG3	2.14	0.48
1:A:242:THR:HG22	1:A:242:THR:O	2.14	0.48
1:A:881:PRO:O	1:A:883:PHE:N	2.46	0.48
1:A:89:VAL:O	1:A:93:VAL:HG23	2.13	0.48
1:A:501:ALA:C	1:A:503:SER:N	2.67	0.48
1:A:787:LEU:HA	1:A:791:GLN:OE1	2.13	0.47
1:A:869:GLN:OE1	1:A:871:THR:O	2.31	0.47
1:A:914:ASN:HD21	1:A:978:ILE:HA	1.79	0.47
1:A:127:GLY:O	1:A:139:ARG:HA	2.13	0.47
1:A:962:LEU:HD12	1:A:967:TRP:CE2	2.50	0.47
1:A:418:ALA:HB3	1:A:475:ILE:HG21	1.96	0.47
1:A:524:ARG:HD2	1:A:588:GLU:O	2.14	0.47
1:A:845:GLY:O	1:A:848:THR:HG22	2.14	0.47
1:A:1:MET:HG3	1:A:225:THR:CG2	2.44	0.47
1:A:416:ILE:HD11	1:A:566:THR:OG1	2.15	0.47
1:A:62:VAL:O	1:A:66:LEU:HB2	2.14	0.47
1:A:711:LEU:HD23	1:A:711:LEU:HA	1.72	0.47
1:A:735:LEU:HD13	1:A:739:ASN:O	2.14	0.47
1:A:899:MET:O	1:A:903:VAL:HG23	2.14	0.47
1:A:975:LEU:N	1:A:976:PRO:CD	2.77	0.47
1:A:65:LEU:HG	1:A:304:VAL:HG13	1.97	0.47
1:A:412:GLU:OE2	1:A:529:ARG:NH1	2.47	0.47
1:A:804:ALA:HA	1:A:807:LEU:HD23	1.96	0.47
1:A:383:SER:C	1:A:384:ILE:HD13	2.35	0.47
1:A:4:ALA:HB1	1:A:7:LYS:HG2	1.95	0.47
1:A:629:LYS:HD2	1:A:654:THR:HG22	1.92	0.47
1:A:898:THR:HG22	1:A:958:LYS:HB2	1.96	0.47
1:A:564:LEU:N	1:A:564:LEU:HD12	2.29	0.47
1:A:436:LYS:CB	1:A:443:THR:HG21	2.45	0.47
1:A:829:ILE:HD13	1:A:837:TYR:HE2	1.79	0.47
1:A:326:MET:HE2	1:A:329:LYS:CD	2.43	0.46
1:A:352:LYS:HE3	1:A:352:LYS:HB3	1.65	0.46
1:A:829:ILE:HD13	1:A:837:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:ASP:N	1:A:952:PRO:HD2	2.30	0.46
1:A:274:ILE:HD12	1:A:776:PHE:CZ	2.49	0.46
1:A:605:LYS:HE2	1:A:605:LYS:HB3	1.74	0.46
1:A:751:ARG:HG2	1:A:816:ILE:HG12	1.97	0.46
1:A:15:TYR:C	1:A:15:TYR:CD2	2.88	0.46
1:A:267:ILE:O	1:A:270:ALA:HB3	2.15	0.46
1:A:288:TRP:CD1	1:A:289:ILE:HG13	2.50	0.46
1:A:65:LEU:HD22	1:A:309:GLU:CG	2.46	0.46
1:A:908:GLU:C	1:A:910:CYS:H	2.19	0.46
1:A:963:ASP:O	1:A:964:LEU:C	2.53	0.46
1:A:20:GLU:HG3	1:A:166:LEU:HD13	1.98	0.46
1:A:463:SER:OG	1:A:466:GLU:HG3	2.16	0.46
1:A:280:ASN:O	1:A:286:GLY:HA2	2.15	0.46
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.65	0.46
1:A:903:VAL:HG22	1:A:970:VAL:HA	1.97	0.46
1:A:922:LEU:HA	1:A:925:MET:O	2.16	0.46
1:A:177:GLN:HB3	1:A:212:THR:CG2	2.45	0.46
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.31	0.46
1:A:565:ALA:HA	1:A:594:VAL:HG23	1.98	0.46
1:A:294:TYR:HD2	1:A:295:TYR:CD2	2.34	0.45
1:A:361:MET:HA	1:A:600:LEU:O	2.16	0.45
1:A:467:ARG:O	1:A:467:ARG:HG3	2.16	0.45
1:A:679:VAL:O	1:A:679:VAL:HG23	2.15	0.45
1:A:965:THR:N	1:A:968:LEU:HD12	2.30	0.45
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.17	0.45
1:A:124:PRO:HB2	1:A:126:MET:HE3	1.98	0.45
1:A:246:LYS:HG3	1:A:251:GLN:CG	2.46	0.45
1:A:308:PRO:HA	1:A:764:LEU:HD12	1.98	0.45
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.16	0.45
1:A:90:GLU:OE2	1:A:790:VAL:HG22	2.16	0.45
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.98	0.45
1:A:70:CYS:O	1:A:74:VAL:HG23	2.16	0.45
1:A:796:ASN:O	1:A:798:VAL:N	2.50	0.45
1:A:85:ILE:C	1:A:87:ALA:N	2.70	0.45
1:A:148:GLY:O	1:A:222:ILE:HG13	2.17	0.45
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.66	0.45
1:A:185:VAL:HG12	1:A:186:SER:N	2.31	0.45
1:A:921:SER:CB	1:A:923:MET:HG2	2.47	0.45
1:A:983:ILE:O	1:A:986:PHE:HB3	2.16	0.45
1:A:855:TRP:NE1	1:A:896:PRO:HD3	2.32	0.45
1:A:86:THR:O	1:A:86:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:HIS:CB	1:A:881:PRO:HD2	2.46	0.45
1:A:807:LEU:HD12	1:A:915:SER:O	2.16	0.45
1:A:962:LEU:HA	1:A:966:GLN:OE1	2.16	0.45
1:A:276:ILE:HD11	1:A:292:ALA:HB2	1.99	0.45
1:A:188:ILE:CG2	1:A:189:LYS:N	2.80	0.44
1:A:145:ILE:HD12	1:A:223:VAL:HG21	1.99	0.44
1:A:865:VAL:CG1	1:A:865:VAL:O	2.65	0.44
1:A:250:GLN:O	1:A:254:ASP:HB2	2.18	0.44
1:A:267:ILE:HG21	1:A:772:VAL:HG11	1.98	0.44
1:A:268:CYS:SG	1:A:303:ALA:HB2	2.58	0.44
1:A:720:MET:O	1:A:728:LYS:HE2	2.18	0.44
1:A:903:VAL:O	1:A:907:ILE:HG22	2.17	0.44
1:A:352:LYS:HA	1:A:356:LEU:HB2	1.98	0.44
1:A:663:LEU:HD12	1:A:663:LEU:HA	1.77	0.44
1:A:88:PHE:O	1:A:91:PRO:HD2	2.16	0.44
1:A:959:LEU:O	1:A:960:LYS:O	2.36	0.44
1:A:120:LYS:C	1:A:122:TYR:H	2.20	0.44
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.16	0.44
1:A:828:LEU:HD12	1:A:828:LEU:O	2.18	0.44
1:A:863:PRO:HG3	1:A:890:ILE:CD1	2.48	0.44
1:A:336:LEU:N	1:A:337:PRO:CD	2.80	0.44
1:A:376:PHE:CZ	1:A:378:SER:HB3	2.53	0.44
1:A:719:ALA:HB2	1:A:731:SER:OG	2.18	0.44
1:A:894:PRO:HB3	1:A:958:LYS:HD3	1.99	0.44
1:A:968:LEU:O	1:A:972:LYS:HD3	2.17	0.44
1:A:241:ALA:C	1:A:243:GLU:H	2.20	0.44
1:A:449:VAL:HA	1:A:452:MET:HG3	2.00	0.44
1:A:51:GLU:O	1:A:54:ILE:HB	2.17	0.44
1:A:880:HIS:HB3	1:A:881:PRO:HD2	2.00	0.44
1:A:230:THR:HG22	1:A:232:ILE:HG22	2.00	0.44
1:A:255:GLU:HG2	1:A:255:GLU:O	2.18	0.44
1:A:273:LEU:O	1:A:275:ASN:N	2.51	0.44
1:A:49:LEU:HD12	1:A:52:LEU:HD23	1.99	0.44
1:A:271:VAL:HG22	1:A:776:PHE:CE1	2.52	0.44
1:A:18:VAL:HG13	1:A:24:LEU:HD12	1.99	0.43
1:A:529:ARG:HH21	1:A:592:THR:HG21	1.83	0.43
1:A:279:PHE:HZ	1:A:288:TRP:O	2.01	0.43
1:A:445:LEU:O	1:A:448:LEU:HB3	2.18	0.43
1:A:962:LEU:HA	1:A:966:GLN:CB	2.40	0.43
1:A:163:ILE:O	1:A:207:MET:HA	2.18	0.43
1:A:836:ARG:HH22	1:A:985:LYS:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:TYR:O	1:A:868:HIS:CD2	2.72	0.43
1:A:991:TYR:CD2	1:A:991:TYR:O	2.71	0.43
1:A:241:ALA:C	1:A:243:GLU:N	2.72	0.43
1:A:253:LEU:HD12	1:A:315:ILE:CD1	2.48	0.43
1:A:533:THR:CG2	1:A:534:ARG:H	2.31	0.43
1:A:164:ARG:NH1	1:A:165:ILE:O	2.51	0.43
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.54	0.43
1:A:909:MET:CE	1:A:909:MET:HA	2.48	0.43
1:A:854:TRP:CD1	1:A:858:TYR:HB2	2.54	0.43
1:A:391:PRO:HD2	1:A:434:TYR:CE1	2.54	0.43
1:A:921:SER:N	1:A:989:ARG:NH2	2.65	0.43
1:A:984:LEU:HA	1:A:984:LEU:HD12	1.87	0.43
1:A:400:LYS:O	1:A:402:ILE:HG23	2.19	0.43
1:A:478:LEU:C	1:A:501:ALA:HB2	2.39	0.43
1:A:581:SER:HA	1:A:584:PHE:CE1	2.54	0.43
1:A:10:GLU:HG3	1:A:11:GLU:H	1.84	0.42
1:A:490:ASP:OD1	1:A:491:ARG:N	2.45	0.42
1:A:855:TRP:HA	1:A:859:ALA:HB2	2.00	0.42
1:A:908:GLU:C	1:A:910:CYS:N	2.72	0.42
1:A:680:GLU:HB3	1:A:681:PRO:HD2	2.00	0.42
1:A:71:ILE:HG13	1:A:72:SER:N	2.34	0.42
1:A:963:ASP:O	1:A:964:LEU:O	2.36	0.42
1:A:238:GLN:O	1:A:239:MET:O	2.37	0.42
1:A:49:LEU:HD12	1:A:52:LEU:CD2	2.49	0.42
1:A:620:ARG:NH2	1:A:622:ILE:HD11	2.34	0.42
1:A:218:LYS:NZ	1:A:422:ASP:O	2.52	0.42
1:A:788:ILE:HG23	1:A:789:PRO:N	2.34	0.42
1:A:336:LEU:HD22	1:A:336:LEU:HA	1.75	0.42
1:A:334:ARG:NH1	1:A:731:SER:O	2.50	0.42
1:A:413:LEU:C	1:A:413:LEU:HD13	2.40	0.42
1:A:762:ARG:CG	1:A:837:TYR:HE1	2.32	0.42
1:A:848:THR:OG1	1:A:904:LEU:HD13	2.20	0.42
1:A:482:GLU:OE1	1:A:482:GLU:HA	2.20	0.42
1:A:510:ASN:O	1:A:511:LYS:HD3	2.20	0.42
1:A:705:VAL:C	1:A:707:ASP:H	2.23	0.42
1:A:86:THR:CG2	1:A:790:VAL:HG21	2.50	0.42
1:A:764:LEU:HA	1:A:764:LEU:HD22	1.68	0.42
1:A:53:VAL:CG1	1:A:106:VAL:HG13	2.50	0.42
1:A:340:GLU:CG	1:A:341:THR:N	2.80	0.42
1:A:894:PRO:HB3	1:A:958:LYS:HB3	2.01	0.42
1:A:239:MET:O	1:A:240:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:ALA:O	1:A:962:LEU:O	2.38	0.41
1:A:977:VAL:CG1	1:A:978:ILE:N	2.83	0.41
1:A:581:SER:HA	1:A:584:PHE:CZ	2.55	0.41
1:A:671:ARG:HG3	1:A:694:TYR:CE2	2.55	0.41
1:A:834:PHE:O	1:A:838:MET:HG2	2.21	0.41
1:A:877:THR:HG22	1:A:878:GLU:N	2.35	0.41
1:A:111:ASN:HB3	1:A:324:ARG:HD2	2.01	0.41
1:A:42:PRO:O	1:A:43:ALA:C	2.59	0.41
1:A:377:CYS:HB3	1:A:544:LYS:HG3	2.01	0.41
1:A:809:PHE:N	1:A:809:PHE:CD2	2.88	0.41
1:A:867:TYR:C	1:A:868:HIS:CG	2.92	0.41
1:A:194:VAL:O	1:A:194:VAL:HG23	2.21	0.41
1:A:889:GLU:HG2	1:A:889:GLU:O	2.21	0.41
1:A:529:ARG:NH2	1:A:568:ASP:OD2	2.54	0.41
1:A:99:ILE:O	1:A:103:ILE:HG13	2.21	0.41
1:A:13:LEU:HD13	1:A:20:GLU:HB2	2.03	0.41
1:A:246:LYS:HG3	1:A:251:GLN:HG2	2.02	0.41
1:A:506:ALA:O	1:A:507:ALA:HB3	2.20	0.41
1:A:119:LEU:HA	1:A:119:LEU:HD23	1.92	0.41
1:A:275:ASN:C	1:A:277:GLY:N	2.73	0.41
1:A:60:LEU:N	1:A:60:LEU:HD23	2.06	0.41
1:A:65:LEU:HD22	1:A:309:GLU:CB	2.51	0.40
1:A:33:LEU:HA	1:A:33:LEU:HD23	1.87	0.40
1:A:763:TYR:CD1	1:A:912:ALA:HB2	2.55	0.40
1:A:10:GLU:O	1:A:11:GLU:C	2.59	0.40
1:A:228:VAL:O	1:A:230:THR:N	2.54	0.40
1:A:379:LEU:HD21	1:A:544:LYS:HD2	2.03	0.40
1:A:489:ARG:HD3	1:A:706:ASN:HB3	2.03	0.40
1:A:124:PRO:O	1:A:126:MET:HE2	2.22	0.40
1:A:60:LEU:N	1:A:60:LEU:CD2	2.72	0.40
1:A:828:LEU:C	1:A:828:LEU:HD12	2.42	0.40
1:A:873:PHE:HD1	1:A:891:PHE:HD1	1.69	0.40
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.57	0.40
1:A:635:ILE:O	1:A:636:CYS:C	2.59	0.40
1:A:843:TYR:CD2	1:A:843:TYR:C	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	991/994 (100%)	838 (85%)	121 (12%)	32 (3%)	4	13

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ALA
1	A	46	GLY
1	A	55	GLU
1	A	239	MET
1	A	244	GLN
1	A	276	ILE
1	A	501	ALA
1	A	866	THR
1	A	876	CYS
1	A	881	PRO
1	A	882	HIS
1	A	892	GLU
1	A	960	LYS
1	A	961	ALA
1	A	962	LEU
1	A	964	LEU
1	A	965	THR
1	A	229	SER
1	A	959	LEU
1	A	121	GLU
1	A	502	LYS
1	A	797	LEU
1	A	863	PRO
1	A	42	PRO
1	A	587	TYR
1	A	316	THR
1	A	155	VAL
1	A	274	ILE

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Mol	Chain	Res	Type
1	A	867	TYR
1	A	26	PRO
1	A	289	ILE
1	A	865	VAL

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	839/839 (100%)	771 (92%)	68 (8%)	11	33

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	VAL
1	A	55	GLU
1	A	60	LEU
1	A	110	ARG
1	A	119	LEU
1	A	136	SER
1	A	139	ARG
1	A	145	ILE
1	A	198	ARG
1	A	225	THR
1	A	239	MET
1	A	244	GLN
1	A	245	ASP
1	A	276	ILE
1	A	284	HIS
1	A	309	GLU
1	A	319	LEU
1	A	336	LEU
1	A	338	SER
1	A	340	GLU
1	A	346	SER
1	A	356	LEU

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Mol	Chain	Res	Type
1	A	379	LEU
1	A	384	ILE
1	A	433	VAL
1	A	445	LEU
1	A	449	VAL
1	A	484	THR
1	A	489	ARG
1	A	491	ARG
1	A	496	VAL
1	A	529	ARG
1	A	532	THR
1	A	554	THR
1	A	558	THR
1	A	581	SER
1	A	656	ARG
1	A	663	LEU
1	A	665	GLU
1	A	678	ARG
1	A	691	LEU
1	A	701	THR
1	A	712	LYS
1	A	716	ILE
1	A	751	ARG
1	A	764	LEU
1	A	788	ILE
1	A	795	VAL
1	A	828	LEU
1	A	861	ASP
1	A	867	TYR
1	A	873	PHE
1	A	880	HIS
1	A	882	HIS
1	A	884	GLU
1	A	890	ILE
1	A	891	PHE
1	A	895	GLU
1	A	909	MET
1	A	917	SER
1	A	943	LEU
1	A	951	ASP
1	A	958	LYS
1	A	962	LEU

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Mol	Chain	Res	Type
1	A	972	LYS
1	A	977	VAL
1	A	982	GLU
1	A	991	TYR

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

Mol	Chain	Res	Type
1	A	111	ASN
1	A	114	ASN
1	A	250	GLN
1	A	259	GLN
1	A	275	ASN
1	A	280	ASN
1	A	284	HIS
1	A	398	ASN
1	A	472	ASN
1	A	706	ASN
1	A	755	ASN
1	A	914	ASN
1	A	920	GLN
1	A	990	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	PHD	A	351	1,2	9,11,12	2.70	4 (44%)	10,15,17	3.57	6 (60%)

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
1	PHD	A	351	1,2	-	4/8/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	PHD	O-C	6.00	1.43	1.19
1	A	351	PHD	P-OD1	3.59	1.64	1.59
1	A	351	PHD	P-OP2	-2.74	1.44	1.54
1	A	351	PHD	P-OP1	2.13	1.57	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	PHD	CB-CA-C	-7.66	97.11	111.47
1	A	351	PHD	OP2-P-OD1	4.62	119.33	105.25
1	A	351	PHD	OP3-P-OP1	-3.91	95.37	110.68
1	A	351	PHD	OD1-CG-CB	3.13	119.72	111.11
1	A	351	PHD	CA-CB-CG	-2.52	107.57	112.86
1	A	351	PHD	OD1-P-OP1	-2.42	100.72	109.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	351	PHD	CA-CB-CG-OD1
1	A	351	PHD	C-CA-CB-CG
1	A	351	PHD	N-CA-CB-CG
1	A	351	PHD	CA-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	351	PHD	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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$
4	AN2	A	1001	-	24,29,29	3.48	11 (45%)	25,45,45	1.98	5 (20%)

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
4	AN2	A	1001	-	-	4/9/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	AN2	PB-O1B	-12.27	1.26	1.46
4	A	1001	AN2	C8-N7	5.26	1.44	1.34
4	A	1001	AN2	PA-O1A	4.56	1.67	1.50
4	A	1001	AN2	C2-N3	4.52	1.39	1.32
4	A	1001	AN2	C2-N1	3.33	1.40	1.33
4	A	1001	AN2	C6-N6	3.24	1.45	1.34
4	A	1001	AN2	C5-C4	2.84	1.48	1.40
4	A	1001	AN2	O4'-C1'	2.79	1.45	1.41
4	A	1001	AN2	C4-N3	-2.69	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	AN2	PB-O3A	2.58	1.62	1.59
4	A	1001	AN2	PB-O2B	2.35	1.63	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	AN2	PA-O3A-PB	-5.01	116.68	132.56
4	A	1001	AN2	C3'-C2'-C1'	4.51	107.77	100.98
4	A	1001	AN2	C4-C5-N7	-3.62	105.62	109.40
4	A	1001	AN2	N3-C2-N1	-3.61	123.03	128.68
4	A	1001	AN2	C5'-C4'-C3'	-3.24	103.04	115.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

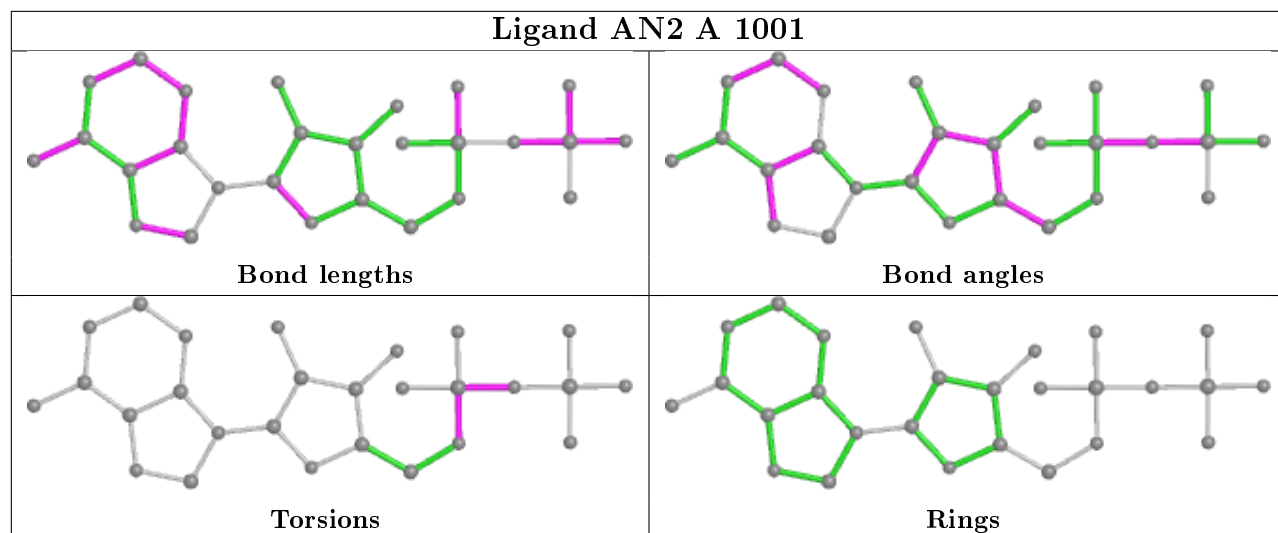
Mol	Chain	Res	Type	Atoms
4	A	1001	AN2	C5'-O5'-PA-O1A
4	A	1001	AN2	PB-O3A-PA-O5'
4	A	1001	AN2	C5'-O5'-PA-O3A
4	A	1001	AN2	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	AN2	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	993/994 (99%)	0.08	42 (4%) 36 26	54, 109, 190, 249	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.8
1	A	993	GLU	7.3
1	A	47	LYS	7.3
1	A	876	CYS	6.3
1	A	877	THR	6.3
1	A	45	GLU	6.2
1	A	506	ALA	6.1
1	A	84	THR	5.2
1	A	874	MET	5.0
1	A	887	ASP	4.9
1	A	891	PHE	4.9
1	A	239	MET	4.7
1	A	883	PHE	4.3
1	A	505	ARG	4.0
1	A	987	ILE	3.9
1	A	837	TYR	3.8
1	A	82	GLU	3.4
1	A	283	VAL	3.3
1	A	880	HIS	3.2
1	A	78	PHE	3.2
1	A	938	CYS	3.1
1	A	44	GLU	2.9
1	A	504	SER	2.9
1	A	282	PRO	2.9
1	A	294	TYR	2.9
1	A	964	LEU	2.8
1	A	782	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	85	ILE	2.7
1	A	852	ALA	2.7
1	A	240	ALA	2.6
1	A	292	ALA	2.6
1	A	994	GLY	2.5
1	A	83	GLU	2.5
1	A	851	ALA	2.5
1	A	80	GLU	2.5
1	A	75	LEU	2.3
1	A	988	ALA	2.3
1	A	46	GLY	2.2
1	A	48	SER	2.2
1	A	787	LEU	2.1
1	A	81	GLY	2.1
1	A	778	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PHD	A	351	12/13	0.95	0.18	46,73,95,98	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

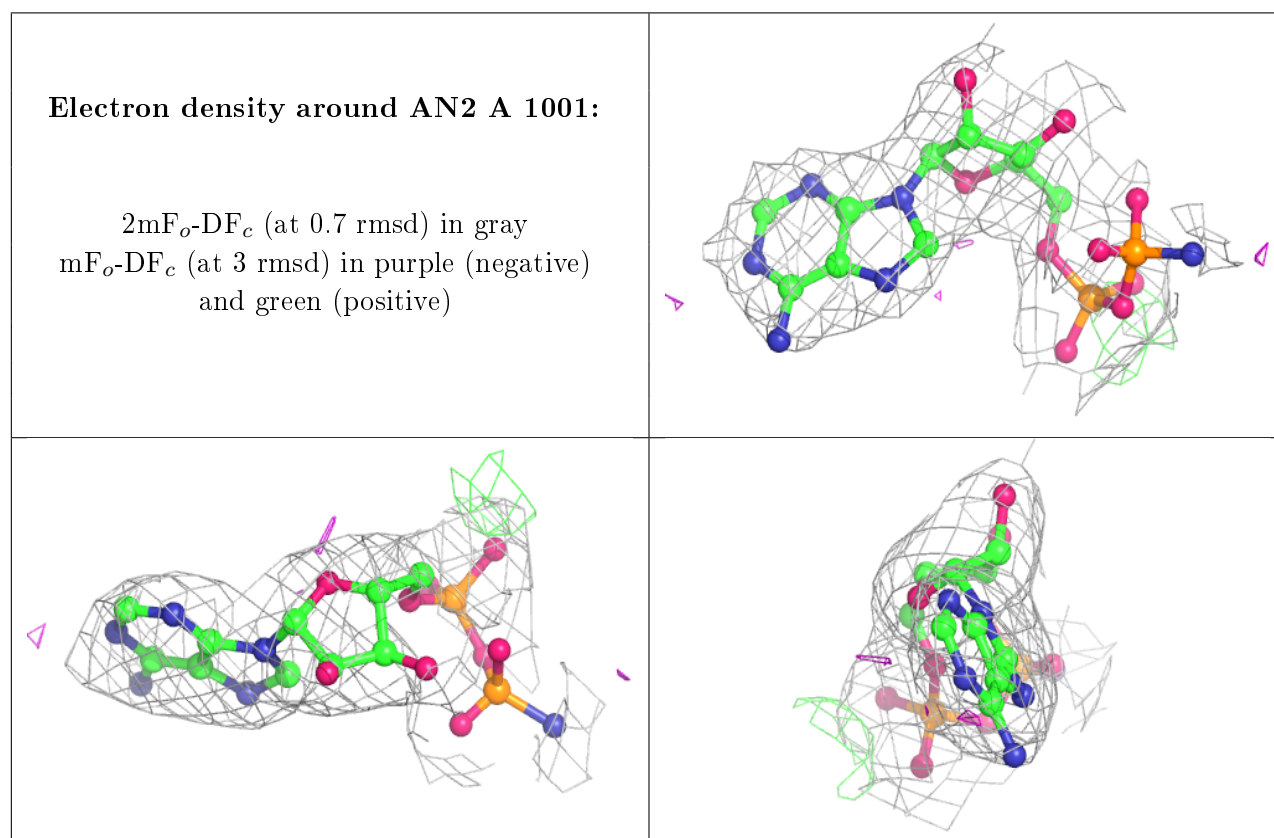
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	1003	1/1	0.89	0.12	95,95,95,95	0
2	CA	A	1004	1/1	0.92	0.14	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	K	A	1006	1/1	0.92	0.23	99,99,99,99	0
2	CA	A	1005	1/1	0.94	0.23	71,71,71,71	0
4	AN2	A	1001	27/27	0.98	0.21	58,68,82,97	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.