



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 AM GMT

PDB ID : 2DQS
Title : Crystal structure of the calcium pump with amppcp in the absence of calcium
Authors : Toyoshima, C.; Norimatsu, Y.; Tsueda, J.
Deposited on : 2006-05-29
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

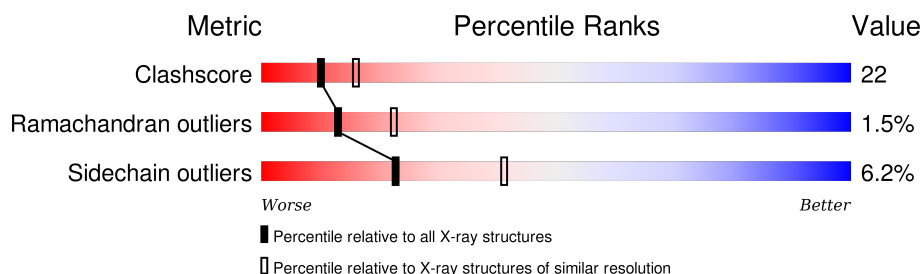
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	995	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8024 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	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

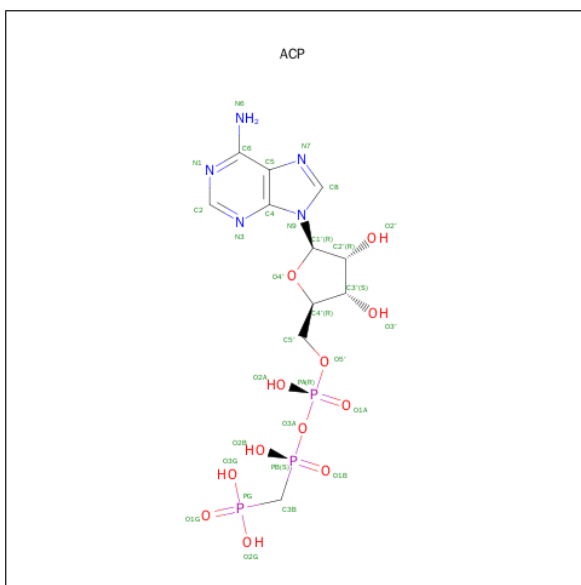
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

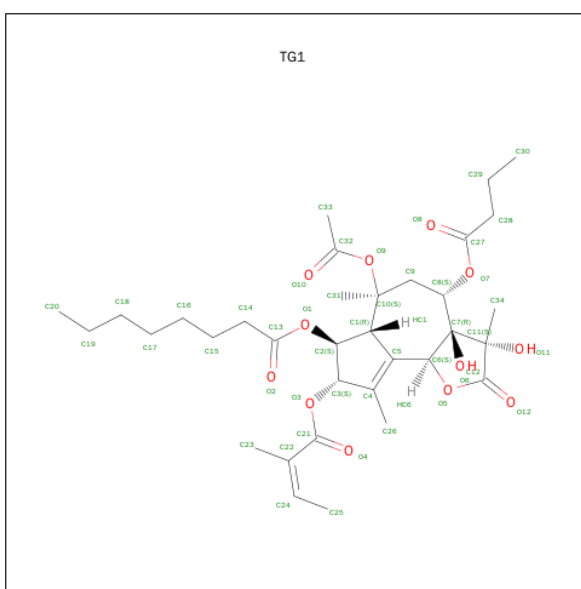
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



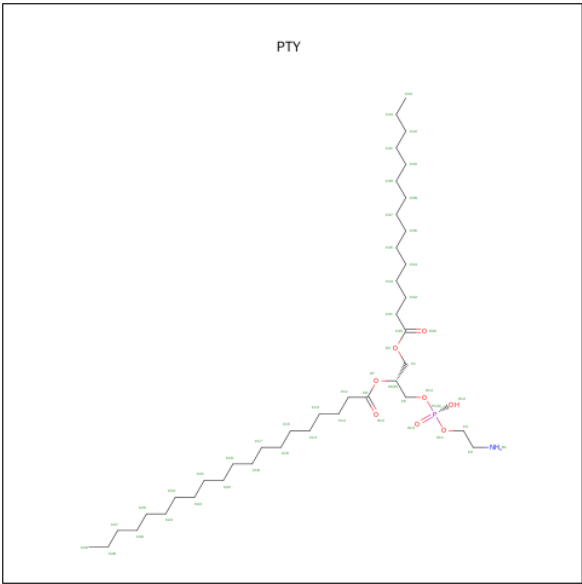
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: C₃₄H₅₀O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			46	34	12		

- Molecule 6 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

- Molecule 7 is water.

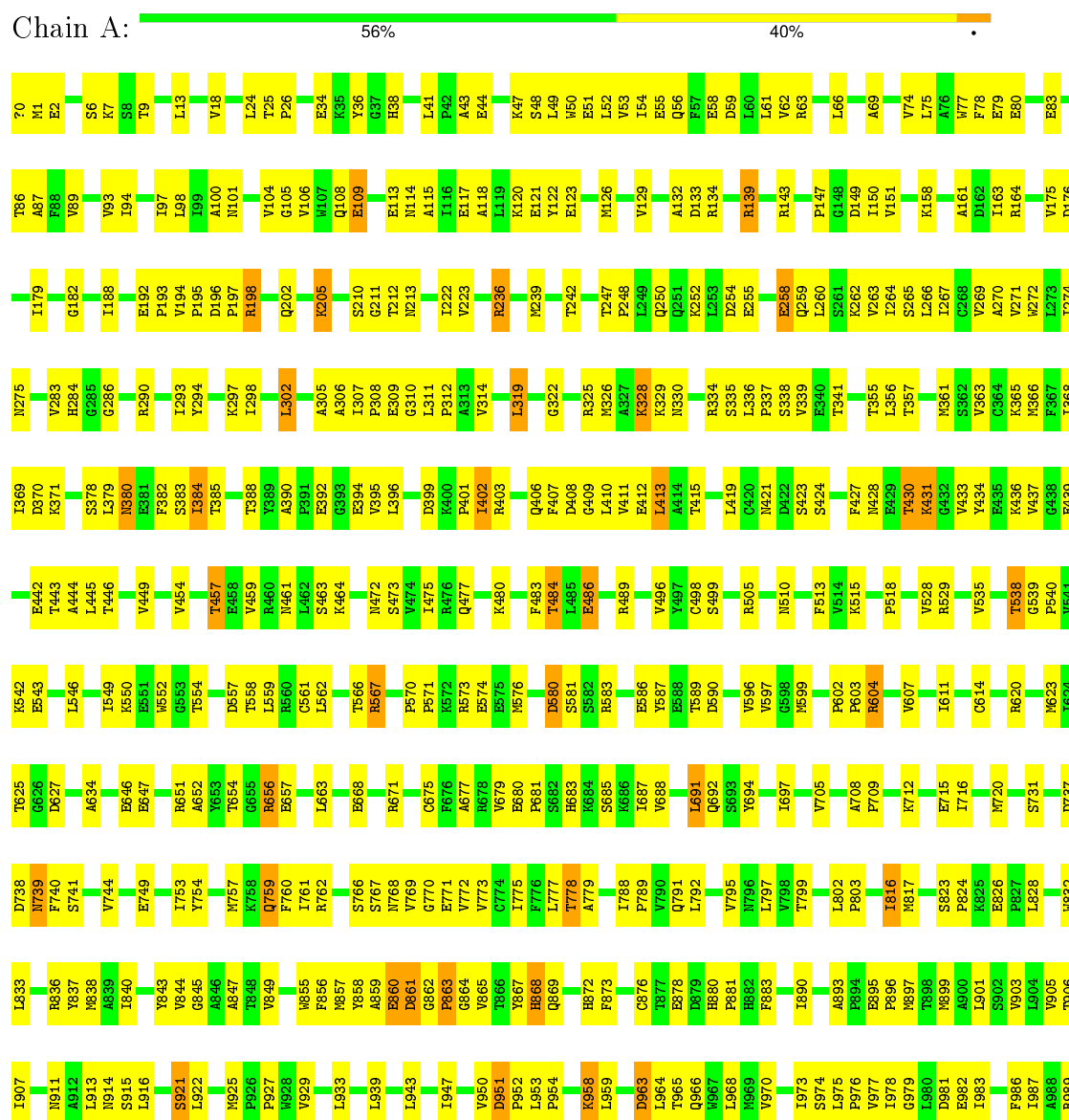
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	232	Total	O	0	0
			232	232		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.42 Å 71.42 Å 589.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.50	Depositor
% Data completeness (in resolution range)	98.8 (14.97-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8024	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

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: MG, TG1, ACE, NA, ACP, PTY

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	0.38	0/7813	0.61	1/10594 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	413	LEU	CA-CB-CG	5.54	128.05	115.30

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	7674	0	7765	342	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	31	0	14	1	0
5	A	46	0	50	2	0
6	A	38	0	22	0	0
7	A	232	0	0	7	0
All	All	8024	0	7851	342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 22.

All (342) 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:663:LEU:HD12	1:A:663:LEU:H	1.32	0.93
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.49	0.92
1:A:484:THR:HB	1:A:496:VAL:HG12	1.53	0.91
1:A:328:LYS:NZ	1:A:328:LYS:HA	1.85	0.90
1:A:739:ASN:HD22	1:A:740:PHE:N	1.72	0.87
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.58	0.86
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.61	0.81
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.63	0.78
1:A:328:LYS:HZ3	1:A:328:LYS:HA	1.47	0.78
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.64	0.78
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.47	0.77
1:A:49:LEU:O	1:A:53:VAL:HG23	1.86	0.75
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.51	0.74
1:A:963:ASP:H	1:A:966:GLN:NE2	1.85	0.74
1:A:205:LYS:HB3	1:A:205:LYS:NZ	2.03	0.73
1:A:843:TYR:OH	1:A:976:PRO:HG2	1.89	0.73
1:A:986:PHE:HA	1:A:989:ARG:HH21	1.55	0.72
1:A:395:VAL:O	1:A:396:LEU:HD23	1.90	0.71
1:A:964:LEU:O	1:A:968:LEU:HD13	1.90	0.71
1:A:179:ILE:O	1:A:705:VAL:HG22	1.91	0.71
1:A:963:ASP:H	1:A:966:GLN:HE21	1.37	0.70
1:A:589:THR:HG22	1:A:590:ASP:N	2.05	0.70
1:A:370:ASP:HB3	1:A:378:SER:OG	1.92	0.70
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.73	0.69
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.73	0.69
1:A:396:LEU:HD22	1:A:401:PRO:HG3	1.75	0.68
1:A:550:LYS:O	1:A:554:THR:HB	1.94	0.68
1:A:176:ASP:O	1:A:212:THR:HG23	1.92	0.68
1:A:880:HIS:N	1:A:881:PRO:HD2	2.09	0.67
1:A:457:THR:O	1:A:459:VAL:HG13	1.95	0.66
1:A:762:ARG:HD2	1:A:833:LEU:HD21	1.77	0.66
1:A:979:GLY:O	1:A:983:ILE:HG13	1.96	0.66
1:A:759:GLN:HG3	1:A:915:SER:O	1.95	0.66
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.78	0.66
1:A:283:VAL:HG13	1:A:284:HIS:ND1	2.11	0.65
1:A:188:ILE:HD13	1:A:486:GLU:HG2	1.76	0.65
1:A:338:SER:HA	1:A:341:THR:HG22	1.78	0.65
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:GLU:H	1:A:860:GLU:CD	2.01	0.64
1:A:974:SER:C	1:A:976:PRO:HD2	2.17	0.64
1:A:436:LYS:HB2	1:A:443:THR:HG21	1.79	0.63
1:A:604:ARG:O	1:A:607:VAL:HG22	1.99	0.63
1:A:847:ALA:HA	1:A:973:ILE:HD11	1.79	0.63
1:A:571:PRO:HG2	1:A:576:MET:SD	2.38	0.63
1:A:663:LEU:CD1	1:A:663:LEU:H	2.10	0.63
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.80	0.63
1:A:242:THR:HB	1:A:712:LYS:HD3	1.79	0.62
1:A:55:GLU:HA	1:A:58:GLU:HG3	1.80	0.62
1:A:52:LEU:HD23	1:A:106:VAL:HG13	1.79	0.62
1:A:293:ILE:O	1:A:297:LYS:HB2	2.00	0.62
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.81	0.62
1:A:983:ILE:O	1:A:987:ILE:HG13	2.00	0.62
1:A:855:TRP:HA	1:A:859:ALA:CB	2.30	0.61
1:A:48:SER:OG	1:A:51:GLU:HG3	1.99	0.61
1:A:922:LEU:HD22	1:A:927:PRO:HG3	1.82	0.61
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.00	0.61
1:A:749:GLU:O	1:A:753:ILE:HG12	2.01	0.61
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.35	0.61
1:A:446:THR:O	1:A:449:VAL:HG22	2.00	0.61
1:A:607:VAL:O	1:A:611:ILE:HG12	2.00	0.61
1:A:739:ASN:C	1:A:739:ASN:HD22	2.03	0.61
1:A:986:PHE:CA	1:A:989:ARG:HH21	2.13	0.61
1:A:188:ILE:H	1:A:188:ILE:HD12	1.65	0.61
1:A:654:THR:HA	1:A:677:ALA:O	2.01	0.61
1:A:668:GLU:O	1:A:671:ARG:HG2	2.00	0.61
1:A:265:SER:O	1:A:269:VAL:HG23	2.01	0.60
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.67	0.60
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.37	0.60
1:A:897:MET:HE1	1:A:958:LYS:HG2	1.84	0.60
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.32	0.60
1:A:267:ILE:HD11	5:A:1003:TG1:H191	1.85	0.59
1:A:52:LEU:HG	1:A:106:VAL:HG22	1.83	0.59
1:A:403:ARG:HB3	1:A:406:GLN:OE1	2.01	0.59
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.84	0.59
1:A:192:GLU:HG3	1:A:193:PRO:HD2	1.84	0.59
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.84	0.59
1:A:133:ASP:O	1:A:134:ARG:HG3	2.03	0.59
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.85	0.59
1:A:567:ARG:CD	1:A:570:PRO:HA	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.16	0.59
1:A:828:LEU:H	1:A:828:LEU:HD12	1.67	0.59
1:A:212:THR:HG22	1:A:213:ASN:N	2.17	0.58
1:A:589:THR:CG2	1:A:590:ASP:N	2.66	0.58
1:A:264:ILE:HG23	1:A:302:LEU:HD12	1.85	0.58
1:A:247:THR:H	1:A:250:GLN:NE2	2.02	0.58
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.04	0.58
1:A:583:ARG:O	1:A:586:GLU:HG2	2.04	0.58
1:A:305:ALA:HB1	1:A:771:GLU:HB3	1.84	0.58
1:A:737:ASP:O	1:A:738:ASP:HB2	2.03	0.58
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.34	0.57
1:A:41:LEU:H	1:A:41:LEU:HD22	1.69	0.57
1:A:428:ASN:ND2	1:A:431:LYS:HD3	2.18	0.57
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.86	0.57
1:A:114:ASN:HD21	1:A:117:GLU:HG3	1.69	0.57
1:A:192:GLU:OE1	1:A:580:ASP:HB3	2.04	0.57
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.06	0.56
1:A:205:LYS:HB3	1:A:205:LYS:HZ2	1.69	0.56
1:A:188:ILE:HD12	1:A:188:ILE:N	2.20	0.56
1:A:260:LEU:HD13	5:A:1003:TG1:H252	1.88	0.56
1:A:668:GLU:CD	1:A:671:ARG:HD3	2.27	0.56
1:A:916:LEU:HD21	1:A:933:LEU:HD22	1.87	0.56
1:A:122:TYR:O	1:A:211:GLY:HA2	2.07	0.55
1:A:716:ILE:N	1:A:716:ILE:HD12	2.21	0.55
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.42	0.55
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.34	0.55
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.88	0.55
1:A:757:MET:HA	1:A:760:PHE:CE2	2.42	0.55
1:A:656:ARG:HG2	1:A:656:ARG:HH11	1.72	0.55
1:A:269:VAL:O	1:A:272:TRP:HB3	2.08	0.54
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.89	0.54
1:A:100:ALA:O	1:A:104:VAL:HG23	2.07	0.54
1:A:712:LYS:HA	7:A:2036:HOH:O	2.06	0.54
1:A:52:LEU:CD2	1:A:106:VAL:HG13	2.37	0.54
1:A:89:VAL:O	1:A:93:VAL:HG23	2.06	0.54
1:A:311:LEU:N	1:A:312:PRO:HD2	2.23	0.54
1:A:720:MET:HE3	1:A:738:ASP:CB	2.38	0.54
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.88	0.54
1:A:720:MET:HE1	1:A:738:ASP:O	2.08	0.54
1:A:1:MET:CE	1:A:7:LYS:HG3	2.38	0.54
1:A:833:LEU:HD11	1:A:837:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ALA:HA	1:A:210:SER:HB2	1.89	0.54
1:A:328:LYS:HA	1:A:328:LYS:HZ2	1.72	0.54
1:A:2:GLU:CD	1:A:2:GLU:H	2.11	0.53
1:A:357:THR:HA	1:A:603:PRO:HA	1.91	0.53
1:A:402:ILE:HD13	1:A:402:ILE:H	1.72	0.53
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.91	0.53
1:A:890:ILE:C	1:A:890:ILE:HD12	2.29	0.53
1:A:41:LEU:N	1:A:41:LEU:HD22	2.24	0.53
1:A:867:TYR:O	1:A:869:GLN:HG2	2.07	0.53
1:A:836:ARG:O	1:A:840:ILE:HG12	2.09	0.53
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.34	0.52
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.45	0.52
1:A:589:THR:CG2	1:A:590:ASP:H	2.23	0.52
1:A:13:LEU:HD23	1:A:222:ILE:HD12	1.91	0.52
1:A:762:ARG:HD3	1:A:828:LEU:O	2.10	0.52
1:A:863:PRO:C	1:A:865:VAL:H	2.12	0.52
1:A:325:ARG:HD2	1:A:749:GLU:OE2	2.09	0.52
1:A:427:PHE:CZ	1:A:464:LYS:HG2	2.44	0.52
1:A:878:GLU:HB3	1:A:880:HIS:CD2	2.44	0.52
1:A:449:VAL:HG21	1:A:472:ASN:OD1	2.10	0.52
1:A:309:GLU:HB2	1:A:797:LEU:HD11	1.91	0.52
1:A:604:ARG:HB2	1:A:607:VAL:HG13	1.92	0.52
1:A:1:MET:HE2	1:A:7:LYS:HG3	1.92	0.52
1:A:97:ILE:O	1:A:101:ASN:HB2	2.09	0.52
1:A:421:ASN:OD1	1:A:442:GLU:HB3	2.10	0.52
1:A:47:LYS:HD2	1:A:109:GLU:OE2	2.10	0.51
1:A:754:TYR:HA	1:A:757:MET:CE	2.40	0.51
1:A:212:THR:CG2	1:A:213:ASN:N	2.73	0.51
1:A:896:PRO:O	1:A:899:MET:HB2	2.10	0.51
1:A:431:LYS:HD2	1:A:431:LYS:H	1.75	0.51
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.39	0.51
1:A:828:LEU:HD12	1:A:828:LEU:N	2.25	0.51
1:A:856:PHE:CZ	1:A:896:PRO:HG3	2.45	0.51
1:A:126:MET:HG3	1:A:139:ARG:NH1	2.26	0.51
1:A:860:GLU:O	1:A:862:GLY:N	2.44	0.51
1:A:604:ARG:NH1	1:A:604:ARG:CG	2.73	0.51
1:A:267:ILE:O	1:A:271:VAL:HG23	2.10	0.51
1:A:294:TYR:O	1:A:298:ILE:HG23	2.10	0.51
1:A:788:ILE:HG13	1:A:791:GLN:HG3	1.94	0.51
1:A:950:VAL:O	1:A:954:PRO:HD2	2.11	0.50
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:SER:O	1:A:477:GLN:HG2	2.11	0.50
1:A:262:LYS:O	1:A:266:LEU:HD23	2.11	0.50
1:A:338:SER:HA	1:A:341:THR:CG2	2.41	0.50
1:A:310:GLY:O	1:A:314:VAL:HG23	2.11	0.50
1:A:656:ARG:NH1	1:A:656:ARG:HG2	2.27	0.50
1:A:198:ARG:HD3	1:A:198:ARG:O	2.12	0.50
1:A:79:GLU:HG2	1:A:80:GLU:N	2.27	0.50
1:A:335:SER:OG	1:A:337:PRO:HD2	2.12	0.50
1:A:120:LYS:HA	1:A:123:GLU:HG2	1.93	0.50
1:A:975:LEU:N	1:A:976:PRO:HD2	2.27	0.50
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.93	0.50
1:A:895:GLU:N	1:A:896:PRO:HD2	2.26	0.49
1:A:515:LYS:HE3	4:A:1002:ACP:N1	2.27	0.49
1:A:499:SER:HB3	1:A:510:ASN:ND2	2.28	0.49
1:A:589:THR:HG22	1:A:590:ASP:H	1.75	0.49
1:A:777:LEU:C	1:A:779:ALA:H	2.14	0.49
1:A:428:ASN:OD1	1:A:430:THR:HB	2.12	0.49
1:A:865:VAL:O	1:A:868:HIS:HB2	2.13	0.49
1:A:925:MET:HG3	1:A:929:VAL:HG21	1.95	0.49
1:A:6:SER:HA	1:A:194:VAL:O	2.12	0.49
1:A:380:ASN:HB3	1:A:382:PHE:CE1	2.48	0.49
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.13	0.49
1:A:542:LYS:O	1:A:546:LEU:HG	2.13	0.49
1:A:855:TRP:CE3	1:A:896:PRO:HD3	2.47	0.48
1:A:845:GLY:O	1:A:849:VAL:HG23	2.12	0.48
1:A:43:ALA:HA	1:A:120:LYS:NZ	2.27	0.48
1:A:778:THR:HG23	1:A:778:THR:O	2.14	0.48
1:A:832:TRP:O	1:A:836:ARG:HG3	2.14	0.48
1:A:867:TYR:C	1:A:869:GLN:H	2.17	0.48
1:A:319:LEU:CD1	1:A:339:VAL:HG21	2.44	0.48
1:A:858:TYR:N	1:A:858:TYR:CD1	2.81	0.48
1:A:480:LYS:O	1:A:498:CYS:HA	2.14	0.48
1:A:873:PHE:HD2	1:A:876:CYS:H	1.62	0.48
1:A:74:VAL:O	1:A:77:TRP:HB3	2.14	0.47
1:A:322:GLY:O	1:A:325:ARG:HB3	2.14	0.47
1:A:838:MET:HA	1:A:838:MET:CE	2.44	0.47
1:A:816:ILE:HG22	1:A:817:MET:HG2	1.95	0.47
1:A:970:VAL:O	1:A:973:ILE:HG22	2.15	0.47
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.45	0.47
1:A:18:VAL:CG2	1:A:24:LEU:HD23	2.45	0.47
1:A:757:MET:HG2	1:A:760:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ALA:HB1	1:A:239:MET:CE	2.44	0.47
1:A:161:ALA:CA	1:A:210:SER:HB2	2.45	0.47
1:A:202:GLN:OE1	1:A:489:ARG:HD3	2.15	0.47
1:A:757:MET:O	1:A:761:ILE:HG13	2.14	0.46
1:A:305:ALA:HB2	1:A:792:LEU:HD13	1.96	0.46
1:A:847:ALA:O	1:A:903:VAL:HG11	2.15	0.46
1:A:576:MET:HE3	1:A:587:TYR:HB3	1.97	0.46
1:A:326:MET:CE	1:A:339:VAL:HG12	2.46	0.46
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.45	0.46
1:A:561:CYS:HB2	7:A:2168:HOH:O	2.16	0.46
1:A:652:ALA:HA	1:A:675:CYS:O	2.16	0.46
1:A:865:VAL:HB	1:A:868:HIS:CD2	2.50	0.46
1:A:44:GLU:HB3	1:A:117:GLU:OE2	2.15	0.46
1:A:483:PHE:HE1	1:A:573:ARG:HD3	1.81	0.46
1:A:329:LYS:O	1:A:330:ASN:HB2	2.15	0.46
1:A:334:ARG:HD3	1:A:731:SER:O	2.16	0.46
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.98	0.45
1:A:434:TYR:OH	1:A:464:LYS:HG3	2.16	0.45
1:A:380:ASN:ND2	1:A:407:PHE:CE2	2.84	0.45
1:A:118:ALA:O	1:A:121:GLU:HG3	2.17	0.45
1:A:697:ILE:N	1:A:697:ILE:HD12	2.31	0.45
1:A:771:GLU:O	1:A:775:ILE:HG12	2.16	0.45
1:A:424:SER:O	1:A:437:VAL:HG23	2.17	0.45
1:A:680:GLU:HB2	1:A:683:HIS:CE1	2.52	0.45
1:A:863:PRO:HG2	1:A:890:ILE:HD13	1.99	0.45
1:A:380:ASN:HD21	1:A:407:PHE:HE2	1.65	0.44
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.46	0.44
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.18	0.44
1:A:336:LEU:HB2	1:A:337:PRO:HD3	2.00	0.44
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.79	0.44
1:A:697:ILE:HD11	1:A:824:PRO:HG2	1.98	0.44
1:A:921:SER:HB2	1:A:989:ARG:HH12	1.82	0.44
1:A:614:CYS:SG	1:A:744:VAL:HG22	2.58	0.44
1:A:720:MET:CE	1:A:738:ASP:HB3	2.47	0.44
1:A:769:VAL:O	1:A:773:VAL:HG23	2.18	0.44
1:A:150:ILE:HD12	1:A:150:ILE:N	2.33	0.44
1:A:679:VAL:CG1	1:A:683:HIS:HB2	2.42	0.44
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.96	0.44
1:A:388:THR:CG2	1:A:390:ALA:HB3	2.48	0.44
1:A:86:THR:HA	1:A:89:VAL:CG2	2.48	0.44
1:A:309:GLU:CB	1:A:797:LEU:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:MET:CG	1:A:929:VAL:HG21	2.48	0.43
1:A:939:LEU:O	1:A:943:LEU:HG	2.18	0.43
1:A:739:ASN:ND2	1:A:741:SER:H	2.16	0.43
1:A:986:PHE:HA	1:A:989:ARG:NH2	2.30	0.43
1:A:385:THR:OG1	1:A:394:GLU:HG2	2.18	0.43
1:A:775:ILE:HA	1:A:778:THR:HG22	2.00	0.43
1:A:611:LEU:HD22	1:A:307:ILE:HD12	2.00	0.43
1:A:906:THR:HG22	1:A:974:SER:HB3	2.00	0.43
1:A:893:ALA:O	1:A:896:PRO:HD2	2.18	0.43
1:A:687:ILE:HG22	1:A:691:LEU:HD22	2.00	0.43
1:A:762:ARG:O	1:A:766:SER:HB2	2.18	0.43
1:A:754:TYR:HA	1:A:757:MET:HE3	2.00	0.43
1:A:768:ASN:O	1:A:772:VAL:HG23	2.17	0.43
1:A:558:THR:HG22	1:A:634:ALA:HB1	2.01	0.43
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.99	0.43
1:A:431:LYS:O	1:A:433:VAL:HG13	2.19	0.43
1:A:977:VAL:HG13	1:A:978:ILE:N	2.33	0.43
1:A:363:VAL:HA	1:A:599:MET:HA	2.01	0.43
1:A:394:GLU:HG3	1:A:396:LEU:HD21	2.00	0.43
1:A:688:VAL:O	1:A:692:GLN:HG3	2.19	0.43
1:A:557:ASP:HB3	1:A:559:LEU:HG	2.01	0.43
1:A:596:VAL:HG12	1:A:597:VAL:N	2.33	0.43
1:A:880:HIS:N	1:A:881:PRO:CD	2.80	0.42
1:A:104:VAL:HG12	1:A:108:GLN:HE21	1.85	0.42
1:A:188:ILE:CD1	1:A:486:GLU:HG2	2.48	0.42
1:A:720:MET:HE3	1:A:738:ASP:CG	2.40	0.42
1:A:423:SER:OG	1:A:442:GLU:HB2	2.18	0.42
1:A:671:ARG:HD2	1:A:694:TYR:OH	2.18	0.42
1:A:126:MET:CE	1:A:139:ARG:HD3	2.49	0.42
1:A:290:ARG:HH11	1:A:290:ARG:HB3	1.84	0.42
1:A:390:ALA:C	1:A:392:GLU:H	2.23	0.42
1:A:326:MET:HE3	1:A:339:VAL:HG12	2.01	0.42
1:A:897:MET:HE3	1:A:958:LYS:HB3	2.02	0.42
1:A:795:VAL:HA	1:A:799:THR:HB	2.02	0.42
1:A:66:LEU:HA	1:A:98:LEU:HD11	2.02	0.42
1:A:236:ARG:HD3	1:A:236:ARG:C	2.39	0.42
1:A:539:GLY:O	1:A:543:GLU:HG2	2.19	0.42
1:A:767:SER:O	1:A:770:GLY:N	2.53	0.42
1:A:259:GLN:O	1:A:263:VAL:HG23	2.20	0.42
1:A:833:LEU:HA	1:A:836:ARG:HD3	2.01	0.42
1:A:120:LYS:HE2	7:A:2041:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:TYR:HA	1:A:757:MET:HE2	2.02	0.42
1:A:844:VAL:HG22	1:A:907:ILE:HG21	2.02	0.42
1:A:901:LEU:HD22	1:A:959:LEU:HD21	2.02	0.42
1:A:270:ALA:O	1:A:274:ILE:HG13	2.20	0.42
1:A:646:GLU:OE1	1:A:651:ARG:NH1	2.53	0.42
1:A:911:ASN:HA	1:A:914:ASN:ND2	2.25	0.41
1:A:715:GLU:CB	1:A:716:ILE:HD12	2.49	0.41
1:A:83:GLU:O	1:A:87:ALA:HB2	2.20	0.41
1:A:182:GLY:HA2	7:A:2077:HOH:O	2.19	0.41
1:A:963:ASP:C	1:A:965:THR:N	2.73	0.41
1:A:554:THR:HG21	7:A:2162:HOH:O	2.20	0.41
1:A:867:TYR:O	1:A:869:GLN:N	2.53	0.41
1:A:38:HIS:CE1	1:A:143:ARG:NH1	2.88	0.41
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.50	0.41
1:A:260:LEU:O	1:A:264:ILE:HG13	2.20	0.41
1:A:427:PHE:CE2	1:A:464:LYS:HG2	2.55	0.41
1:A:59:ASP:HB3	1:A:62:VAL:HG22	2.02	0.41
1:A:513:PHE:CD1	1:A:566:THR:HG22	2.51	0.41
1:A:75:LEU:O	1:A:79:GLU:HB2	2.20	0.41
1:A:63:ARG:HH11	1:A:63:ARG:HG2	1.85	0.41
1:A:708:ALA:HB3	1:A:709:PRO:HD3	2.02	0.41
1:A:951:ASP:O	1:A:952:PRO:C	2.58	0.41
1:A:412:GLU:OE1	1:A:529:ARG:CD	2.68	0.41
1:A:415:THR:HA	1:A:475:ILE:HG21	2.01	0.41
1:A:43:ALA:HA	1:A:120:LYS:HZ1	1.84	0.41
1:A:195:PRO:HG2	7:A:2172:HOH:O	2.20	0.41
1:A:857:MET:O	1:A:864:GLY:HA2	2.21	0.41
1:A:25:THR:HB	1:A:26:PRO:HD2	2.03	0.41
1:A:788:ILE:HG12	1:A:791:GLN:OE1	2.20	0.41
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.89	0.41
1:A:0:ACE:H3	1:A:36:TYR:CE1	2.54	0.41
1:A:122:TYR:CE1	1:A:179:ILE:HG21	2.56	0.41
1:A:663:LEU:HD12	1:A:663:LEU:N	2.15	0.41
1:A:212:THR:CG2	1:A:213:ASN:H	2.34	0.41
1:A:860:GLU:C	1:A:862:GLY:H	2.23	0.41
1:A:627:ASP:O	1:A:677:ALA:HB1	2.21	0.41
1:A:867:TYR:C	1:A:869:GLN:N	2.74	0.41
1:A:266:LEU:HD13	1:A:266:LEU:HA	1.96	0.41
1:A:773:VAL:O	1:A:777:LEU:HG	2.21	0.41
1:A:379:LEU:HD23	1:A:379:LEU:N	2.36	0.41
1:A:408:ASP:O	1:A:409:GLY:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:SER:C	1:A:384:ILE:HD13	2.41	0.41
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.51	0.41
1:A:248:PRO:O	1:A:252:LYS:HG2	2.21	0.41
1:A:623:MET:HE3	1:A:625:THR:HG21	2.03	0.41
1:A:18:VAL:HG23	1:A:24:LEU:HD23	2.03	0.40
1:A:499:SER:HB3	1:A:510:ASN:HD21	1.85	0.40
1:A:461:ASN:HA	1:A:461:ASN:HD22	1.66	0.40
1:A:254:ASP:O	1:A:258:GLU:HG2	2.21	0.40
1:A:855:TRP:CZ3	1:A:896:PRO:HD3	2.57	0.40
1:A:44:GLU:HA	7:A:2035:HOH:O	2.22	0.40
1:A:899:MET:O	1:A:903:VAL:HG23	2.21	0.40
1:A:366:MET:HA	1:A:596:VAL:O	2.22	0.40
1:A:966:GLN:HE21	1:A:966:GLN:HB2	1.64	0.40
1:A:408:ASP:HA	1:A:411:VAL:HG23	2.03	0.40
1:A:388:THR:HG21	1:A:390:ALA:HB3	2.04	0.40
1:A:538:THR:HB	1:A:540:PRO:HD2	2.03	0.40
1:A:823:SER:O	1:A:826:GLU:HB3	2.21	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	993/995 (100%)	906 (91%)	72 (7%)	15 (2%)	13	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	883	PHE
1	A	463	SER
1	A	861	ASP
1	A	951	ASP

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Mol	Chain	Res	Type
1	A	132	ALA
1	A	430	THR
1	A	457	THR
1	A	863	PRO
1	A	868	HIS
1	A	78	PHE
1	A	778	THR
1	A	860	GLU
1	A	505	ARG
1	A	789	PRO
1	A	286	GLY

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	840/840 (100%)	788 (94%)	52 (6%)	23	41

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	34	GLU
1	A	109	GLU
1	A	113	GLU
1	A	139	ARG
1	A	158	LYS
1	A	164	ARG
1	A	198	ARG
1	A	205	LYS
1	A	236	ARG
1	A	255	GLU
1	A	258	GLU
1	A	275	ASN
1	A	302	LEU
1	A	319	LEU

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Mol	Chain	Res	Type
1	A	328	LYS
1	A	356	LEU
1	A	371	LYS
1	A	380	ASN
1	A	384	ILE
1	A	399	ASP
1	A	402	ILE
1	A	413	LEU
1	A	431	LYS
1	A	439	GLU
1	A	445	LEU
1	A	484	THR
1	A	486	GLU
1	A	535	VAL
1	A	538	THR
1	A	562	LEU
1	A	567	ARG
1	A	574	GLU
1	A	580	ASP
1	A	581	SER
1	A	604	ARG
1	A	620	ARG
1	A	647	GLU
1	A	656	ARG
1	A	685	SER
1	A	691	LEU
1	A	739	ASN
1	A	759	GLN
1	A	816	ILE
1	A	861	ASP
1	A	872	HIS
1	A	921	SER
1	A	958	LYS
1	A	963	ASP
1	A	981	ASP
1	A	982	GLU
1	A	990	ASN

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

Mol	Chain	Res	Type
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	380	ASN
1	A	461	ASN
1	A	510	ASN
1	A	612	GLN
1	A	739	ASN
1	A	869	GLN
1	A	872	HIS
1	A	880	HIS
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	ACP	A	1002	2	25,33,33	2.04	4 (16%)	31,52,52	2.21	6 (19%)
5	TG1	A	1003	-	43,48,48	1.92	9 (20%)	42,72,72	1.85	9 (21%)
6	PTY	A	1011	-	17,18,49	1.26	3 (17%)	18,23,54	1.35	2 (11%)
6	PTY	A	1012	-	17,18,49	1.18	3 (17%)	18,23,54	1.25	2 (11%)

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	ACP	A	1002	2	-	0/15/38/38	0/3/3/3
5	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
6	PTY	A	1011	-	-	0/20/20/53	0/0/0/0
6	PTY	A	1012	-	-	0/20/20/53	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ACP	PB-O2B	-3.98	1.46	1.56
4	A	1002	ACP	PG-O2G	-2.21	1.49	1.54
6	A	1012	PTY	P1-O13	2.07	1.58	1.51
5	A	1003	TG1	C1-C5	2.15	1.54	1.51
6	A	1011	PTY	P1-O13	2.16	1.59	1.51
6	A	1011	PTY	C5-C6	2.38	1.57	1.50
6	A	1012	PTY	C1-C6	2.39	1.57	1.50
6	A	1012	PTY	C5-C6	2.44	1.57	1.50
5	A	1003	TG1	C7-C6	2.51	1.58	1.54
5	A	1003	TG1	C1-C2	2.82	1.59	1.54
5	A	1003	TG1	C34-C11	2.89	1.57	1.53
5	A	1003	TG1	C9-C8	2.89	1.55	1.52
6	A	1011	PTY	C1-C6	2.95	1.59	1.50
5	A	1003	TG1	O6-C7	2.99	1.48	1.43
4	A	1002	ACP	C2-N3	3.10	1.37	1.32
5	A	1003	TG1	C11-C7	3.48	1.59	1.55
5	A	1003	TG1	O4-C21	4.45	1.31	1.21
4	A	1002	ACP	PB-O3A	6.93	1.66	1.58
5	A	1003	TG1	C7-C8	7.74	1.64	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ACP	N3-C2-N1	-7.65	123.04	128.89
4	A	1002	ACP	C5'-C4'-C3'	-5.03	95.23	115.21
5	A	1003	TG1	O12-C12-C11	-4.68	123.96	128.26
5	A	1003	TG1	O5-C6-C7	-3.04	101.39	104.08
5	A	1003	TG1	O11-C11-C12	-2.31	98.99	106.08
5	A	1003	TG1	C23-C22-C21	-2.22	110.27	116.04
6	A	1012	PTY	O4-C1-C6	2.07	114.27	108.69
4	A	1002	ACP	O2A-PA-O5'	2.24	119.76	108.46
5	A	1003	TG1	C24-C22-C21	2.45	131.16	120.67
4	A	1002	ACP	O2B-PB-C3B	2.51	117.84	106.88
5	A	1003	TG1	O3-C21-O4	2.53	128.35	123.30
5	A	1003	TG1	O5-C12-O12	2.63	125.46	121.62
6	A	1011	PTY	O4-C1-C6	2.69	115.93	108.69
4	A	1002	ACP	C4-C5-N7	3.11	112.34	109.48
6	A	1012	PTY	O7-C8-C11	3.12	116.99	111.10
6	A	1011	PTY	O7-C8-C11	3.43	117.56	111.10
5	A	1003	TG1	C2-O1-C13	4.37	125.48	117.75
4	A	1002	ACP	O5'-C5'-C4'	5.01	127.60	109.12
5	A	1003	TG1	C10-O9-C32	6.03	134.28	121.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	ACP	1	0
5	A	1003	TG1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.