Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:46 AM GMT

PDB ID	:	2EAU
Title	:	Crystal structure of the SR CA2+-ATPASE with bound CPA in the presence of curcumin
Authors	:	Takahashi, M.; Kondou, Y.; Toyoshima, C.
Deposited on	:	2007-02-02
Resolution	:	2.80 Å(reported)

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

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

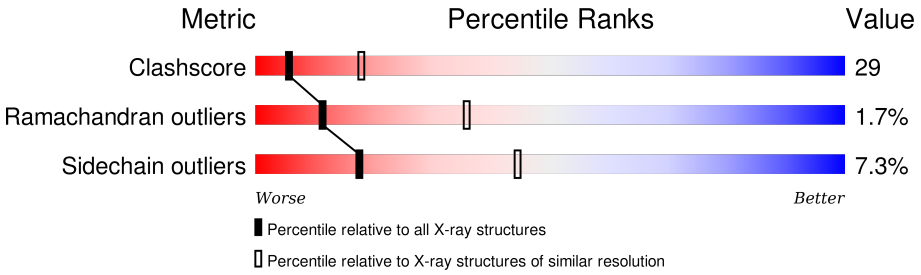
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	53% 42% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CZA	A	1005	X	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7756 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.

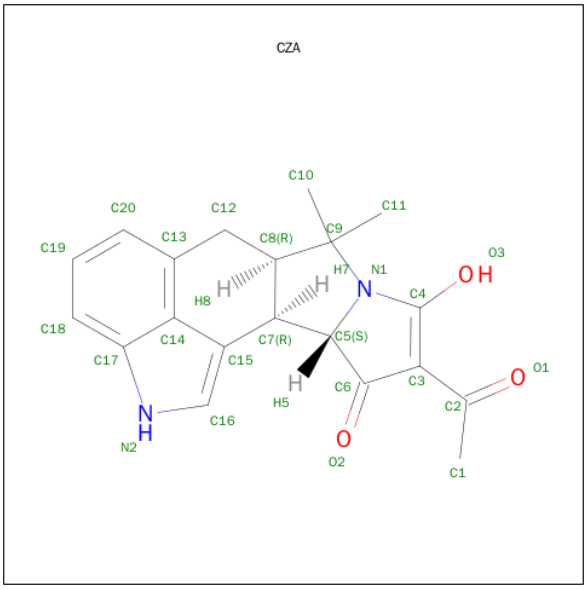
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	1	0	0
			7674	4878	1287	1452	57			

There is a discrepancy between the modelled and reference sequences:

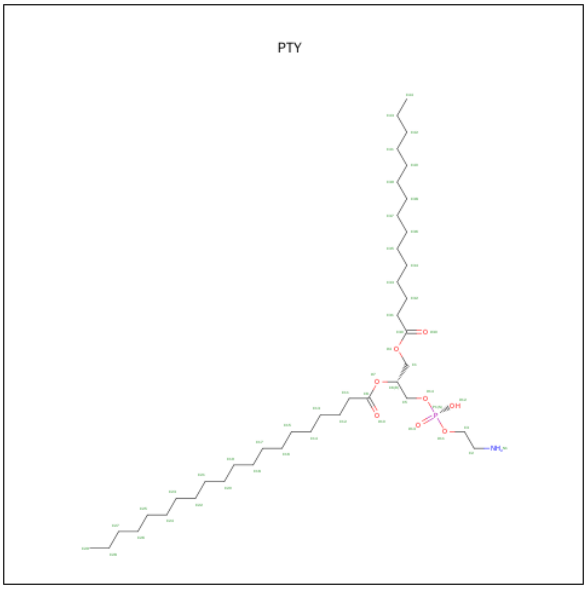
Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula: $C_{20}H_{20}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

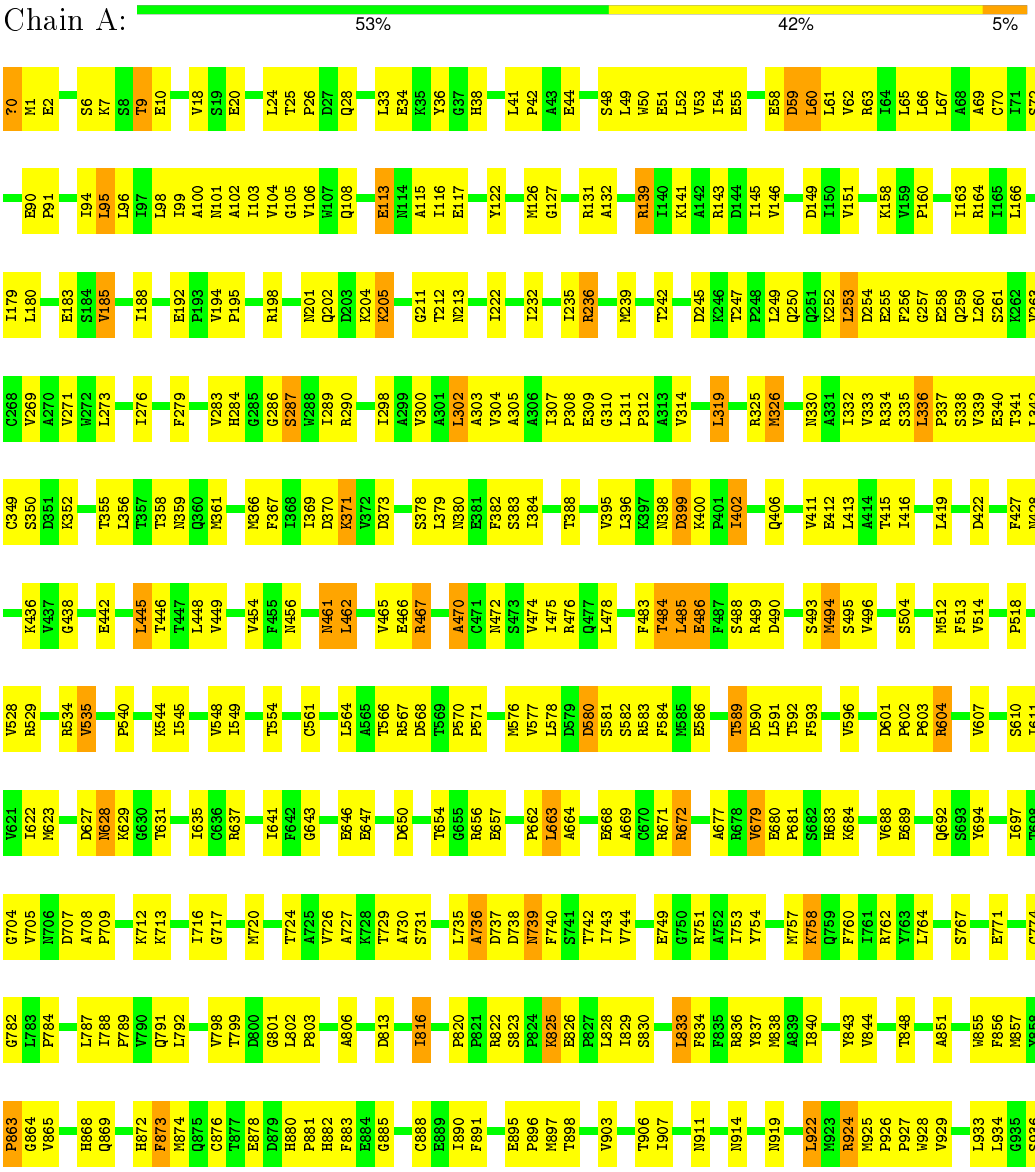
3 Residue-property plots (i)

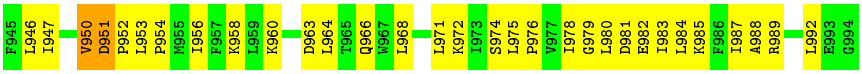
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

Chain A:




F945
L946
T947
V950
D951
P952
L953
P954
M955
I956
F957
K958
L959
K960
D963
I964
T965
Q966
M967
L968
L971
K972
I973
S974
L975
P976
W977
I978
G979
L980
D981
E982
I983
L984
K985
F986
I987
A988
R989
L992
E993
G994

4 Data and refinement statistics (i)

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	71.65Å 71.65Å 586.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.6 (15.00-2.80)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7756	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CZA, ACE, 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	0.53	1/7813 (0.0%)	0.66	2/10594 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	-24.41	0.78	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	0	ACE	C-N-CA	9.78	146.16	121.70
1	A	0	ACE	O-C-N	-6.93	111.62	122.70

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	7767	453	0
2	A	25	0	19	23	0
3	A	57	0	33	2	0
All	All	7756	0	7819	453	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 (453) 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:101:ASN:HB3	2:A:1005:CZA:C18	1.69	1.21
1:A:0:ACE:CH3	1:A:1:MET:N	2.07	1.18
1:A:0:ACE:C	1:A:1:MET:CA	2.19	1.11
1:A:101:ASN:CB	2:A:1005:CZA:C18	2.34	1.04
1:A:101:ASN:HD22	2:A:1005:CZA:C19	1.77	0.98
1:A:101:ASN:HB3	2:A:1005:CZA:H18	1.45	0.96
1:A:271:VAL:HG11	1:A:298:ILE:HD11	1.48	0.95
1:A:749:GLU:O	1:A:753:ILE:HG12	1.67	0.94
1:A:312:PRO:HD3	2:A:1005:CZA:H101	1.50	0.93
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.48	0.93
1:A:628:ASN:ND2	1:A:631:THR:H	1.68	0.90
1:A:762:ARG:HD2	1:A:837:TYR:CE2	2.06	0.90
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.55	0.89
1:A:312:PRO:HD3	2:A:1005:CZA:C10	2.01	0.89
1:A:122:TYR:O	1:A:158:LYS:HD3	1.72	0.88
1:A:865:VAL:HB	1:A:868:HIS:HB3	1.54	0.88
1:A:101:ASN:CB	2:A:1005:CZA:C19	2.53	0.87
1:A:526:ASN:ND2	1:A:590:ASP:HA	1.90	0.86
1:A:924:ARG:HA	1:A:924:ARG:HE	1.40	0.86
1:A:101:ASN:CB	2:A:1005:CZA:H18	2.04	0.86
1:A:914:ASN:HD21	1:A:978:ILE:HA	1.41	0.86
1:A:963:ASP:H	1:A:966:GLN:HE21	1.23	0.85
1:A:101:ASN:HD22	2:A:1005:CZA:C20	1.90	0.85
1:A:256:PHE:HD2	2:A:1005:CZA:H12	1.42	0.84
1:A:9:THR:HG22	1:A:10:GLU:OE2	1.78	0.83
1:A:183:GLU:HG3	1:A:183:GLU:O	1.79	0.83
1:A:256:PHE:HB3	2:A:1005:CZA:H11	1.62	0.82
1:A:101:ASN:HB2	2:A:1005:CZA:C19	2.10	0.82
1:A:0:ACE:C	1:A:1:MET:H1	0.55	0.80
1:A:101:ASN:HB2	2:A:1005:CZA:H19	1.64	0.80
1:A:968:LEU:O	1:A:972:LYS:HG3	1.81	0.80
1:A:467:ARG:HA	1:A:470:ALA:HB2	1.64	0.79
1:A:628:ASN:HD21	1:A:631:THR:H	1.29	0.79
1:A:65:LEU:HD21	1:A:94:ILE:HG23	1.64	0.79
1:A:298:ILE:O	1:A:302:LEU:HB2	1.84	0.76
1:A:180:LEU:HA	1:A:705:VAL:HG22	1.67	0.76
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ARG:HB3	1:A:816:ILE:CD1	2.17	0.75
1:A:963:ASP:H	1:A:966:GLN:NE2	1.84	0.75
1:A:922:LEU:HD22	1:A:927:PRO:HG3	1.68	0.75
1:A:252:LYS:HB3	1:A:828:LEU:HD11	1.68	0.75
1:A:925:MET:HA	1:A:925:MET:HE3	1.67	0.75
1:A:256:PHE:CD2	2:A:1005:CZA:H12	2.22	0.75
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.22	0.75
1:A:758:LYS:HE2	1:A:762:ARG:HH12	1.51	0.74
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.87	0.74
1:A:688:VAL:O	1:A:692:GLN:HG3	1.86	0.74
1:A:242:THR:HG21	1:A:712:LYS:HG3	1.69	0.73
1:A:101:ASN:ND2	2:A:1005:CZA:C19	2.51	0.73
1:A:754:TYR:CE2	1:A:822:ARG:HD2	2.23	0.73
1:A:739:ASN:HD22	1:A:740:PHE:N	1.86	0.73
1:A:415:THR:HA	1:A:475:ILE:HG21	1.70	0.73
1:A:212:THR:HG22	1:A:213:ASN:N	2.03	0.73
1:A:370:ASP:HB3	1:A:378:SER:OG	1.89	0.72
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.71	0.72
1:A:950:VAL:O	1:A:954:PRO:HD2	1.88	0.72
1:A:319:LEU:HB3	1:A:336:LEU:HD12	1.70	0.71
1:A:308:PRO:HG2	2:A:1005:CZA:H111	1.73	0.71
1:A:865:VAL:HB	1:A:868:HIS:CB	2.20	0.71
1:A:762:ARG:HD2	1:A:837:TYR:HE2	1.56	0.70
1:A:604:ARG:O	1:A:607:VAL:HG22	1.91	0.70
1:A:979:GLY:O	1:A:983:ILE:HG13	1.92	0.70
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.75	0.69
1:A:338:SER:HA	1:A:341:THR:HG22	1.75	0.69
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.74	0.69
1:A:751:ARG:HB3	1:A:816:ILE:HD12	1.75	0.69
1:A:0:ACE:CH3	1:A:1:MET:H3	1.89	0.68
1:A:256:PHE:HD2	2:A:1005:CZA:C1	2.06	0.68
1:A:101:ASN:HB2	2:A:1005:CZA:C18	2.21	0.68
1:A:336:LEU:O	1:A:339:VAL:HG22	1.93	0.68
1:A:264:ILE:CD1	1:A:307:ILE:HD11	2.23	0.68
1:A:514:VAL:HG21	1:A:591:LEU:HD22	1.75	0.68
1:A:963:ASP:N	1:A:966:GLN:HE21	1.90	0.67
1:A:534:ARG:HG2	1:A:535:VAL:N	2.08	0.67
1:A:0:ACE:C	1:A:1:MET:H2	1.22	0.67
1:A:472:ASN:HB3	1:A:476:ARG:HH12	1.60	0.67
1:A:952:PRO:O	1:A:956:ILE:HG13	1.95	0.67
1:A:61:LEU:HD13	1:A:307:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:OE1	1:A:185:VAL:HB	1.94	0.67
1:A:689:GLU:HB2	1:A:713:LYS:NZ	2.10	0.67
1:A:643:GLY:H	1:A:646:GLU:HG2	1.59	0.67
1:A:484:THR:HB	1:A:496:VAL:HG12	1.77	0.66
1:A:247:THR:H	1:A:250:GLN:NE2	1.93	0.66
1:A:589:THR:HG22	1:A:590:ASP:H	1.60	0.66
1:A:874:MET:HG2	1:A:891:PHE:CD2	2.31	0.66
1:A:941:MET:O	1:A:944:HIS:HB3	1.96	0.66
1:A:868:HIS:CE1	1:A:881:PRO:HB2	2.30	0.66
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.30	0.66
1:A:175:VAL:HG12	1:A:212:THR:HG21	1.78	0.66
1:A:963:ASP:HB3	1:A:966:GLN:HG3	1.77	0.65
1:A:975:LEU:N	1:A:976:PRO:HD2	2.10	0.65
1:A:116:ILE:HG12	1:A:239:MET:HB3	1.79	0.65
1:A:352:LYS:HG3	1:A:623:MET:HE2	1.77	0.65
1:A:720:MET:HB3	1:A:738:ASP:OD1	1.97	0.65
1:A:287:SER:OG	1:A:289:ILE:HG22	1.96	0.65
1:A:436:LYS:HE2	1:A:438:GLY:O	1.97	0.65
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.62	0.64
1:A:330:ASN:O	1:A:742:THR:HG21	1.97	0.64
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.80	0.64
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.80	0.64
1:A:174:ARG:CZ	1:A:188:ILE:HD11	2.28	0.64
1:A:984:LEU:HA	1:A:987:ILE:HD12	1.80	0.63
1:A:472:ASN:HB3	1:A:476:ARG:NH1	2.13	0.63
1:A:449:VAL:HG21	1:A:472:ASN:OD1	1.99	0.63
1:A:577:VAL:HG23	1:A:583:ARG:NH1	2.13	0.63
1:A:356:LEU:HD23	1:A:623:MET:CE	2.29	0.63
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.12	0.63
1:A:988:ALA:HA	1:A:992:LEU:HB2	1.81	0.63
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.81	0.63
1:A:462:LEU:HD22	1:A:466:GLU:HB3	1.79	0.63
1:A:478:LEU:H	1:A:478:LEU:HD12	1.64	0.62
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.29	0.62
1:A:212:THR:CG2	1:A:213:ASN:N	2.62	0.62
1:A:175:VAL:HG12	1:A:212:THR:CG2	2.30	0.62
1:A:176:ASP:O	1:A:212:THR:HG23	1.99	0.62
1:A:369:ILE:HD13	1:A:379:LEU:HD23	1.81	0.62
1:A:349:CYS:HA	1:A:622:ILE:O	1.99	0.62
1:A:806:ALA:HB1	1:A:933:LEU:HA	1.82	0.62
1:A:101:ASN:ND2	1:A:312:PRO:HG3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:HB3	1:A:51:GLU:HB2	1.83	0.61
1:A:67:LEU:O	1:A:70:CYS:HB2	2.01	0.61
1:A:267:ILE:HG21	1:A:302:LEU:HD11	1.83	0.61
1:A:650:ASP:O	1:A:672:ARG:HD2	2.00	0.61
1:A:704:GLY:HA2	1:A:724:THR:HG21	1.82	0.61
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.82	0.61
1:A:369:ILE:HD13	1:A:379:LEU:CD2	2.30	0.60
1:A:571:PRO:HG2	1:A:576:MET:SD	2.41	0.60
1:A:868:HIS:NE2	1:A:881:PRO:HB2	2.16	0.60
1:A:247:THR:HG23	1:A:250:GLN:NE2	2.16	0.60
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.82	0.60
1:A:788:ILE:HG13	1:A:791:GLN:HG3	1.83	0.60
1:A:428:ASN:ND2	1:A:431:LYS:HD3	2.17	0.60
1:A:252:LYS:HD3	1:A:255:GLU:OE2	2.01	0.60
1:A:946:LEU:HD12	1:A:950:VAL:HG21	1.83	0.60
1:A:256:PHE:CD2	2:A:1005:CZA:C1	2.84	0.59
1:A:256:PHE:HE2	1:A:260:LEU:HD22	1.67	0.59
1:A:102:ALA:O	1:A:106:VAL:HG23	2.01	0.59
1:A:762:ARG:CZ	1:A:833:LEU:HD23	2.33	0.59
1:A:332:ILE:HD12	1:A:332:ILE:N	2.17	0.59
1:A:65:LEU:HD23	1:A:65:LEU:O	2.01	0.59
1:A:964:LEU:O	1:A:968:LEU:HD13	2.03	0.59
1:A:235:ILE:HD13	1:A:705:VAL:O	2.02	0.59
1:A:813:ASP:O	1:A:816:ILE:HB	2.02	0.59
1:A:192:GLU:OE2	1:A:580:ASP:HB3	2.03	0.59
1:A:105:GLY:O	1:A:108:GLN:HG2	2.03	0.59
1:A:361:MET:SD	1:A:601:ASP:HB2	2.42	0.59
1:A:256:PHE:CE2	1:A:260:LEU:HD22	2.38	0.59
1:A:179:ILE:HD12	1:A:232:ILE:HD11	1.84	0.59
1:A:983:ILE:O	1:A:987:ILE:HG13	2.03	0.59
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.84	0.59
1:A:44:GLU:HB3	1:A:117:GLU:OE2	2.02	0.59
1:A:798:VAL:O	1:A:801:GLY:N	2.36	0.58
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.86	0.58
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.86	0.58
1:A:115:ALA:HB2	1:A:730:ALA:HB2	1.86	0.58
1:A:483:PHE:HE2	1:A:485:LEU:HD21	1.68	0.58
1:A:212:THR:CG2	1:A:213:ASN:H	2.16	0.57
1:A:663:LEU:H	1:A:663:LEU:HD12	1.67	0.57
1:A:325:ARG:HD2	1:A:749:GLU:OE2	2.03	0.57
1:A:671:ARG:HD2	1:A:694:TYR:OH	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:THR:HG21	1:A:960:LYS:O	2.05	0.57
1:A:758:LYS:O	1:A:762:ARG:HG3	2.04	0.57
1:A:878:GLU:HB3	1:A:880:HIS:CD2	2.40	0.57
1:A:880:HIS:N	1:A:881:PRO:HD2	2.20	0.56
1:A:356:LEU:HD23	1:A:623:MET:HE3	1.86	0.56
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.87	0.56
1:A:366:MET:HE1	1:A:448:LEU:HD21	1.87	0.56
1:A:65:LEU:HD22	1:A:98:LEU:HD21	1.86	0.56
1:A:65:LEU:HD22	1:A:98:LEU:HD11	1.87	0.56
1:A:345:THR:HA	1:A:697:ILE:HG22	1.88	0.56
1:A:20:GLU:HG3	1:A:166:LEU:HD13	1.88	0.56
1:A:311:LEU:N	1:A:312:PRO:HD2	2.20	0.56
1:A:869:GLN:HB3	1:A:872:HIS:HB2	1.87	0.56
1:A:212:THR:HG22	1:A:213:ASN:H	1.71	0.56
1:A:179:ILE:O	1:A:705:VAL:HG13	2.06	0.56
1:A:751:ARG:HB3	1:A:816:ILE:HD11	1.87	0.55
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.89	0.55
1:A:307:ILE:HG22	2:A:1005:CZA:H113	1.89	0.55
1:A:319:LEU:HG	1:A:339:VAL:CG2	2.36	0.55
1:A:44:GLU:HG3	1:A:44:GLU:O	2.06	0.55
1:A:396:LEU:HD13	1:A:399:ASP:HA	1.89	0.55
1:A:775:ILE:O	1:A:778:THR:HG22	2.07	0.55
1:A:300:VAL:O	1:A:304:VAL:HG23	2.07	0.55
1:A:514:VAL:HG21	1:A:591:LEU:CD2	2.37	0.55
1:A:0:ACE:C	1:A:1:MET:H3	1.11	0.55
1:A:55:GLU:O	1:A:58:GLU:HB3	2.07	0.54
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.89	0.54
1:A:330:ASN:HB3	1:A:736:ALA:HB3	1.89	0.54
1:A:326:MET:HE3	1:A:333:VAL:HG21	1.89	0.54
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.72	0.54
1:A:974:SER:C	1:A:976:PRO:HD2	2.27	0.54
1:A:326:MET:HE2	1:A:339:VAL:HG12	1.90	0.54
1:A:264:ILE:HD11	1:A:307:ILE:HD11	1.87	0.54
1:A:431:LYS:HB3	1:A:433:VAL:HG22	1.90	0.53
1:A:518:PRO:HD3	1:A:561:CYS:O	2.08	0.53
1:A:762:ARG:CZ	1:A:833:LEU:CD2	2.87	0.53
1:A:383:SER:C	1:A:384:ILE:HD13	2.28	0.53
1:A:116:ILE:CG1	1:A:239:MET:HB3	2.38	0.53
1:A:126:MET:SD	1:A:141:LYS:HD3	2.48	0.53
1:A:0:ACE:CH3	1:A:1:MET:H2	2.01	0.53
1:A:739:ASN:C	1:A:739:ASN:HD22	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LEU:O	1:A:737:ASP:N	2.42	0.53
1:A:963:ASP:CB	1:A:966:GLN:HE21	2.22	0.53
1:A:762:ARG:HD3	1:A:829:ILE:HG12	1.91	0.52
1:A:25:THR:HB	1:A:26:PRO:HD2	1.91	0.52
1:A:874:MET:HG2	1:A:891:PHE:CE2	2.44	0.52
1:A:419:LEU:HD12	1:A:513:PHE:HE2	1.75	0.52
1:A:305:ALA:HB2	1:A:792:LEU:HD13	1.91	0.52
1:A:139:ARG:HG3	1:A:139:ARG:O	2.09	0.52
1:A:461:ASN:N	1:A:461:ASN:ND2	2.55	0.52
1:A:264:ILE:HD11	1:A:307:ILE:CD1	2.40	0.52
1:A:95:LEU:O	1:A:98:LEU:HB2	2.10	0.52
1:A:689:GLU:HB2	1:A:713:LYS:HZ2	1.73	0.52
1:A:367:PHE:HZ	1:A:545:ILE:HG23	1.75	0.52
1:A:628:ASN:HD21	1:A:631:THR:N	2.03	0.52
1:A:868:HIS:O	1:A:868:HIS:ND1	2.43	0.52
1:A:654:THR:HA	1:A:677:ALA:O	2.10	0.52
1:A:334:ARG:NH2	1:A:729:THR:HA	2.25	0.52
1:A:983:ILE:HG22	1:A:987:ILE:HD11	1.91	0.51
1:A:379:LEU:CD1	1:A:548:VAL:HG21	2.40	0.51
1:A:554:THR:O	1:A:554:THR:HG22	2.09	0.51
1:A:398:ASN:C	1:A:400:LYS:H	2.13	0.51
1:A:583:ARG:O	1:A:586:GLU:HB3	2.10	0.51
1:A:643:GLY:N	1:A:646:GLU:HG2	2.26	0.51
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.41	0.51
1:A:863:PRO:HG2	1:A:890:ILE:HD13	1.93	0.51
1:A:924:ARG:NE	1:A:924:ARG:HA	2.19	0.51
1:A:338:SER:HA	1:A:341:THR:CG2	2.40	0.51
1:A:131:ARG:NH2	1:A:149:ASP:OD2	2.30	0.51
1:A:65:LEU:CD2	1:A:94:ILE:HG23	2.37	0.51
1:A:413:LEU:CD2	1:A:564:LEU:HD12	2.38	0.51
1:A:461:ASN:HD22	1:A:461:ASN:N	2.09	0.51
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.87	0.51
1:A:946:LEU:HD12	1:A:950:VAL:CG2	2.41	0.51
1:A:628:ASN:ND2	1:A:631:THR:HB	2.26	0.51
1:A:833:LEU:HG	1:A:837:TYR:HE2	1.76	0.50
1:A:25:THR:HA	1:A:132:ALA:HB3	1.93	0.50
1:A:840:ILE:O	1:A:844:VAL:HG23	2.12	0.50
1:A:946:LEU:CD1	1:A:950:VAL:HG21	2.41	0.50
1:A:446:THR:O	1:A:449:VAL:HG22	2.11	0.50
1:A:483:PHE:CE2	1:A:485:LEU:HD21	2.46	0.50
1:A:753:ILE:O	1:A:757:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:MET:HG2	1:A:865:VAL:HG23	1.94	0.50
1:A:874:MET:HG2	1:A:891:PHE:HD2	1.77	0.50
1:A:757:MET:HA	1:A:760:PHE:CE2	2.47	0.50
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.41	0.50
1:A:188:ILE:HD12	1:A:188:ILE:N	2.27	0.50
1:A:236:ARG:HD3	1:A:236:ARG:C	2.33	0.50
1:A:166:LEU:HD11	1:A:222:ILE:HB	1.94	0.49
1:A:762:ARG:HA	1:A:829:ILE:CD1	2.42	0.49
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.93	0.49
1:A:334:ARG:HD3	1:A:731:SER:O	2.12	0.49
1:A:260:LEU:O	1:A:264:ILE:HG13	2.12	0.49
1:A:356:LEU:HD23	1:A:623:MET:HE2	1.94	0.49
1:A:179:ILE:CD1	1:A:232:ILE:HD11	2.42	0.49
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.47	0.49
1:A:856:PHE:CZ	1:A:896:PRO:HG3	2.47	0.49
1:A:174:ARG:NH2	1:A:188:ILE:HD11	2.27	0.49
1:A:370:ASP:HB3	1:A:378:SER:O	2.13	0.49
1:A:604:ARG:NH1	1:A:604:ARG:CG	2.71	0.49
1:A:106:VAL:O	1:A:106:VAL:HG12	2.13	0.49
1:A:593:PHE:CZ	1:A:596:VAL:HG23	2.47	0.49
1:A:717:GLY:O	1:A:731:SER:HB2	2.13	0.49
1:A:442:GLU:O	1:A:445:LEU:HB2	2.12	0.49
1:A:836:ARG:HH12	1:A:919:ASN:HD22	1.60	0.49
1:A:470:ALA:O	1:A:474:VAL:HG23	2.13	0.48
1:A:484:THR:CB	1:A:496:VAL:HG12	2.43	0.48
1:A:735:LEU:HD22	1:A:742:THR:HB	1.94	0.48
1:A:42:PRO:HG2	1:A:236:ARG:CZ	2.42	0.48
1:A:628:ASN:HD22	1:A:628:ASN:N	2.10	0.48
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.95	0.48
1:A:828:LEU:H	1:A:828:LEU:HD12	1.78	0.48
1:A:106:VAL:C	1:A:108:GLN:H	2.17	0.48
1:A:59:ASP:CB	1:A:62:VAL:HG12	2.43	0.48
1:A:259:GLN:HB3	3:A:1011:PTY:HC21	1.96	0.48
1:A:580:ASP:HB2	1:A:583:ARG:HG3	1.95	0.48
1:A:307:ILE:HB	1:A:309:GLU:OE2	2.14	0.48
1:A:202:GLN:OE1	1:A:489:ARG:NH1	2.47	0.48
1:A:205:LYS:HB3	1:A:205:LYS:NZ	2.29	0.48
1:A:326:MET:HE3	1:A:342:LEU:HD23	1.96	0.48
1:A:33:LEU:HD13	1:A:146:VAL:CG1	2.44	0.48
1:A:798:VAL:O	1:A:799:THR:C	2.52	0.47
1:A:802:LEU:HB3	1:A:936:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:MET:HG3	1:A:139:ARG:NH1	2.29	0.47
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.49	0.47
1:A:882:HIS:CD2	1:A:885:GLY:HA3	2.48	0.47
1:A:355:THR:OG1	1:A:720:MET:HE2	2.15	0.47
1:A:24:LEU:HG	1:A:149:ASP:HA	1.96	0.47
1:A:254:ASP:O	1:A:258:GLU:HG2	2.14	0.47
1:A:122:TYR:CE2	1:A:726:VAL:CG2	2.98	0.47
1:A:971:LEU:HA	1:A:975:LEU:HD23	1.96	0.47
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.44	0.47
1:A:925:MET:HE3	1:A:929:VAL:HG21	1.96	0.47
1:A:100:ALA:O	1:A:104:VAL:HG23	2.14	0.47
1:A:702:GLY:HA3	1:A:707:ASP:OD2	2.14	0.47
1:A:911:ASN:HA	1:A:914:ASN:HB2	1.95	0.47
1:A:828:LEU:HD12	1:A:828:LEU:N	2.29	0.47
1:A:975:LEU:HD22	1:A:975:LEU:N	2.30	0.47
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.14	0.47
1:A:873:PHE:HE2	1:A:876:CYS:HA	1.80	0.47
1:A:122:TYR:CE2	1:A:726:VAL:HG21	2.50	0.47
1:A:366:MET:CE	1:A:448:LEU:HD11	2.45	0.47
1:A:629:LYS:HB2	1:A:654:THR:CG2	2.45	0.47
1:A:18:VAL:CG2	1:A:24:LEU:HD23	2.44	0.47
1:A:834:PHE:O	1:A:838:MET:HB2	2.15	0.47
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.97	0.47
1:A:720:MET:HE3	1:A:738:ASP:CB	2.45	0.47
1:A:90:GLU:OE1	1:A:789:PRO:HG2	2.15	0.47
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.87	0.47
1:A:833:LEU:HG	1:A:837:TYR:CE2	2.49	0.47
1:A:72:SER:OG	1:A:91:PRO:HD3	2.15	0.47
1:A:61:LEU:HD11	1:A:260:LEU:HD23	1.97	0.47
1:A:628:ASN:HD21	1:A:631:THR:CB	2.28	0.47
1:A:762:ARG:HA	1:A:829:ILE:HD11	1.96	0.46
1:A:784:PRO:HG3	1:A:874:MET:SD	2.54	0.46
1:A:286:GLY:O	1:A:287:SER:HB2	2.14	0.46
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.45	0.46
1:A:593:PHE:HZ	1:A:596:VAL:HG23	1.80	0.46
1:A:326:MET:CE	1:A:333:VAL:HG21	2.45	0.46
1:A:307:ILE:CG2	2:A:1005:CZA:H113	2.45	0.46
1:A:257:GLY:HA3	2:A:1005:CZA:O1	2.16	0.46
1:A:897:MET:HE1	1:A:958:LYS:HG2	1.97	0.46
1:A:922:LEU:CD2	1:A:927:PRO:HG3	2.43	0.46
1:A:416:ILE:HD11	1:A:566:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:OG1	1:A:602:PRO:HG2	2.15	0.46
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.15	0.46
1:A:851:ALA:HB2	1:A:903:VAL:HG21	1.98	0.46
1:A:980:LEU:O	1:A:984:LEU:HD12	2.15	0.46
1:A:371:LYS:HE2	1:A:373:ASP:HB2	1.97	0.46
1:A:857:MET:HA	1:A:865:VAL:H	1.80	0.46
1:A:527:TYR:O	1:A:592:THR:HA	2.16	0.46
1:A:544:LYS:O	1:A:548:VAL:HG23	2.16	0.46
1:A:65:LEU:HD23	1:A:65:LEU:C	2.36	0.46
1:A:689:GLU:HB2	1:A:713:LYS:HZ3	1.78	0.46
1:A:428:ASN:CG	1:A:431:LYS:HD3	2.37	0.45
1:A:42:PRO:HG2	1:A:236:ARG:NH2	2.31	0.45
1:A:355:THR:OG1	1:A:720:MET:CE	2.64	0.45
1:A:764:LEU:O	1:A:767:SER:HB3	2.16	0.45
1:A:856:PHE:O	1:A:865:VAL:HG22	2.16	0.45
1:A:249:LEU:HD22	1:A:340:GLU:HG3	1.98	0.45
1:A:0:ACE:O	1:A:1:MET:CA	2.50	0.45
1:A:179:ILE:HD13	1:A:211:GLY:O	2.16	0.45
1:A:350:SER:HB3	1:A:356:LEU:HD11	1.98	0.45
1:A:115:ALA:HB1	1:A:239:MET:HE1	1.98	0.45
1:A:332:ILE:CD1	1:A:332:ILE:N	2.79	0.45
1:A:358:THR:O	1:A:359:ASN:HB3	2.15	0.45
1:A:38:HIS:CE1	1:A:143:ARG:HH12	2.35	0.45
1:A:880:HIS:C	1:A:882:HIS:H	2.20	0.45
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.47	0.45
1:A:534:ARG:NH2	1:A:568:ASP:OD2	2.50	0.45
1:A:874:MET:HA	1:A:891:PHE:CE2	2.52	0.45
1:A:289:ILE:HG23	1:A:290:ARG:N	2.31	0.45
1:A:485:LEU:HB3	1:A:584:PHE:CD2	2.52	0.45
1:A:96:LEU:O	1:A:99:ILE:N	2.50	0.45
1:A:981:ASP:HA	1:A:984:LEU:HD12	1.98	0.44
1:A:662:PRO:O	1:A:664:ALA:N	2.50	0.44
1:A:267:ILE:CG2	1:A:302:LEU:HD11	2.47	0.44
1:A:383:SER:O	1:A:384:ILE:HD13	2.17	0.44
1:A:49:LEU:O	1:A:53:VAL:HG23	2.17	0.44
1:A:981:ASP:O	1:A:985:LYS:HG3	2.17	0.44
1:A:82:GLU:C	1:A:84:THR:H	2.21	0.44
1:A:688:VAL:HG11	1:A:713:LYS:HB3	1.99	0.44
1:A:359:ASN:HA	1:A:601:ASP:OD1	2.17	0.44
1:A:263:VAL:O	1:A:264:ILE:C	2.56	0.44
1:A:192:GLU:CD	1:A:580:ASP:HB3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:HB3	1:A:466:GLU:HB2	2.00	0.44
1:A:348:ILE:HD13	1:A:743:ILE:HG21	1.98	0.44
1:A:422:ASP:HB2	1:A:442:GLU:OE2	2.17	0.44
1:A:6:SER:HA	1:A:194:VAL:O	2.18	0.44
1:A:303:ALA:O	1:A:307:ILE:HG12	2.17	0.43
1:A:427:PHE:HB3	1:A:465:VAL:HG22	1.99	0.43
1:A:607:VAL:O	1:A:611:ILE:HG12	2.17	0.43
1:A:355:THR:HA	1:A:738:ASP:O	2.18	0.43
1:A:865:VAL:O	1:A:868:HIS:CB	2.67	0.43
1:A:873:PHE:CE2	1:A:876:CYS:HA	2.53	0.43
1:A:699:ALA:HA	1:A:716:ILE:O	2.17	0.43
1:A:865:VAL:O	1:A:868:HIS:HB3	2.18	0.43
1:A:338:SER:O	1:A:342:LEU:HB2	2.19	0.43
1:A:475:ILE:HA	1:A:478:LEU:HD13	2.00	0.43
1:A:527:TYR:CG	1:A:534:ARG:HD3	2.54	0.43
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.83	0.43
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.80	0.43
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.99	0.43
1:A:60:LEU:HD22	1:A:261:SER:OG	2.19	0.43
1:A:256:PHE:CB	2:A:1005:CZA:H11	2.42	0.43
1:A:906:THR:HG22	1:A:974:SER:HB3	2.01	0.43
1:A:704:GLY:H	1:A:727:ALA:HB2	1.84	0.43
1:A:641:ILE:HG22	1:A:641:ILE:O	2.19	0.42
1:A:862:GLY:O	1:A:864:GLY:N	2.52	0.42
1:A:833:LEU:O	1:A:837:TYR:HB2	2.20	0.42
1:A:580:ASP:C	1:A:582:SER:N	2.71	0.42
1:A:398:ASN:O	1:A:400:LYS:N	2.51	0.42
1:A:486:GLU:CD	1:A:486:GLU:H	2.22	0.42
1:A:252:LYS:O	1:A:255:GLU:HG2	2.19	0.42
1:A:518:PRO:HB3	1:A:549:ILE:HD13	2.01	0.42
1:A:24:LEU:HD12	1:A:149:ASP:HB3	2.01	0.42
1:A:273:LEU:HA	1:A:276:ILE:HG13	2.01	0.42
1:A:1:MET:HG2	1:A:1:MET:O	2.19	0.42
1:A:158:LYS:HA	1:A:212:THR:O	2.19	0.42
1:A:975:LEU:N	1:A:976:PRO:CD	2.81	0.42
1:A:488:SER:OG	1:A:490:ASP:HB3	2.20	0.42
1:A:127:GLY:HA3	1:A:145:ILE:HD11	2.02	0.42
1:A:545:ILE:HD13	1:A:593:PHE:CE2	2.54	0.42
1:A:269:VAL:O	1:A:273:LEU:HG	2.20	0.42
1:A:865:VAL:O	1:A:865:VAL:HG23	2.18	0.42
1:A:52:LEU:HD13	1:A:106:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PHE:HA	1:A:380:ASN:O	2.19	0.42
1:A:100:ALA:HA	1:A:103:ILE:HD12	2.01	0.42
1:A:366:MET:HG3	1:A:382:PHE:HB2	2.02	0.42
1:A:113:GLU:OE1	1:A:113:GLU:N	2.53	0.42
1:A:577:VAL:HG23	1:A:583:ARG:HH12	1.85	0.42
1:A:310:GLY:O	1:A:314:VAL:HG23	2.20	0.42
1:A:855:TRP:CZ3	1:A:896:PRO:HD3	2.54	0.42
1:A:863:PRO:O	1:A:865:VAL:HG13	2.19	0.42
1:A:989:ARG:HD2	3:A:1012:PTY:HC22	2.02	0.42
1:A:631:THR:O	1:A:635:ILE:HG13	2.20	0.41
1:A:527:TYR:HB3	1:A:534:ARG:HG3	2.02	0.41
1:A:860:GLU:C	1:A:862:GLY:H	2.23	0.41
1:A:833:LEU:O	1:A:837:TYR:HD2	2.02	0.41
1:A:442:GLU:O	1:A:445:LEU:N	2.52	0.41
1:A:493:SER:OG	1:A:524:ARG:NH2	2.52	0.41
1:A:816:ILE:HD13	1:A:816:ILE:O	2.21	0.41
1:A:335:SER:O	1:A:338:SER:HB2	2.20	0.41
1:A:72:SER:HB3	1:A:91:PRO:HB3	2.02	0.41
1:A:44:GLU:HG2	1:A:117:GLU:OE1	2.21	0.41
1:A:857:MET:HG2	1:A:865:VAL:CG2	2.50	0.41
1:A:895:GLU:N	1:A:896:PRO:HD2	2.36	0.41
1:A:581:SER:HA	1:A:584:PHE:CD2	2.56	0.41
1:A:869:GLN:HB3	1:A:872:HIS:CB	2.50	0.41
1:A:276:ILE:O	1:A:279:PHE:HB2	2.20	0.41
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.61	0.41
1:A:823:SER:C	1:A:825:LYS:H	2.23	0.41
1:A:0:ACE:H3	1:A:36:TYR:CE1	2.55	0.41
1:A:252:LYS:HE2	1:A:826:GLU:O	2.20	0.41
1:A:628:ASN:HD21	1:A:631:THR:HB	1.86	0.41
1:A:669:ALA:HA	1:A:672:ARG:NH1	2.36	0.41
1:A:771:GLU:CD	1:A:792:LEU:HD22	2.41	0.41
1:A:494:MET:HG3	1:A:495:SER:N	2.36	0.41
1:A:554:THR:CG2	1:A:554:THR:O	2.68	0.41
1:A:63:ARG:O	1:A:66:LEU:N	2.54	0.41
1:A:55:GLU:O	1:A:58:GLU:CB	2.68	0.41
1:A:283:VAL:HG13	1:A:284:HIS:N	2.35	0.41
1:A:637:ARG:NH1	1:A:643:GLY:O	2.54	0.41
1:A:926:PRO:HB3	1:A:928:TRP:CZ2	2.56	0.41
1:A:628:ASN:ND2	1:A:628:ASN:N	2.69	0.40
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.35	0.40
1:A:683:HIS:O	1:A:684:LYS:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HA	1:A:28:GLN:OE1	2.21	0.40
1:A:946:LEU:O	1:A:953:LEU:HD12	2.21	0.40
1:A:628:ASN:HD22	1:A:628:ASN:C	2.23	0.40
1:A:971:LEU:CA	1:A:975:LEU:HD23	2.51	0.40
1:A:663:LEU:N	1:A:663:LEU:HD12	2.36	0.40
1:A:194:VAL:HA	1:A:195:PRO:HD2	1.82	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%)	863 (87%)	113 (11%)	17 (2%)	11 36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	951	ASP
1	A	663	LEU
1	A	736	ALA
1	A	950	VAL
1	A	185	VAL
1	A	399	ASP
1	A	406	GLN
1	A	462	LEU
1	A	863	PRO
1	A	883	PHE
1	A	287	SER
1	A	456	ASN
1	A	470	ALA
1	A	504	SER
1	A	627	ASP

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Mol	Chain	Res	Type
1	A	782	GLY
1	A	820	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	840/840 (100%)	779 (93%)	61 (7%)	17 44

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	7	LYS
1	A	9	THR
1	A	34	GLU
1	A	41	LEU
1	A	59	ASP
1	A	60	LEU
1	A	95	LEU
1	A	113	GLU
1	A	139	ARG
1	A	160	PRO
1	A	164	ARG
1	A	198	ARG
1	A	205	LYS
1	A	236	ARG
1	A	245	ASP
1	A	253	LEU
1	A	266	LEU
1	A	302	LEU
1	A	319	LEU
1	A	326	MET
1	A	336	LEU
1	A	371	LYS
1	A	388	THR

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Mol	Chain	Res	Type
1	A	402	ILE
1	A	431	LYS
1	A	445	LEU
1	A	461	ASN
1	A	467	ARG
1	A	484	THR
1	A	485	LEU
1	A	486	GLU
1	A	494	MET
1	A	535	VAL
1	A	540	PRO
1	A	578	LEU
1	A	580	ASP
1	A	589	THR
1	A	604	ARG
1	A	612	GLN
1	A	613	LEU
1	A	620	ARG
1	A	628	ASN
1	A	647	GLU
1	A	656	ARG
1	A	668	GLU
1	A	672	ARG
1	A	679	VAL
1	A	739	ASN
1	A	758	LYS
1	A	816	ILE
1	A	825	LYS
1	A	830	SER
1	A	833	LEU
1	A	848	THR
1	A	873	PHE
1	A	888	CYS
1	A	922	LEU
1	A	924	ARG
1	A	951	ASP
1	A	982	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	359	ASN
1	A	461	ASN
1	A	510	ASN
1	A	628	ASN
1	A	706	ASN
1	A	739	ASN
1	A	880	HIS
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CZA	A	1005	-	25,29,29	2.49	9 (36%)	22,48,48	2.17	5 (22%)
3	PTY	A	1011	-	17,18,49	1.48	4 (23%)	18,23,54	1.50	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PTY	A	1012	-	17,18,49	1.46	4 (23%)	18,23,54	1.28	2 (11%)
3	PTY	A	1013	-	17,18,49	1.33	3 (17%)	18,23,54	1.53	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CZA	A	1005	-	3/3/9/9	0/4/52/52	0/5/5/5
3	PTY	A	1011	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1012	-	-	0/20/20/53	0/0/0/0
3	PTY	A	1013	-	-	0/20/20/53	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	CZA	C3-C2	-3.83	1.34	1.46
2	A	1005	CZA	C1-C2	-3.53	1.42	1.50
2	A	1005	CZA	O3-C4	-2.65	1.23	1.31
2	A	1005	CZA	C4-N1	-2.50	1.36	1.39
2	A	1005	CZA	C13-C14	-2.39	1.39	1.44
2	A	1005	CZA	C7-C8	2.03	1.59	1.55
3	A	1012	PTY	O7-C8	2.07	1.40	1.35
3	A	1011	PTY	C1-C6	2.09	1.56	1.50
3	A	1011	PTY	P1-O12	2.14	1.64	1.54
3	A	1013	PTY	P1-O13	2.29	1.59	1.51
3	A	1012	PTY	P1-O13	2.36	1.59	1.51
2	A	1005	CZA	C19-C20	2.44	1.43	1.38
3	A	1013	PTY	C5-C6	2.50	1.57	1.50
3	A	1013	PTY	C1-C6	2.59	1.58	1.50
3	A	1012	PTY	C1-C6	2.73	1.58	1.50
3	A	1012	PTY	C5-C6	2.74	1.58	1.50
3	A	1011	PTY	C5-C6	3.28	1.60	1.50
3	A	1011	PTY	P1-O13	3.55	1.64	1.51
2	A	1005	CZA	C3-C4	3.92	1.47	1.40
2	A	1005	CZA	O1-C2	8.26	1.41	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1005	CZA	C12-C13-C14	-5.08	115.07	119.49
3	A	1011	PTY	O12-P1-O13	-2.98	96.38	112.53
3	A	1013	PTY	C5-C6-C1	-2.97	105.14	112.07
2	A	1005	CZA	C19-C18-C17	-2.68	115.77	120.06
2	A	1005	CZA	O3-C4-C3	-2.02	124.59	130.14
3	A	1013	PTY	O4-C1-C6	2.03	114.16	108.69
2	A	1005	CZA	C13-C12-C8	2.15	117.22	112.40
3	A	1012	PTY	O4-C1-C6	2.77	116.14	108.69
3	A	1011	PTY	C5-C6-C1	2.85	118.74	112.07
3	A	1012	PTY	O7-C8-C11	2.85	116.48	111.10
3	A	1011	PTY	O11-P1-O13	2.94	121.04	109.62
3	A	1013	PTY	O7-C8-C11	3.18	117.11	111.10
2	A	1005	CZA	C13-C14-C15	7.11	130.26	123.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1005	CZA	C5
2	A	1005	CZA	C8
2	A	1005	CZA	C7

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	CZA	23	0
3	A	1011	PTY	1	0
3	A	1012	PTY	1	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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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