



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:43 AM GMT

PDB ID : 2C8K  
Title : CRYSTAL STRUCTURE OF (SR) CALCIUM-ATPASE E2(TG) WITH PARTIALLY OCCUPIED AMPPCP SITE  
Authors : Jensen, A.M.; Sorensen, T.L.; Olesen, C.; Moller, J.V.; Nissen, P.  
Deposited on : 2005-12-06  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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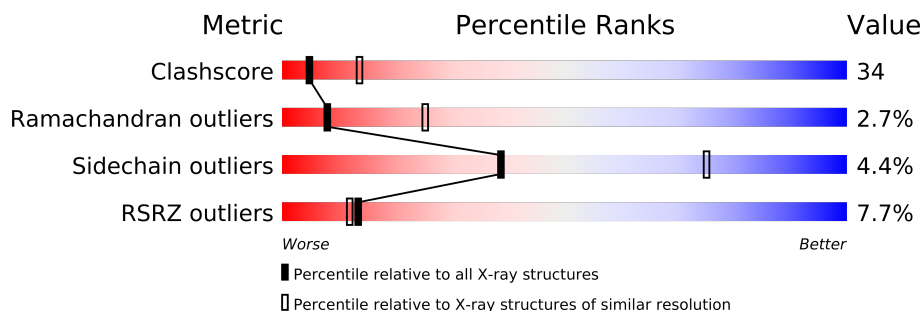
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	994	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACP	A	1996	-	X
4	MG	A	1997	-	X
5	NA	A	1998	-	X

## 2 Entry composition i

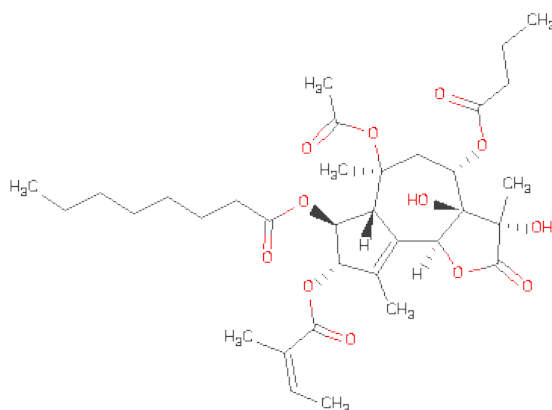
There are 5 unique types of molecules in this entry. The entry contains 7750 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ARCOPLASMIC/ENDOPLASMICRETICULUM CALCIUM ATPASE 1.

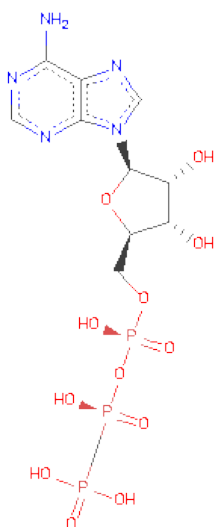
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

- Molecule 2 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-YLESTER (three-letter code: TG1) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONICACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0

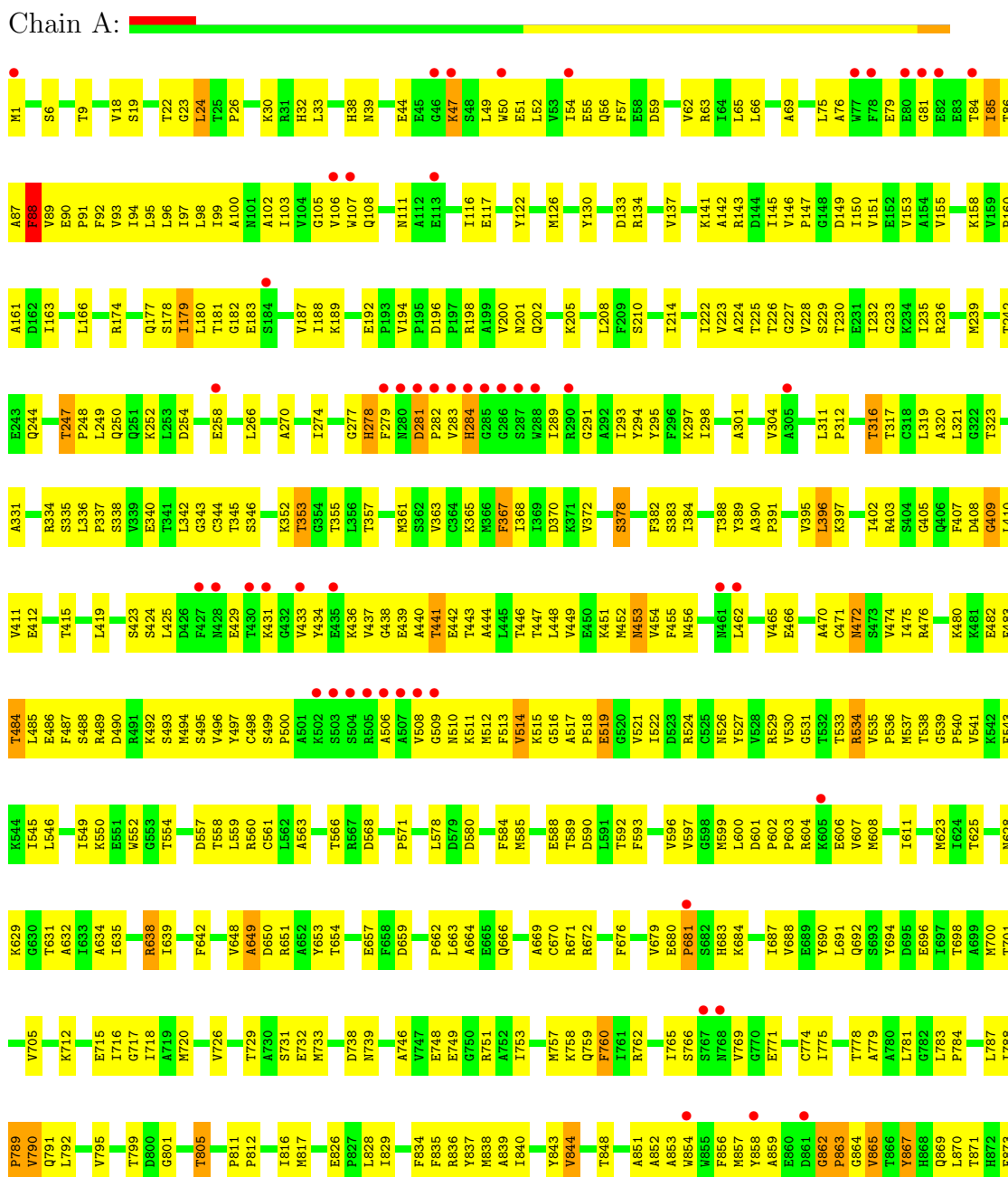
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

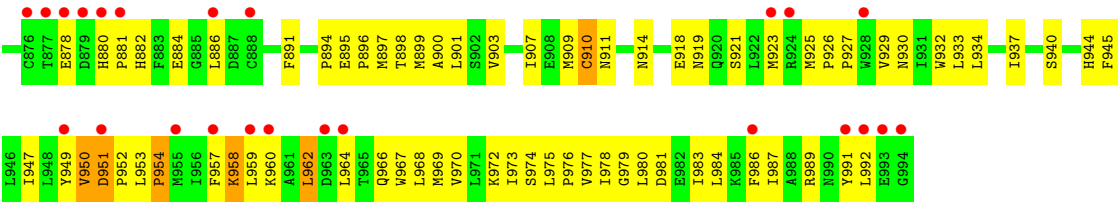
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0

### 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.

#### • Molecule 1: ARCOPLASMIC/ENDOPLASMICRETICULUM CALCIUM ATPASE 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.34Å 71.34Å 587.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.95 – 2.80 29.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (14.95-2.80) 92.7 (29.83-2.80)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.252 , 0.308 0.270 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 36357 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, ACP, TG1

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	0.40	0/7812	0.66	2/10592 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLY	N-CA-C	8.55	134.47	113.10
1	A	962	LEU	N-CA-C	-5.84	95.23	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7764	532	0
2	A	46	0	50	2	0
3	A	31	0	14	9	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
All	All	7750	0	7828	532	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (532) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:334:ARG:HH12	1:A:729:THR:HA	1.05	1.18
1:A:521:VAL:HG21	1:A:563:ALA:HB3	1.29	1.07
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.37	1.05
1:A:453:ASN:HB3	1:A:471:CYS:SG	1.97	1.04
1:A:530:VAL:HG23	1:A:533:THR:HG23	1.39	1.02
1:A:1:MET:HB2	1:A:225:THR:HG22	1.40	1.02
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.24	1.02
1:A:76:ALA:HB1	1:A:87:ALA:O	1.60	1.01
1:A:527:TYR:HB2	1:A:592:THR:HG22	1.36	1.01
1:A:247:THR:HG22	1:A:250:GLN:H	1.20	0.99
1:A:79:GLU:HG2	1:A:84:THR:HG21	1.44	0.97
1:A:342:LEU:O	1:A:345:THR:HG23	1.64	0.97
1:A:334:ARG:NH1	1:A:729:THR:HA	1.78	0.96
1:A:248:PRO:HG2	1:A:340:GLU:OE2	1.67	0.94
1:A:352:LYS:HE3	1:A:635:ILE:HD13	1.51	0.92
1:A:411:VAL:HG12	1:A:454:VAL:CG1	1.99	0.90
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.51	0.90
1:A:530:VAL:HG23	1:A:533:THR:CG2	2.02	0.89
1:A:680:GLU:H	1:A:683:HIS:HD2	1.21	0.88
1:A:560:ARG:HH21	3:A:1996:ACP:H3'	1.39	0.88
1:A:530:VAL:CG2	1:A:533:THR:HG23	2.03	0.87
1:A:192:GLU:OE1	1:A:580:ASP:HB2	1.76	0.86
1:A:950:VAL:O	1:A:954:PRO:HG2	1.77	0.85
1:A:788:ILE:HG12	1:A:897:MET:CE	2.07	0.84
1:A:865:VAL:HG11	1:A:869:GLN:HB2	1.57	0.84
1:A:161:ALA:HA	1:A:210:SER:HB2	1.60	0.84
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.07	0.83
1:A:862:GLY:H	1:A:863:PRO:HD3	1.43	0.83
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.62	0.81
1:A:411:VAL:HG12	1:A:454:VAL:HG11	1.63	0.81
1:A:795:VAL:HA	1:A:799:THR:OG1	1.81	0.81
1:A:680:GLU:N	1:A:683:HIS:HD2	1.78	0.81
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.61	0.81
1:A:788:ILE:HG12	1:A:897:MET:HE3	1.61	0.81
1:A:549:ILE:HD11	1:A:596:VAL:HG11	1.63	0.81
1:A:521:VAL:CG2	1:A:563:ALA:HB3	2.10	0.80
1:A:1:MET:CE	1:A:229:SER:HB3	2.12	0.80
1:A:700:MET:HE3	1:A:701:THR:H	1.45	0.80
1:A:352:LYS:HB2	1:A:625:THR:HG22	1.64	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:788:ILE:HG22	1:A:790:VAL:HG23	1.64	0.79
1:A:945:PHE:HD1	1:A:949:TYR:HE2	1.28	0.78
1:A:484:THR:HB	1:A:496:VAL:HG12	1.64	0.78
1:A:180:LEU:HA	1:A:705:VAL:HG12	1.63	0.78
1:A:680:GLU:H	1:A:683:HIS:CD2	2.02	0.78
1:A:909:MET:CE	1:A:937:ILE:HA	2.13	0.77
1:A:177:GLN:HE22	1:A:189:LYS:NZ	1.80	0.77
1:A:436:LYS:CG	1:A:443:THR:HG21	2.14	0.77
1:A:865:VAL:HG11	1:A:869:GLN:CB	2.14	0.77
1:A:397:LYS:HB3	1:A:402:ILE:HD11	1.67	0.76
1:A:312:PRO:O	1:A:316:THR:HG23	1.85	0.76
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.68	0.76
1:A:449:VAL:HG11	1:A:472:ASN:ND2	2.01	0.76
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.68	0.75
1:A:909:MET:HE3	1:A:937:ILE:HA	1.68	0.75
1:A:958:LYS:N	1:A:958:LYS:HD2	2.01	0.75
1:A:751:ARG:HD2	1:A:817:MET:CE	2.17	0.75
1:A:606:GLU:CD	1:A:606:GLU:H	1.87	0.75
1:A:958:LYS:HD2	1:A:958:LYS:H	1.52	0.75
1:A:835:PHE:O	1:A:838:MET:HB3	1.86	0.75
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.69	0.75
1:A:447:THR:HG22	1:A:451:LYS:HE2	1.69	0.74
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.27	0.74
1:A:281:ASP:OD1	1:A:282:PRO:HD3	1.87	0.74
1:A:89:VAL:O	1:A:93:VAL:HG23	1.88	0.73
1:A:471:CYS:O	1:A:474:VAL:HG22	1.87	0.73
1:A:352:LYS:CB	1:A:625:THR:HG22	2.18	0.73
1:A:748:GLU:HA	1:A:817:MET:CE	2.18	0.72
1:A:560:ARG:NH2	3:A:1996:ACP:H8	2.04	0.72
1:A:654:THR:HG22	1:A:657:GLU:CG	2.20	0.72
1:A:334:ARG:HH12	1:A:729:THR:CA	1.96	0.71
1:A:153:VAL:HB	1:A:214:ILE:HD11	1.71	0.71
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.72	0.70
1:A:382:PHE:CE2	1:A:410:LEU:HD11	2.26	0.70
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.21	0.70
1:A:252:LYS:HE2	1:A:826:GLU:O	1.91	0.70
1:A:439:GLU:O	1:A:443:THR:HG22	1.91	0.70
1:A:1:MET:HE3	1:A:229:SER:HB3	1.73	0.70
1:A:651:ARG:HH11	1:A:651:ARG:HG2	1.57	0.70
1:A:62:VAL:HG23	1:A:98:LEU:HD22	1.74	0.69
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.22	0.69
1:A:19:SER:OG	1:A:22:THR:HB	1.92	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:560:ARG:NH2	3:A:1996:ACP:H3'	2.07	0.69
1:A:791:GLN:HB3	1:A:901:LEU:CD1	2.23	0.69
1:A:100:ALA:HA	1:A:103:ILE:HD12	1.75	0.69
1:A:453:ASN:CB	1:A:471:CYS:SG	2.77	0.68
1:A:298:ILE:CD1	1:A:779:ALA:HB2	2.24	0.68
1:A:334:ARG:O	1:A:335:SER:HB3	1.94	0.68
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.59	0.68
1:A:363:VAL:HG13	1:A:597:VAL:HG13	1.75	0.68
1:A:1:MET:HG3	1:A:1:MET:O	1.93	0.68
1:A:388:THR:HG22	1:A:389:TYR:N	2.10	0.67
1:A:515:LYS:HE3	3:A:1996:ACP:N1	2.09	0.67
1:A:99:ILE:O	1:A:103:ILE:HG13	1.94	0.67
1:A:87:ALA:O	1:A:88:PHE:HD1	1.78	0.67
1:A:431:LYS:O	1:A:433:VAL:HG23	1.95	0.67
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.15	0.66
1:A:979:GLY:O	1:A:983:ILE:HG13	1.96	0.65
1:A:247:THR:HG23	1:A:249:LEU:H	1.61	0.65
1:A:133:ASP:O	1:A:134:ARG:HG3	1.96	0.65
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.77	0.65
1:A:775:ILE:O	1:A:778:THR:HG22	1.96	0.65
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.79	0.65
1:A:508:VAL:HG11	1:A:511:LYS:NZ	2.11	0.65
1:A:951:ASP:C	1:A:954:PRO:HD2	2.16	0.65
1:A:247:THR:HG22	1:A:250:GLN:HG3	1.78	0.65
1:A:122:TYR:O	1:A:158:LYS:HD3	1.97	0.64
1:A:788:ILE:CG2	1:A:790:VAL:HG23	2.27	0.64
1:A:521:VAL:HG21	1:A:563:ALA:CB	2.18	0.64
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.79	0.64
1:A:950:VAL:CG1	1:A:951:ASP:N	2.61	0.64
1:A:545:ILE:O	1:A:549:ILE:HG12	1.98	0.64
1:A:944:HIS:O	1:A:947:ILE:HG12	1.96	0.64
1:A:79:GLU:CG	1:A:84:THR:HG21	2.24	0.63
1:A:748:GLU:HA	1:A:817:MET:HE3	1.80	0.63
1:A:448:LEU:O	1:A:452:MET:HG2	1.99	0.63
1:A:472:ASN:O	1:A:476:ARG:HG3	1.98	0.63
1:A:317:THR:O	1:A:321:LEU:HG	1.97	0.63
1:A:177:GLN:NE2	1:A:189:LYS:NZ	2.46	0.63
1:A:900:ALA:O	1:A:903:VAL:HG12	1.98	0.63
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.81	0.63
1:A:958:LYS:N	1:A:958:LYS:CD	2.62	0.62
1:A:295:TYR:O	1:A:298:ILE:HG22	1.98	0.62
1:A:411:VAL:CG1	1:A:454:VAL:HG11	2.30	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:508:VAL:HG11	1:A:511:LYS:HZ1	1.65	0.62
1:A:402:ILE:HG22	1:A:403:ARG:N	2.13	0.62
1:A:748:GLU:HA	1:A:817:MET:HE1	1.81	0.62
1:A:247:THR:HG22	1:A:250:GLN:N	2.04	0.61
1:A:75:LEU:HD13	1:A:297:LYS:HB3	1.82	0.61
1:A:757:MET:HA	1:A:760:PHE:CE2	2.35	0.61
1:A:500:PRO:HG3	1:A:506:ALA:HA	1.81	0.61
1:A:183:GLU:HG3	1:A:183:GLU:O	2.00	0.61
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.83	0.61
1:A:559:LEU:HD23	1:A:600:LEU:HB2	1.83	0.61
1:A:909:MET:HE3	1:A:937:ILE:HG12	1.82	0.61
1:A:161:ALA:CA	1:A:210:SER:HB2	2.29	0.61
1:A:412:GLU:CD	1:A:529:ARG:HE	2.04	0.61
1:A:84:THR:O	1:A:86:THR:N	2.34	0.60
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.36	0.60
1:A:526:ASN:ND2	1:A:590:ASP:HA	2.16	0.60
1:A:91:PRO:O	1:A:95:LEU:HG	2.01	0.60
1:A:870:LEU:HD12	1:A:873:PHE:HB3	1.83	0.60
1:A:247:THR:HG23	1:A:340:GLU:OE1	2.01	0.60
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.83	0.60
1:A:541:VAL:O	1:A:545:ILE:HG13	2.02	0.60
1:A:903:VAL:O	1:A:907:ILE:HG13	2.02	0.60
1:A:470:ALA:O	1:A:474:VAL:HG13	2.02	0.60
1:A:859:ALA:O	1:A:863:PRO:HG3	2.02	0.60
1:A:865:VAL:HG11	1:A:869:GLN:CG	2.32	0.59
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.01	0.59
1:A:177:GLN:HE22	1:A:189:LYS:HZ3	1.49	0.59
1:A:700:MET:HE3	1:A:701:THR:N	2.16	0.59
1:A:361:MET:HB3	1:A:599:MET:HE3	1.84	0.59
1:A:527:TYR:O	1:A:592:THR:HA	2.02	0.59
1:A:298:ILE:HD13	1:A:779:ALA:HB2	1.85	0.59
1:A:550:LYS:O	1:A:554:THR:HB	2.03	0.59
1:A:411:VAL:O	1:A:415:THR:HG23	2.02	0.59
1:A:895:GLU:OE2	1:A:959:LEU:HD11	2.01	0.59
1:A:749:GLU:O	1:A:753:ILE:HG12	2.02	0.59
1:A:951:ASP:H	1:A:952:PRO:HD2	1.68	0.59
1:A:688:VAL:O	1:A:692:GLN:HG3	2.01	0.59
1:A:895:GLU:CD	1:A:959:LEU:HD11	2.23	0.58
1:A:720:MET:HB3	1:A:738:ASP:OD1	2.03	0.58
1:A:441:THR:HA	1:A:599:MET:HE2	1.85	0.58
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.39	0.58
1:A:483:PHE:HE1	1:A:485:LEU:HD21	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:LEU:O	1:A:99:ILE:HG12	2.04	0.58
1:A:865:VAL:HG11	1:A:869:GLN:HG2	1.84	0.58
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.32	0.58
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.85	0.58
1:A:974:SER:O	1:A:977:VAL:HG23	2.03	0.58
1:A:518:PRO:HD3	1:A:561:CYS:O	2.04	0.58
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.33	0.58
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.39	0.58
1:A:277:GLY:C	1:A:279:PHE:H	2.07	0.58
1:A:911:ASN:HA	1:A:914:ASN:ND2	2.06	0.57
1:A:759:GLN:HE22	1:A:762:ARG:HH11	1.52	0.57
1:A:717:GLY:N	1:A:732:GLU:OE1	2.38	0.57
1:A:331:ALA:HB1	1:A:733:MET:CE	2.34	0.57
1:A:436:LYS:HG3	1:A:443:THR:CG2	2.31	0.57
1:A:851:ALA:O	1:A:854:TRP:HB3	2.05	0.57
1:A:26:PRO:O	1:A:30:LYS:HG3	2.03	0.57
1:A:75:LEU:HD22	1:A:293:ILE:HG13	1.86	0.57
1:A:298:ILE:HD11	1:A:779:ALA:HB2	1.87	0.57
1:A:146:VAL:HG13	1:A:147:PRO:CD	2.34	0.57
1:A:248:PRO:O	1:A:252:LYS:HG3	2.05	0.56
1:A:177:GLN:HE22	1:A:189:LYS:HZ1	1.50	0.56
1:A:408:ASP:O	1:A:411:VAL:HG22	2.05	0.56
1:A:278:HIS:HA	1:A:282:PRO:HG2	1.88	0.56
1:A:352:LYS:CE	1:A:635:ILE:HD13	2.29	0.56
1:A:895:GLU:N	1:A:896:PRO:HD2	2.19	0.56
1:A:388:THR:HG22	1:A:390:ALA:H	1.69	0.56
1:A:950:VAL:HG12	1:A:951:ASP:N	2.20	0.56
1:A:519:GLU:OE1	1:A:519:GLU:N	2.27	0.56
1:A:47:LYS:HB3	1:A:51:GLU:OE1	2.06	0.56
1:A:517:ALA:HB2	3:A:1996:ACP:H4'	1.87	0.56
1:A:895:GLU:O	1:A:899:MET:HG2	2.06	0.56
1:A:607:VAL:O	1:A:611:ILE:HG12	2.05	0.56
1:A:452:MET:O	1:A:454:VAL:N	2.39	0.55
1:A:244:GLN:CD	1:A:244:GLN:H	2.09	0.55
1:A:969:MET:O	1:A:973:ILE:HG13	2.06	0.55
1:A:411:VAL:HG12	1:A:454:VAL:HG13	1.88	0.55
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.87	0.55
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.86	0.55
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.87	0.55
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.70	0.55
1:A:411:VAL:CB	1:A:454:VAL:HG11	2.36	0.55
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:659:ASP:OD1	1:A:683:HIS:HE1	1.89	0.55
1:A:691:LEU:O	1:A:696:GLU:HB2	2.07	0.55
1:A:412:GLU:OE1	1:A:529:ARG:NE	2.38	0.55
1:A:483:PHE:CE1	1:A:578:LEU:HD22	2.42	0.55
1:A:122:TYR:HE2	1:A:726:VAL:CG2	2.19	0.55
1:A:530:VAL:O	1:A:530:VAL:HG23	2.07	0.55
1:A:910:CYS:SG	1:A:978:ILE:HD11	2.47	0.55
1:A:651:ARG:HG2	1:A:651:ARG:NH1	2.22	0.54
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.37	0.54
1:A:603:PRO:HG2	1:A:638:ARG:HD3	1.88	0.54
1:A:361:MET:HE3	1:A:599:MET:HG3	1.87	0.54
1:A:465:VAL:O	1:A:465:VAL:HG12	2.07	0.54
1:A:92:PHE:CE2	1:A:96:LEU:HD11	2.41	0.54
1:A:367:PHE:C	1:A:367:PHE:CD1	2.81	0.54
1:A:840:ILE:O	1:A:844:VAL:HG13	2.07	0.54
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.37	0.54
1:A:784:PRO:HG3	1:A:873:PHE:CD2	2.42	0.54
1:A:654:THR:CG2	1:A:657:GLU:H	2.20	0.54
1:A:196:ASP:OD1	1:A:198:ARG:N	2.36	0.54
1:A:278:HIS:HA	1:A:282:PRO:CG	2.38	0.54
1:A:608:MET:SD	1:A:639:ILE:HA	2.48	0.54
1:A:962:LEU:O	1:A:966:GLN:HB2	2.08	0.54
1:A:353:THR:HA	1:A:357:THR:OG1	2.07	0.54
1:A:515:LYS:HE3	3:A:1996:ACP:C6	2.38	0.54
1:A:894:PRO:O	1:A:898:THR:HG23	2.08	0.54
1:A:436:LYS:CD	1:A:443:THR:HG21	2.38	0.54
1:A:535:VAL:HG13	1:A:536:PRO:HD2	1.90	0.54
1:A:909:MET:CE	1:A:940:SER:HB2	2.38	0.53
1:A:853:ALA:O	1:A:856:PHE:HB2	2.07	0.53
1:A:235:ILE:HD13	1:A:705:VAL:HG22	1.89	0.53
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.90	0.53
1:A:363:VAL:CG1	1:A:597:VAL:HG13	2.38	0.53
1:A:402:ILE:CG2	1:A:403:ARG:N	2.72	0.53
1:A:239:MET:O	1:A:242:THR:HG22	2.09	0.53
1:A:986:PHE:CE1	1:A:989:ARG:HD2	2.43	0.53
1:A:593:PHE:CZ	1:A:596:VAL:HG12	2.44	0.53
1:A:76:ALA:HB1	1:A:88:PHE:HD1	1.73	0.53
1:A:23:GLY:HA3	1:A:130:TYR:O	2.09	0.53
1:A:254:ASP:O	1:A:258:GLU:HG2	2.09	0.53
1:A:455:PHE:O	1:A:456:ASN:HB2	2.09	0.53
1:A:527:TYR:CE2	1:A:534:ARG:NH2	2.77	0.53
1:A:281:ASP:CG	1:A:282:PRO:HD3	2.28	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.91	0.53
1:A:676:PHE:CE2	1:A:687:ILE:HD13	2.43	0.53
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.91	0.52
1:A:489:ARG:O	1:A:492:LYS:HE3	2.10	0.52
1:A:235:ILE:HG21	1:A:705:VAL:HG22	1.91	0.52
1:A:200:VAL:HG12	1:A:681:PRO:HG3	1.92	0.52
1:A:894:PRO:CB	1:A:958:LYS:HG3	2.39	0.52
1:A:962:LEU:N	1:A:966:GLN:OE1	2.41	0.52
1:A:865:VAL:HG12	1:A:867:TYR:H	1.73	0.52
1:A:59:ASP:O	1:A:62:VAL:HG12	2.10	0.52
1:A:486:GLU:OE2	1:A:584:PHE:HE2	1.91	0.52
1:A:76:ALA:CB	1:A:87:ALA:O	2.48	0.52
1:A:748:GLU:CG	1:A:817:MET:HE3	2.39	0.52
1:A:57:PHE:HE1	1:A:102:ALA:HB2	1.74	0.52
1:A:462:LEU:HB3	1:A:466:GLU:CD	2.29	0.52
1:A:49:LEU:HD23	1:A:52:LEU:HD12	1.92	0.52
1:A:178:SER:O	1:A:180:LEU:N	2.42	0.52
1:A:538:THR:OG1	1:A:541:VAL:HG23	2.10	0.51
1:A:446:THR:HB	1:A:472:ASN:OD1	2.10	0.51
1:A:388:THR:CG2	1:A:389:TYR:N	2.73	0.51
1:A:865:VAL:CG1	1:A:869:GLN:H	2.23	0.51
1:A:898:THR:HG22	1:A:958:LYS:HB2	1.91	0.51
1:A:304:VAL:HG21	1:A:789:PRO:HA	1.91	0.51
1:A:844:VAL:O	1:A:848:THR:HG23	2.11	0.51
1:A:284:HIS:ND1	1:A:284:HIS:O	2.43	0.51
1:A:829:ILE:HG21	2:A:1995:TG1:H333	1.91	0.51
1:A:945:PHE:HD1	1:A:949:TYR:CE2	2.17	0.51
1:A:623:MET:HG2	1:A:625:THR:HG23	1.93	0.51
1:A:950:VAL:HG13	1:A:952:PRO:HD2	1.92	0.51
1:A:480:LYS:O	1:A:498:CYS:HA	2.11	0.51
1:A:517:ALA:O	1:A:521:VAL:HG22	2.11	0.50
1:A:99:ILE:HG22	1:A:103:ILE:HD11	1.92	0.50
1:A:153:VAL:CB	1:A:214:ILE:HD11	2.40	0.50
1:A:662:PRO:O	1:A:664:ALA:N	2.44	0.50
1:A:301:ALA:HA	1:A:789:PRO:HG3	1.92	0.50
1:A:107:TRP:CD1	1:A:111:ASN:ND2	2.80	0.50
1:A:964:LEU:O	1:A:968:LEU:HD12	2.11	0.50
1:A:629:LYS:O	1:A:632:ALA:HB3	2.12	0.50
1:A:244:GLN:CD	1:A:244:GLN:N	2.65	0.50
1:A:474:VAL:HG23	1:A:475:ILE:N	2.26	0.50
1:A:277:GLY:O	1:A:279:PHE:N	2.45	0.50
1:A:519:GLU:H	1:A:519:GLU:CD	2.04	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:MET:SD	1:A:141:LYS:HG2	2.52	0.50
1:A:50:TRP:NE1	1:A:54:ILE:HD11	2.27	0.50
1:A:18:VAL:HG22	1:A:19:SER:N	2.26	0.50
1:A:352:LYS:HD2	1:A:625:THR:CG2	2.42	0.49
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.77	0.49
1:A:967:TRP:O	1:A:970:VAL:HB	2.12	0.49
1:A:650:ASP:OD2	1:A:672:ARG:HD3	2.12	0.49
1:A:765:ILE:O	1:A:769:VAL:HG23	2.11	0.49
1:A:783:LEU:HD12	1:A:784:PRO:HD2	1.94	0.49
1:A:856:PHE:O	1:A:864:GLY:N	2.45	0.49
1:A:51:GLU:O	1:A:55:GLU:HG3	2.12	0.49
1:A:415:THR:HA	1:A:475:ILE:HG21	1.95	0.49
1:A:32:HIS:HB3	1:A:146:VAL:HG11	1.95	0.49
1:A:408:ASP:HB2	1:A:531:GLY:HA2	1.95	0.49
1:A:512:MET:HE1	1:A:571:PRO:HD2	1.93	0.49
1:A:361:MET:HB3	1:A:599:MET:CE	2.43	0.49
1:A:150:ILE:HD12	1:A:150:ILE:N	2.28	0.49
1:A:331:ALA:HB1	1:A:733:MET:HE1	1.94	0.49
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.48	0.49
1:A:604:ARG:HH11	1:A:739:ASN:ND2	2.11	0.49
1:A:901:LEU:HD23	1:A:901:LEU:C	2.32	0.49
1:A:909:MET:HE1	1:A:940:SER:HB2	1.95	0.48
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.94	0.48
1:A:319:LEU:HG	1:A:757:MET:HE1	1.94	0.48
1:A:150:ILE:N	1:A:150:ILE:CD1	2.76	0.48
1:A:926:PRO:HG2	1:A:929:VAL:HG23	1.95	0.48
1:A:516:GLY:HA2	3:A:1996:ACP:N3	2.28	0.48
1:A:79:GLU:HG2	1:A:84:THR:CG2	2.31	0.48
1:A:788:ILE:HG12	1:A:897:MET:HE1	1.94	0.48
1:A:151:VAL:CG2	1:A:223:VAL:HG23	2.43	0.48
1:A:900:ALA:C	1:A:903:VAL:HG12	2.34	0.48
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.48	0.48
1:A:227:GLY:O	1:A:230:THR:HG22	2.13	0.48
1:A:950:VAL:O	1:A:954:PRO:CG	2.57	0.48
1:A:670:CYS:HG	1:A:690:TYR:HD2	1.62	0.48
1:A:352:LYS:HD2	1:A:625:THR:HG21	1.96	0.48
1:A:897:MET:SD	1:A:958:LYS:HE2	2.54	0.48
1:A:950:VAL:CG1	1:A:951:ASP:H	2.27	0.48
1:A:397:LYS:HB3	1:A:402:ILE:CD1	2.41	0.48
1:A:415:THR:HA	1:A:475:ILE:HD13	1.95	0.48
1:A:857:MET:O	1:A:858:TYR:HB2	2.14	0.48
1:A:968:LEU:O	1:A:972:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:894:PRO:HB2	1:A:958:LYS:HB3	1.95	0.47
1:A:781:LEU:O	1:A:871:THR:HG23	2.14	0.47
1:A:715:GLU:C	1:A:716:ILE:HD12	2.35	0.47
1:A:85:ILE:HG23	1:A:86:THR:N	2.28	0.47
1:A:945:PHE:CD1	1:A:949:TYR:HE2	2.19	0.47
1:A:291:GLY:O	1:A:294:TYR:HB3	2.14	0.47
1:A:918:GLU:HG2	1:A:919:ASN:OD1	2.13	0.47
1:A:758:LYS:HG3	1:A:828:LEU:HD22	1.95	0.47
1:A:865:VAL:HG21	1:A:869:GLN:HB2	1.96	0.47
1:A:230:THR:HG23	1:A:233:GLY:H	1.78	0.47
1:A:771:GLU:O	1:A:774:CYS:HB3	2.14	0.47
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.49	0.47
1:A:527:TYR:HB2	1:A:592:THR:CG2	2.26	0.47
1:A:898:THR:CG2	1:A:958:LYS:HB2	2.44	0.47
1:A:153:VAL:HB	1:A:214:ILE:HD12	1.93	0.47
1:A:512:MET:O	1:A:566:THR:HA	2.15	0.47
1:A:355:THR:HG21	1:A:720:MET:CE	2.45	0.47
1:A:1:MET:SD	1:A:229:SER:HB3	2.55	0.47
1:A:527:TYR:CB	1:A:592:THR:HG22	2.26	0.47
1:A:687:ILE:O	1:A:691:LEU:HG	2.14	0.47
1:A:648:VAL:O	1:A:649:ALA:C	2.52	0.47
1:A:921:SER:OG	1:A:923:MET:HG2	2.15	0.47
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.97	0.47
1:A:94:ILE:O	1:A:97:ILE:HB	2.15	0.47
1:A:482:GLU:HG3	1:A:497:TYR:HD2	1.80	0.47
1:A:192:GLU:CD	1:A:580:ASP:HB2	2.34	0.46
1:A:361:MET:SD	1:A:601:ASP:HB2	2.55	0.46
1:A:766:SER:O	1:A:769:VAL:HB	2.16	0.46
1:A:896:PRO:O	1:A:899:MET:HB2	2.16	0.46
1:A:593:PHE:HZ	1:A:596:VAL:HG12	1.79	0.46
1:A:880:HIS:N	1:A:881:PRO:HD2	2.30	0.46
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.97	0.46
1:A:950:VAL:HG13	1:A:951:ASP:H	1.80	0.46
1:A:495:SER:HB3	1:A:514:VAL:HB	1.98	0.46
1:A:487:PHE:HA	1:A:493:SER:O	2.15	0.46
1:A:388:THR:C	1:A:390:ALA:H	2.19	0.46
1:A:388:THR:HG22	1:A:389:TYR:H	1.80	0.46
1:A:969:MET:HE3	1:A:969:MET:O	2.16	0.46
1:A:429:GLU:N	1:A:429:GLU:CD	2.69	0.46
1:A:628:ASN:OD1	1:A:631:THR:HB	2.16	0.46
1:A:895:GLU:HG3	1:A:959:LEU:HD11	1.96	0.46
1:A:405:GLY:C	1:A:407:PHE:H	2.19	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:788:ILE:HG22	1:A:790:VAL:H	1.80	0.46
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.46	0.46
1:A:949:TYR:C	1:A:950:VAL:O	2.53	0.46
1:A:181:THR:OG1	1:A:183:GLU:HG2	2.15	0.46
1:A:909:MET:HE3	1:A:937:ILE:CA	2.43	0.46
1:A:174:ARG:NE	1:A:188:ILE:HG12	2.31	0.46
1:A:546:LEU:O	1:A:549:ILE:HB	2.15	0.45
1:A:480:LYS:N	1:A:499:SER:O	2.35	0.45
1:A:760:PHE:C	1:A:760:PHE:CD1	2.90	0.45
1:A:44:GLU:OE2	1:A:117:GLU:HB2	2.16	0.45
1:A:408:ASP:O	1:A:409:GLY:C	2.54	0.45
1:A:953:LEU:N	1:A:954:PRO:CD	2.79	0.45
1:A:372:VAL:HG13	1:A:541:VAL:HG22	1.97	0.45
1:A:596:VAL:HG23	1:A:597:VAL:N	2.30	0.45
1:A:177:GLN:NE2	1:A:189:LYS:HZ3	2.13	0.45
1:A:65:LEU:HA	1:A:65:LEU:HD23	1.83	0.45
1:A:39:ASN:CG	1:A:226:THR:OG1	2.54	0.45
1:A:666:GLN:HG2	1:A:690:TYR:CE2	2.52	0.45
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.97	0.45
1:A:733:MET:HE1	1:A:746:ALA:CB	2.46	0.45
1:A:331:ALA:HB1	1:A:733:MET:HE2	1.98	0.45
1:A:388:THR:HG22	1:A:390:ALA:N	2.32	0.45
1:A:684:LYS:O	1:A:688:VAL:HG23	2.17	0.45
1:A:498:CYS:O	1:A:510:ASN:HA	2.16	0.45
1:A:33:LEU:HD11	1:A:38:HIS:ND1	2.32	0.45
1:A:408:ASP:O	1:A:410:LEU:N	2.50	0.45
1:A:895:GLU:CG	1:A:959:LEU:HD11	2.47	0.45
1:A:446:THR:O	1:A:449:VAL:HB	2.16	0.45
1:A:834:PHE:O	1:A:838:MET:HB2	2.17	0.45
1:A:837:TYR:HB2	2:A:1995:TG1:C33	2.47	0.45
1:A:222:ILE:O	1:A:222:ILE:HG23	2.16	0.45
1:A:270:ALA:O	1:A:274:ILE:HG12	2.17	0.45
1:A:568:ASP:OD2	1:A:592:THR:HG21	2.17	0.45
1:A:202:GLN:OE1	1:A:489:ARG:NH1	2.50	0.44
1:A:642:PHE:CZ	1:A:648:VAL:HG13	2.52	0.44
1:A:166:LEU:HD11	1:A:222:ILE:HB	1.99	0.44
1:A:984:LEU:HA	1:A:987:ILE:HG12	1.99	0.44
1:A:783:LEU:HD12	1:A:784:PRO:CD	2.48	0.44
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.18	0.44
1:A:974:SER:C	1:A:976:PRO:HD2	2.38	0.44
1:A:969:MET:HE3	1:A:972:LYS:HG3	1.99	0.44
1:A:50:TRP:O	1:A:54:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:539:GLY:N	1:A:540:PRO:HD2	2.33	0.44
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.84	0.44
1:A:278:HIS:HA	1:A:282:PRO:CD	2.48	0.44
1:A:242:THR:HG23	1:A:712:LYS:NZ	2.33	0.44
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.82	0.44
1:A:717:GLY:O	1:A:731:SER:HB2	2.18	0.44
1:A:395:VAL:C	1:A:396:LEU:HD23	2.38	0.44
1:A:886:LEU:N	1:A:886:LEU:HD23	2.33	0.44
1:A:865:VAL:CG1	1:A:869:GLN:HB2	2.41	0.44
1:A:909:MET:HE3	1:A:937:ILE:HG23	2.00	0.44
1:A:39:ASN:OD1	1:A:226:THR:OG1	2.33	0.44
1:A:383:SER:C	1:A:384:ILE:HD12	2.38	0.44
1:A:559:LEU:CD2	1:A:600:LEU:HB2	2.46	0.43
1:A:482:GLU:HG3	1:A:497:TYR:CD2	2.53	0.43
1:A:628:ASN:O	1:A:628:ASN:OD1	2.36	0.43
1:A:949:TYR:O	1:A:950:VAL:O	2.36	0.43
1:A:865:VAL:HG11	1:A:869:GLN:H	1.83	0.43
1:A:147:PRO:HA	1:A:223:VAL:CG1	2.49	0.43
1:A:38:HIS:CD2	1:A:143:ARG:HH22	2.36	0.43
1:A:412:GLU:O	1:A:415:THR:N	2.52	0.43
1:A:411:VAL:HA	1:A:454:VAL:HG21	2.00	0.43
1:A:236:ARG:HG2	1:A:236:ARG:O	2.17	0.43
1:A:90:GLU:OE2	1:A:789:PRO:HB2	2.19	0.43
1:A:790:VAL:HB	1:A:957:PHE:CE1	2.53	0.43
1:A:444:ALA:O	1:A:447:THR:N	2.51	0.43
1:A:281:ASP:H	1:A:282:PRO:CD	2.32	0.43
1:A:543:GLU:OE1	1:A:543:GLU:HA	2.17	0.43
1:A:423:SER:OG	1:A:442:GLU:HB2	2.19	0.43
1:A:654:THR:HG22	1:A:657:GLU:H	1.82	0.43
1:A:784:PRO:HG3	1:A:873:PHE:CG	2.54	0.43
1:A:340:GLU:O	1:A:343:GLY:N	2.52	0.43
1:A:870:LEU:O	1:A:870:LEU:HD12	2.19	0.43
1:A:792:LEU:O	1:A:795:VAL:HB	2.19	0.43
1:A:283:VAL:O	1:A:284:HIS:C	2.56	0.43
1:A:585:MET:O	1:A:589:THR:HG23	2.18	0.43
1:A:980:LEU:O	1:A:980:LEU:HD12	2.19	0.43
1:A:407:PHE:O	1:A:411:VAL:HG13	2.19	0.43
1:A:106:VAL:HG13	1:A:107:TRP:N	2.34	0.43
1:A:521:VAL:CG2	1:A:563:ALA:CB	2.90	0.43
1:A:521:VAL:HG23	1:A:522:ILE:N	2.34	0.42
1:A:79:GLU:OE1	1:A:79:GLU:N	2.52	0.42
1:A:178:SER:C	1:A:180:LEU:N	2.72	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:783:LEU:CD1	1:A:784:PRO:HD2	2.49	0.42
1:A:370:ASP:HB3	1:A:378:SER:O	2.19	0.42
1:A:142:ALA:HA	1:A:145:ILE:CD1	2.49	0.42
1:A:546:LEU:O	1:A:549:ILE:N	2.52	0.42
1:A:933:LEU:O	1:A:937:ILE:HG13	2.19	0.42
1:A:391:PRO:HD2	1:A:434:TYR:CD2	2.54	0.42
1:A:966:GLN:O	1:A:970:VAL:HG23	2.20	0.42
1:A:524:ARG:HD2	1:A:588:GLU:O	2.18	0.42
1:A:791:GLN:H	1:A:791:GLN:HG3	1.62	0.42
1:A:716:ILE:N	1:A:716:ILE:HD12	2.34	0.42
1:A:894:PRO:CG	1:A:959:LEU:HG	2.50	0.42
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.45	0.42
1:A:449:VAL:HG21	1:A:472:ASN:HD21	1.85	0.42
1:A:500:PRO:HG3	1:A:509:GLY:HA2	2.00	0.42
1:A:840:ILE:O	1:A:843:TYR:HB3	2.20	0.42
1:A:277:GLY:C	1:A:279:PHE:N	2.73	0.42
1:A:1:MET:SD	1:A:229:SER:CB	3.08	0.42
1:A:748:GLU:CA	1:A:817:MET:HE3	2.48	0.42
1:A:200:VAL:O	1:A:201:ASN:C	2.58	0.42
1:A:24:LEU:HD22	1:A:149:ASP:CB	2.44	0.42
1:A:32:HIS:HB2	1:A:146:VAL:HG11	2.00	0.42
1:A:63:ARG:O	1:A:66:LEU:N	2.53	0.42
1:A:560:ARG:HH21	3:A:1996:ACP:H8	1.79	0.42
1:A:440:ALA:HA	1:A:443:THR:CG2	2.49	0.42
1:A:839:ALA:O	1:A:840:ILE:C	2.58	0.42
1:A:174:ARG:HA	1:A:187:VAL:O	2.20	0.42
1:A:684:LYS:HD3	1:A:700:MET:CE	2.49	0.42
1:A:472:ASN:HA	1:A:472:ASN:HD22	1.75	0.41
1:A:653:TYR:O	1:A:676:PHE:HA	2.19	0.41
1:A:49:LEU:HA	1:A:52:LEU:HD12	2.02	0.41
1:A:283:VAL:O	1:A:283:VAL:HG23	2.20	0.41
1:A:205:LYS:NZ	1:A:488:SER:HB3	2.35	0.41
1:A:163:ILE:HB	1:A:208:LEU:HB2	2.01	0.41
1:A:336:LEU:N	1:A:337:PRO:CD	2.84	0.41
1:A:372:VAL:HG11	1:A:541:VAL:HG21	2.01	0.41
1:A:178:SER:O	1:A:181:THR:N	2.54	0.41
1:A:278:HIS:CA	1:A:282:PRO:HG2	2.50	0.41
1:A:6:SER:HA	1:A:194:VAL:O	2.19	0.41
1:A:424:SER:O	1:A:437:VAL:HB	2.20	0.41
1:A:801:GLY:O	1:A:805:THR:HG23	2.19	0.41
1:A:865:VAL:C	1:A:867:TYR:H	2.22	0.41
1:A:367:PHE:CE2	1:A:596:VAL:HG13	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:388:THR:CG2	1:A:389:TYR:H	2.34	0.41
1:A:92:PHE:O	1:A:96:LEU:HG	2.21	0.41
1:A:836:ARG:HH21	1:A:981:ASP:CG	2.24	0.41
1:A:59:ASP:CB	1:A:62:VAL:HG12	2.45	0.41
1:A:18:VAL:CG2	1:A:19:SER:N	2.84	0.41
1:A:116:ILE:HG23	1:A:236:ARG:HG3	2.03	0.41
1:A:474:VAL:CG2	1:A:475:ILE:N	2.84	0.41
1:A:247:THR:CG2	1:A:249:LEU:H	2.32	0.41
1:A:733:MET:HE1	1:A:746:ALA:HB1	2.03	0.41
1:A:701:THR:HA	1:A:718:ILE:O	2.21	0.41
1:A:653:TYR:CE2	1:A:669:ALA:HB1	2.55	0.41
1:A:535:VAL:CG1	1:A:536:PRO:HD2	2.49	0.41
1:A:320:ALA:O	1:A:323:THR:HB	2.20	0.41
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.93	0.41
1:A:862:GLY:H	1:A:863:PRO:CD	2.21	0.41
1:A:909:MET:HE2	1:A:940:SER:HB2	2.02	0.41
1:A:601:ASP:HA	1:A:602:PRO:HD2	1.83	0.41
1:A:854:TRP:O	1:A:857:MET:O	2.38	0.41
1:A:151:VAL:HG21	1:A:223:VAL:HG23	2.03	0.40
1:A:854:TRP:O	1:A:857:MET:N	2.55	0.40
1:A:930:ASN:OD1	1:A:932:TRP:HB2	2.21	0.40
1:A:873:PHE:HB2	1:A:891:PHE:CG	2.56	0.40
1:A:898:THR:CG2	1:A:958:LYS:CB	2.99	0.40
1:A:411:VAL:CA	1:A:454:VAL:HG11	2.50	0.40
1:A:1:MET:HA	1:A:224:ALA:O	2.20	0.40
1:A:954:PRO:HA	1:A:958:LYS:O	2.21	0.40
1:A:178:SER:O	1:A:182:GLY:N	2.55	0.40
1:A:483:PHE:CE1	1:A:485:LEU:HD21	2.53	0.40
1:A:517:ALA:HA	3:A:1996:ACP:O2'	2.21	0.40
1:A:352:LYS:HB3	1:A:625:THR:HG22	1.98	0.40
1:A:991:TYR:CG	1:A:992:LEU:N	2.89	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	992/994 (100%)	864 (87%)	101 (10%)	27 (3%)	8	25

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ILE
1	A	453	ASN
1	A	882	HIS
1	A	884	GLU
1	A	958	LYS
1	A	960	LYS
1	A	278	HIS
1	A	663	LEU
1	A	950	VAL
1	A	47	LYS
1	A	284	HIS
1	A	649	ALA
1	A	878	GLU
1	A	155	VAL
1	A	438	GLY
1	A	863	PRO
1	A	88	PHE
1	A	108	GLN
1	A	179	ILE
1	A	281	ASP
1	A	409	GLY
1	A	975	LEU
1	A	289	ILE
1	A	681	PRO
1	A	865	VAL
1	A	862	GLY
1	A	951	ASP

### 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%)	803 (96%)	37 (4%)	39	75

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	24	LEU
1	A	88	PHE
1	A	160	PRO
1	A	179	ILE
1	A	228	VAL
1	A	232	ILE
1	A	247	THR
1	A	316	THR
1	A	338	SER
1	A	344	CYS
1	A	346	SER
1	A	353	THR
1	A	367	PHE
1	A	378	SER
1	A	396	LEU
1	A	441	THR
1	A	472	ASN
1	A	484	THR
1	A	490	ASP
1	A	494	MET
1	A	514	VAL
1	A	519	GLU
1	A	534	ARG
1	A	537	MET
1	A	638	ARG
1	A	698	THR
1	A	760	PHE
1	A	789	PRO
1	A	790	VAL
1	A	805	THR
1	A	816	ILE
1	A	844	VAL
1	A	867	TYR
1	A	910	CYS
1	A	925	MET
1	A	954	PRO

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

Mol	Chain	Res	Type
1	A	138	GLN
1	A	177	GLN
1	A	472	ASN
1	A	526	ASN
1	A	683	HIS
1	A	706	ASN
1	A	759	GLN
1	A	796	ASN
1	A	875	GLN
1	A	914	ASN
1	A	944	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	TG1	A	1995	-	48,48,48	2.11	15 (31%)	72,72,72	2.02	19 (26%)
3	ACP	A	1996	4	33,33,33	4.01	9 (27%)	52,52,52	2.30	16 (30%)



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	TG1	A	1995	-	-	0/33/99/99	0/0/3/3
3	ACP	A	1996	4	-	0/20/38/38	0/1/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1996	ACP	PB-C3B	-19.54	1.62	1.79
3	A	1996	ACP	PG-C3B	-8.59	1.72	1.79
2	A	1995	TG1	C6-C5	7.75	1.59	1.50
2	A	1995	TG1	O4-C21	5.45	1.33	1.21
3	A	1996	ACP	PB-O2B	-3.95	1.46	1.56
2	A	1995	TG1	O3-C3	3.66	1.52	1.44
2	A	1995	TG1	C7-C8	3.40	1.59	1.53
2	A	1995	TG1	O1-C13	3.34	1.44	1.34
2	A	1995	TG1	O6-C7	3.25	1.49	1.43
3	A	1996	ACP	C2'-C1'	-3.22	1.48	1.53
2	A	1995	TG1	C34-C11	3.02	1.57	1.53
2	A	1995	TG1	C10-C1	2.92	1.62	1.54
3	A	1996	ACP	PG-O2G	-2.78	1.49	1.54
2	A	1995	TG1	C31-C10	2.46	1.58	1.52
2	A	1995	TG1	O7-C27	2.43	1.41	1.34
3	A	1996	ACP	C2-N3	2.36	1.36	1.32
2	A	1995	TG1	C21-C22	2.31	1.59	1.50
2	A	1995	TG1	C1-C2	2.19	1.58	1.54
2	A	1995	TG1	C4-C5	2.19	1.37	1.33
2	A	1995	TG1	O11-C11	2.19	1.47	1.42
3	A	1996	ACP	C1'-N9	2.12	1.55	1.48
3	A	1996	ACP	C3'-C4'	-2.09	1.47	1.53
2	A	1995	TG1	C9-C8	2.06	1.54	1.52
3	A	1996	ACP	C5-N7	-2.01	1.32	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1996	ACP	N3-C2-N1	-6.61	123.18	128.71
2	A	1995	TG1	O12-C12-C11	-6.00	124.38	128.26
2	A	1995	TG1	C10-O9-C32	5.71	136.82	122.10
2	A	1995	TG1	O3-C3-C2	-5.02	99.69	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1996	ACP	O2B-PB-C3B	4.94	117.98	106.61
3	A	1996	ACP	C8-N9-C4	-4.53	103.44	106.90
3	A	1996	ACP	O3A-PB-O1B	-4.51	101.95	111.51
3	A	1996	ACP	O5'-C5'-C4'	4.27	124.63	108.94
2	A	1995	TG1	O5-C6-C7	-4.18	99.21	104.28
3	A	1996	ACP	O3G-PG-C3B	-4.15	96.34	106.40
2	A	1995	TG1	C7-C6-C5	4.09	124.88	115.55
3	A	1996	ACP	C5'-C4'-C3'	-3.89	99.62	115.21
3	A	1996	ACP	C4-C5-N7	3.74	112.73	109.52
3	A	1996	ACP	O3A-PB-C3B	3.58	117.90	106.62
3	A	1996	ACP	PA-O3A-PB	3.47	142.18	131.74
2	A	1995	TG1	C11-C7-C6	-3.38	96.63	102.71
2	A	1995	TG1	O11-C11-C7	3.13	119.60	107.52
2	A	1995	TG1	C6-O5-C12	-3.13	106.13	110.79
3	A	1996	ACP	C8-N9-C1'	3.00	132.29	126.38
2	A	1995	TG1	C9-C10-C1	2.99	120.45	114.04
2	A	1995	TG1	C6-C5-C4	2.98	128.45	123.41
2	A	1995	TG1	C24-C22-C21	2.90	133.41	120.66
2	A	1995	TG1	C3-O3-C21	2.76	120.30	116.40
2	A	1995	TG1	O5-C12-O12	2.76	125.81	121.67
2	A	1995	TG1	O9-C10-C31	-2.53	97.47	107.74
2	A	1995	TG1	C23-C22-C21	-2.52	109.44	116.05
3	A	1996	ACP	O2A-PA-O5'	2.48	121.04	108.51
2	A	1995	TG1	O9-C10-C1	2.40	112.56	103.50
2	A	1995	TG1	C2-O1-C13	-2.37	114.12	117.92
2	A	1995	TG1	C1-C2-C3	2.36	108.93	104.83
3	A	1996	ACP	C6-C5-C4	-2.36	112.92	117.25
3	A	1996	ACP	O1B-PB-C3B	-2.36	103.58	109.49
3	A	1996	ACP	O4'-C1'-N9	-2.35	106.26	108.44
2	A	1995	TG1	O11-C11-C12	-2.29	99.84	105.80
3	A	1996	ACP	O2G-PG-C3B	2.02	111.31	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	994/994 (100%)	0.17	75 (7%)	14 12	16, 59, 133, 185	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	994	GLY	11.7
1	A	877	THR	11.5
1	A	881	PRO	8.2
1	A	281	ASP	8.1
1	A	286	GLY	7.5
1	A	878	GLU	7.3
1	A	505	ARG	6.9
1	A	992	LEU	6.2
1	A	283	VAL	5.8
1	A	507	ALA	5.4
1	A	964	LEU	5.4
1	A	78	PHE	5.1
1	A	504	SER	5.1
1	A	184	SER	5.0
1	A	951	ASP	4.8
1	A	876	CYS	4.8
1	A	80	GLU	4.8
1	A	879	ASP	4.7
1	A	957	PHE	4.5
1	A	993	GLU	4.4
1	A	1	MET	4.4
1	A	84	THR	4.2
1	A	280	ASN	4.2
1	A	46	GLY	4.2
1	A	880	HIS	4.1
1	A	503	SER	4.0
1	A	888	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	959	LEU	3.8
1	A	461	ASN	3.8
1	A	82	GLU	3.7
1	A	282	PRO	3.7
1	A	861	ASP	3.7
1	A	50	TRP	3.7
1	A	502	LYS	3.5
1	A	963	ASP	3.4
1	A	433	VAL	3.4
1	A	47	LYS	3.3
1	A	81	GLY	3.3
1	A	991	TYR	3.3
1	A	427	PHE	3.2
1	A	279	PHE	3.2
1	A	767	SER	3.2
1	A	435	GLU	3.1
1	A	858	TYR	3.1
1	A	428	ASN	3.0
1	A	284	HIS	3.0
1	A	430	THR	3.0
1	A	924	ARG	3.0
1	A	886	LEU	3.0
1	A	960	LYS	2.9
1	A	506	ALA	2.9
1	A	287	SER	2.9
1	A	949	TYR	2.8
1	A	288	TRP	2.7
1	A	54	ILE	2.7
1	A	508	VAL	2.6
1	A	768	ASN	2.6
1	A	77	TRP	2.6
1	A	431	LYS	2.5
1	A	509	GLY	2.4
1	A	107	TRP	2.4
1	A	258	GLU	2.4
1	A	113	GLU	2.4
1	A	290	ARG	2.3
1	A	106	VAL	2.3
1	A	681	PRO	2.2
1	A	986	PHE	2.2
1	A	854	TRP	2.1
1	A	955	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	462	LEU	2.1
1	A	923	MET	2.1
1	A	605	LYS	2.1
1	A	928	TRP	2.1
1	A	305	ALA	2.0
1	A	285	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	A	1997	1/1	1.81	165.25	66,66,66,66	1
3	ACP	A	1996	31/31	0.52	12.74	29,33,36,36	31
5	NA	A	1998	1/1	0.24	2.16	41,41,41,41	0
2	TG1	A	1995	46/46	0.23	0.41	63,74,89,89	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.