Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:39 PM GMT

PDB ID	:	4J2T
Title	:	Inhibitor-bound Ca2+ ATPase
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Deposited on	:	2013-02-05
Resolution	:	3.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
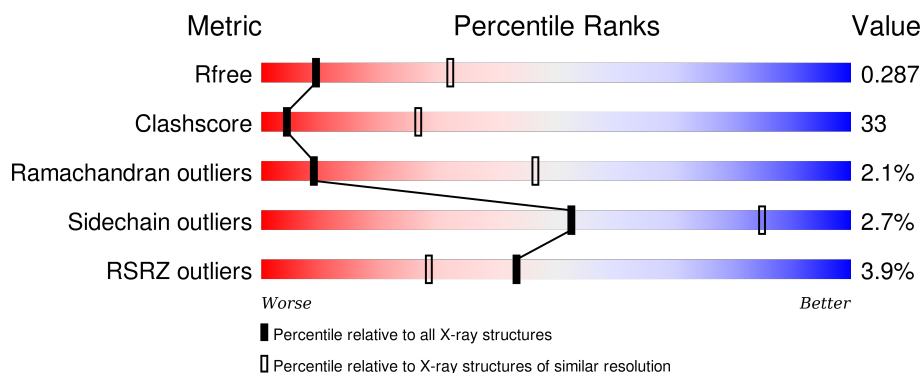
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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.

Mol	Chain	Length	Quality of chain
1	A	994	

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	1HT	A	1001	-	-	-	X

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| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PTY	A	1002	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7748 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 SERCA1a.

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

- Molecule 2 is (3S,3AR,4S,6S,6AR,7S,8S,9BS)-6-(ACETYLOXY)-3A,4-BIS(BUTANOYLO XY)-3-HYDROXY-3,6,9-TRIMETHYL-8-{[(2E)-2-METHYLBUT-2-ENOYL]OXY}-2-O XO-2,3,3A,4,5,6,6A,7,8,9B-DECAHYDROAZULENO[4,5-B]FURAN-7-YL OCTANOATE (three-letter code: 1HT) (formula: $C_{38}H_{56}O_{13}$).
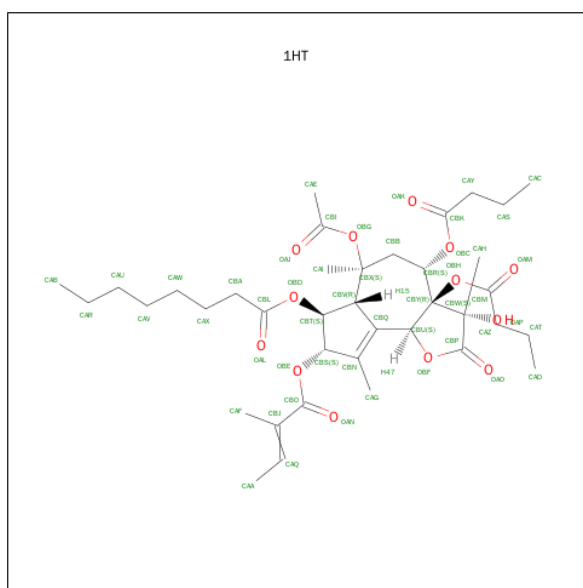
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 51	C 38	O 13	0	0

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

PTY
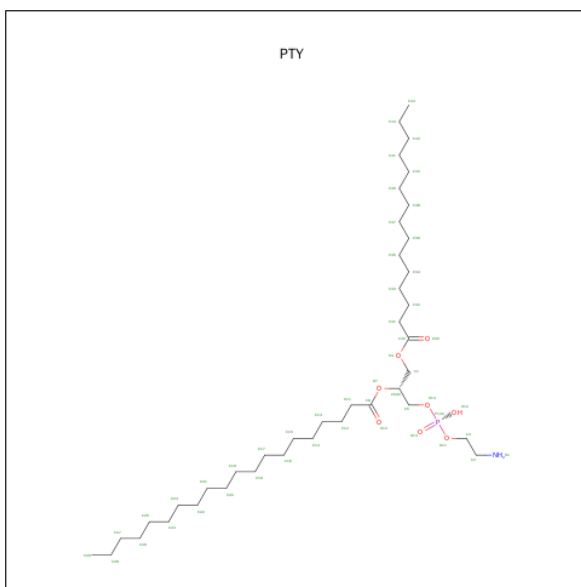
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	24	14	1	8	1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
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: SERCA1a

C888 E889 I890 F891 E892 A893 P894 E895 P896 M897 T898 M899 A900 L901 S902 V903 L904 V905 T906 I907 E908 M909 L916 S917 Q920 R924 M925 P926 P927 W928 V929 L933 S936 I937 M941 H944 Y949 V950 D951 P952 L953 P954 F957 K958 L959 K960 A961 L962 Q966 W967

L968 M969 V970 L971 K972 I973 S974 L975 P976 V977 I978 G979 I983 L984 K985 F986 N990 Y991 L992 E993 G994
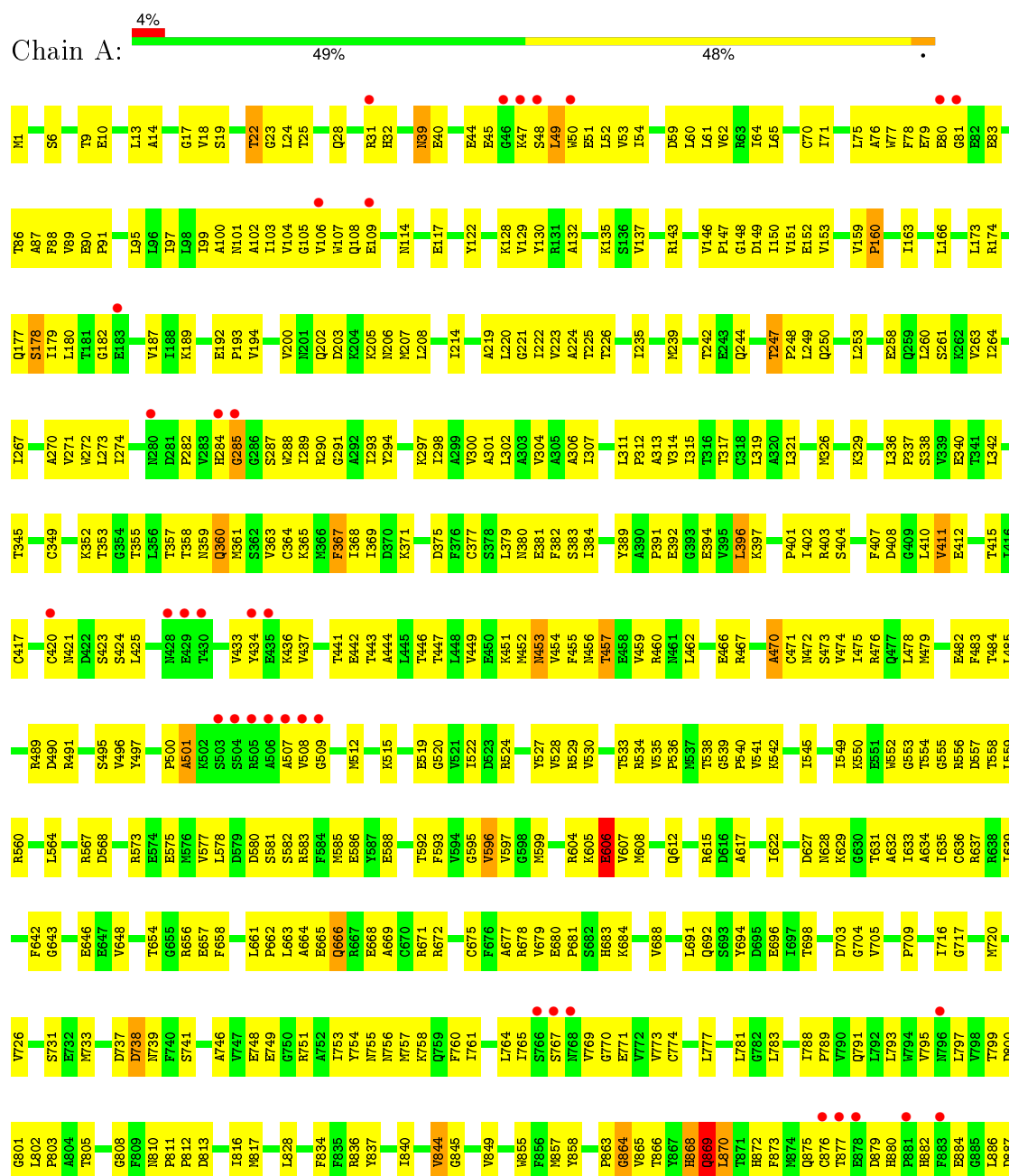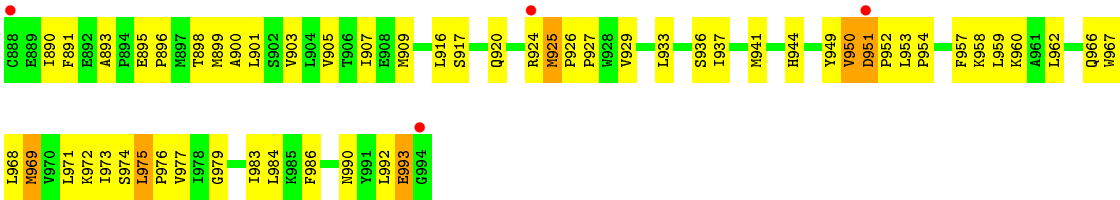
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	70.90Å 70.90Å 587.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 3.20 28.71 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.71-3.20) 99.6 (28.71-3.01)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$<I/\sigma(I)>$ [1]	2.88 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.260 , 0.286 0.267 , 0.287	Depositor DCC
R_{free} test set	1669 reflections (6.80%)	DCC
Wilson B-factor (Å^2)	73.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\lvert L \rvert> = 0.35, <L^2> = 0.18$	Xtriage
Outliers	0 of 31414 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7748	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PTY, 1HT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.46	1/7812 (0.0%)	0.69	1/10592 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ASN	C-N	-5.05	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	870	LEU	N-CA-C	-5.64	95.78	111.00

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	7671	0	7764	515	0
2	A	51	0	55	8	0
3	A	24	0	21	4	0
4	A	1	0	0	0	0
5	A	1	0	0	2	0
All	All	7748	0	7840	515	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 33.

All (515) 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:527:TYR:HB2	1:A:592:THR:CG2	1.45	1.45
1:A:527:TYR:CB	1:A:592:THR:HG22	1.40	1.45
1:A:483:PHE:CE1	1:A:578:LEU:HD21	1.73	1.22
1:A:534:ARG:HD2	1:A:592:THR:HG21	1.40	1.02
1:A:834:PHE:HE2	2:A:1001:1HT:OAM	1.43	1.01
1:A:425:LEU:HD11	1:A:447:THR:HG22	1.44	0.99
1:A:863:PRO:HG3	1:A:890:ILE:HD13	1.42	0.99
1:A:247:THR:HG22	1:A:250:GLN:H	1.24	0.98
1:A:483:PHE:CE1	1:A:578:LEU:CD2	2.48	0.96
1:A:311:LEU:HD13	1:A:764:LEU:HD12	1.49	0.94
1:A:909:MET:HE3	1:A:937:ILE:HG12	1.47	0.94
1:A:97:ILE:HD11	1:A:797:LEU:HD11	1.50	0.94
1:A:483:PHE:CZ	1:A:578:LEU:HD21	2.02	0.93
1:A:32:HIS:HB3	1:A:146:VAL:HG11	1.48	0.93
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.51	0.93
1:A:304:VAL:HB	1:A:793:LEU:HD21	1.48	0.93
1:A:65:LEU:HG	1:A:307:ILE:CD1	2.00	0.90
1:A:248:PRO:HG2	1:A:340:GLU:OE2	1.73	0.89
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.54	0.89
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.56	0.87
1:A:880:HIS:HA	1:A:884:GLU:HB2	1.57	0.87
1:A:535:VAL:HG13	1:A:536:PRO:HD2	1.55	0.86
1:A:1:MET:HB2	1:A:225:THR:HG22	1.57	0.86
1:A:527:TYR:CG	1:A:592:THR:HG22	2.11	0.84
1:A:361:MET:HE3	1:A:599:MET:HG3	1.59	0.83
1:A:1:MET:HA	1:A:224:ALA:O	1.79	0.83
1:A:75:LEU:HD13	1:A:297:LYS:HB3	1.60	0.82
1:A:834:PHE:CE2	2:A:1001:1HT:OAM	2.31	0.82
1:A:879:ASP:OD1	1:A:882:HIS:HB3	1.80	0.81
1:A:453:ASN:HB3	1:A:471:CYS:SG	2.21	0.81
1:A:558:THR:HG22	1:A:634:ALA:CB	2.12	0.80
1:A:47:LYS:HA	1:A:51:GLU:OE1	1.81	0.80
1:A:628:ASN:HB3	1:A:678:ARG:NH2	1.95	0.80
1:A:986:PHE:CZ	1:A:990:ASN:OD1	2.34	0.80
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.64	0.80
1:A:287:SER:HB2	1:A:290:ARG:HB3	1.63	0.79
1:A:986:PHE:CE1	1:A:990:ASN:OD1	2.36	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:O	1:A:274:ILE:HG12	1.82	0.79
1:A:396:LEU:HD23	1:A:401:PRO:HA	1.64	0.78
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.65	0.78
1:A:857:MET:O	1:A:858:TYR:HB2	1.83	0.78
1:A:65:LEU:HG	1:A:307:ILE:HD12	1.65	0.78
1:A:267:ILE:HD11	2:A:1001:1HT:H2	1.65	0.77
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.14	0.76
1:A:106:VAL:C	1:A:108:GLN:H	1.88	0.76
1:A:239:MET:O	1:A:242:THR:HG22	1.85	0.76
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.16	0.76
1:A:549:ILE:HD11	1:A:596:VAL:HG11	1.66	0.76
1:A:342:LEU:O	1:A:345:THR:HG23	1.86	0.74
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.69	0.74
1:A:628:ASN:HB3	1:A:678:ARG:HH21	1.52	0.74
1:A:247:THR:HG22	1:A:250:GLN:N	2.01	0.74
1:A:769:VAL:HG22	2:A:1001:1HT:H58	1.68	0.73
1:A:748:GLU:HA	1:A:817:MET:HE3	1.68	0.73
1:A:865:VAL:HG23	1:A:868:HIS:NE2	2.02	0.73
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.71	0.73
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.71	0.72
1:A:751:ARG:HD2	1:A:817:MET:CE	2.19	0.72
1:A:106:VAL:C	1:A:108:GLN:N	2.41	0.72
1:A:969:MET:HA	1:A:969:MET:HE3	1.72	0.72
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.72	0.71
1:A:654:THR:HG22	1:A:657:GLU:CG	2.19	0.71
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.20	0.71
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.71	0.71
1:A:717:GLY:O	1:A:731:SER:HB2	1.91	0.71
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.73	0.71
1:A:65:LEU:HG	1:A:307:ILE:HD13	1.74	0.70
1:A:441:THR:HG21	1:A:560:ARG:NH1	2.07	0.70
1:A:535:VAL:CG1	1:A:536:PRO:HD2	2.20	0.69
1:A:870:LEU:O	1:A:873:PHE:HB3	1.92	0.69
1:A:361:MET:HE2	1:A:441:THR:HG22	1.75	0.69
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.75	0.68
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.75	0.68
1:A:813:ASP:O	1:A:816:ILE:HG13	1.93	0.68
1:A:97:ILE:CD1	1:A:797:LEU:HD11	2.21	0.68
1:A:969:MET:O	1:A:973:ILE:HG13	1.93	0.68
1:A:971:LEU:HD22	1:A:975:LEU:HD11	1.74	0.68
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:PHE:HB2	1:A:457:THR:HG23	1.74	0.68
1:A:79:GLU:HG3	1:A:87:ALA:CB	2.25	0.67
1:A:530:VAL:HG23	1:A:533:THR:OG1	1.95	0.67
1:A:192:GLU:OE1	1:A:580:ASP:HB2	1.95	0.67
1:A:909:MET:CE	1:A:937:ILE:HA	2.25	0.67
1:A:791:GLN:HB3	1:A:901:LEU:CD1	2.24	0.67
1:A:411:VAL:O	1:A:415:THR:HG23	1.94	0.67
1:A:179:ILE:HG13	1:A:180:LEU:N	2.09	0.66
1:A:837:TYR:HB2	2:A:1001:1HT:H16	1.77	0.66
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.77	0.66
1:A:757:MET:HA	1:A:760:PHE:CE2	2.30	0.66
1:A:903:VAL:O	1:A:907:ILE:HG13	1.96	0.65
1:A:541:VAL:O	1:A:545:ILE:HG13	1.96	0.65
1:A:781:LEU:HB2	1:A:783:LEU:HD13	1.77	0.65
1:A:235:ILE:HG23	1:A:709:PRO:HG3	1.78	0.65
1:A:863:PRO:CG	1:A:890:ILE:HD13	2.22	0.65
1:A:857:MET:HA	1:A:864:GLY:HA2	1.79	0.65
1:A:553:GLY:O	1:A:631:THR:HG22	1.96	0.65
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.77	0.65
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.79	0.65
1:A:397:LYS:HB3	1:A:402:ILE:HD11	1.78	0.65
1:A:105:GLY:O	1:A:108:GLN:HB3	1.96	0.65
1:A:247:THR:HG23	1:A:340:GLU:OE1	1.96	0.65
1:A:527:TYR:CD2	1:A:592:THR:CG2	2.80	0.64
1:A:44:GLU:H	1:A:44:GLU:CD	1.99	0.64
1:A:951:ASP:O	1:A:954:PRO:HD2	1.96	0.64
1:A:99:ILE:O	1:A:103:ILE:HG12	1.97	0.64
1:A:153:VAL:HB	1:A:214:ILE:HD11	1.78	0.64
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.27	0.64
1:A:606:GLU:CD	1:A:606:GLU:H	2.00	0.64
1:A:527:TYR:CB	1:A:592:THR:CG2	2.30	0.64
1:A:527:TYR:HB2	1:A:592:THR:CB	2.23	0.64
1:A:49:LEU:O	1:A:53:VAL:HG23	1.98	0.64
1:A:304:VAL:HB	1:A:793:LEU:CD2	2.24	0.64
1:A:282:PRO:HB2	1:A:284:HIS:NE2	2.13	0.64
1:A:484:THR:HG22	1:A:496:VAL:HG12	1.80	0.64
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.25	0.64
1:A:9:THR:HG23	1:A:166:LEU:HD22	1.79	0.63
1:A:420:CYS:SG	1:A:515:LYS:HG2	2.39	0.63
1:A:527:TYR:CD2	1:A:592:THR:HG22	2.33	0.63
1:A:192:GLU:OE1	1:A:580:ASP:CB	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HB2	1:A:83:GLU:OE1	1.97	0.63
1:A:18:VAL:CG2	1:A:24:LEU:HD23	2.29	0.63
1:A:662:PRO:HG2	1:A:665:GLU:OE1	1.98	0.63
1:A:317:THR:O	1:A:321:LEU:HG	1.99	0.63
1:A:869:GLN:CB	1:A:872:HIS:ND1	2.62	0.62
1:A:244:GLN:HB3	5:A:1101:HOH:O	1.98	0.62
1:A:483:PHE:CD1	1:A:578:LEU:CD2	2.82	0.62
1:A:508:VAL:HG23	1:A:508:VAL:O	2.00	0.62
1:A:263:VAL:HG11	2:A:1001:1HT:OAN	2.00	0.62
1:A:65:LEU:CG	1:A:307:ILE:HD12	2.30	0.62
1:A:907:ILE:HG12	1:A:974:SER:CB	2.30	0.61
1:A:577:VAL:HG21	1:A:583:ARG:NH1	2.15	0.61
1:A:962:LEU:HD12	1:A:967:TRP:CD1	2.35	0.61
1:A:6:SER:HA	1:A:194:VAL:O	2.01	0.61
1:A:629:LYS:HA	1:A:632:ALA:HB3	1.83	0.61
1:A:358:THR:HG22	1:A:360:GLN:HG3	1.82	0.61
1:A:59:ASP:O	1:A:62:VAL:HG12	2.01	0.61
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.36	0.61
1:A:45:GLU:OE2	1:A:47:LYS:HG3	2.00	0.61
1:A:870:LEU:HD12	1:A:891:PHE:HE1	1.66	0.61
1:A:203:ASP:HA	1:A:205:LYS:HE3	1.81	0.61
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.36	0.61
1:A:483:PHE:CD2	1:A:578:LEU:HD11	2.36	0.60
1:A:900:ALA:HA	1:A:903:VAL:HG12	1.82	0.60
1:A:748:GLU:HA	1:A:817:MET:CE	2.31	0.60
1:A:865:VAL:HG23	1:A:868:HIS:CD2	2.36	0.60
1:A:22:THR:HG23	1:A:132:ALA:HB2	1.83	0.60
1:A:545:ILE:O	1:A:549:ILE:HG12	2.02	0.60
1:A:367:PHE:CD1	1:A:379:LEU:HD23	2.37	0.60
1:A:836:ARG:O	1:A:840:ILE:HG12	2.00	0.60
1:A:500:PRO:O	1:A:501:ALA:HB3	2.02	0.60
1:A:900:ALA:O	1:A:903:VAL:HG12	2.02	0.60
1:A:24:LEU:HG	1:A:149:ASP:HA	1.83	0.59
1:A:65:LEU:CD2	1:A:307:ILE:HD12	2.32	0.59
1:A:876:CYS:SG	1:A:884:GLU:HG2	2.42	0.59
1:A:636:CYS:HB3	1:A:642:PHE:CD2	2.37	0.59
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.32	0.58
1:A:415:THR:HA	1:A:475:ILE:HD13	1.86	0.58
1:A:9:THR:HG23	1:A:166:LEU:CD2	2.33	0.58
1:A:441:THR:HA	1:A:599:MET:HE2	1.84	0.58
1:A:193:PRO:HA	1:A:206:ASN:ND2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:SER:HA	1:A:476:ARG:HD2	1.84	0.58
1:A:895:GLU:N	1:A:896:PRO:HD2	2.17	0.58
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.84	0.58
1:A:507:ALA:O	1:A:508:VAL:HG22	2.04	0.58
1:A:355:THR:HG21	1:A:720:MET:CE	2.33	0.58
1:A:61:LEU:HD21	1:A:260:LEU:HD23	1.85	0.58
1:A:688:VAL:O	1:A:692:GLN:HG3	2.03	0.58
1:A:363:VAL:HA	1:A:599:MET:HA	1.85	0.58
1:A:840:ILE:O	1:A:844:VAL:HG13	2.03	0.58
1:A:473:SER:HA	1:A:476:ARG:HB2	1.84	0.57
1:A:539:GLY:N	1:A:540:PRO:HD2	2.18	0.57
1:A:71:ILE:HB	1:A:300:VAL:CG1	2.35	0.57
1:A:367:PHE:HZ	1:A:545:ILE:HG23	1.69	0.57
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.85	0.57
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.34	0.57
1:A:917:SER:OG	1:A:920:GLN:HB2	2.04	0.57
1:A:369:ILE:HD13	1:A:528:VAL:HB	1.86	0.57
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.87	0.57
1:A:326:MET:O	1:A:329:LYS:N	2.37	0.57
1:A:301:ALA:HA	1:A:789:PRO:HG3	1.87	0.57
1:A:869:GLN:HB2	1:A:872:HIS:ND1	2.20	0.57
1:A:441:THR:HA	1:A:599:MET:CE	2.35	0.56
1:A:10:GLU:N	1:A:10:GLU:OE1	2.38	0.56
1:A:654:THR:HG23	1:A:656:ARG:H	1.69	0.56
1:A:79:GLU:HG3	1:A:87:ALA:HB1	1.86	0.56
1:A:444:ALA:HB3	1:A:599:MET:HE1	1.88	0.56
1:A:79:GLU:HG3	1:A:87:ALA:HB2	1.88	0.56
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.87	0.56
1:A:483:PHE:CD1	1:A:578:LEU:HD22	2.40	0.56
1:A:61:LEU:CD2	1:A:260:LEU:HD23	2.36	0.56
1:A:617:ALA:HB1	1:A:751:ARG:HH12	1.69	0.56
1:A:875:GLN:HG3	1:A:875:GLN:O	2.06	0.56
1:A:363:VAL:CG1	1:A:597:VAL:HG13	2.35	0.56
1:A:863:PRO:HG3	1:A:890:ILE:HG21	1.87	0.56
1:A:189:LYS:HD2	1:A:205:LYS:O	2.06	0.56
1:A:104:VAL:O	1:A:108:GLN:HB2	2.06	0.56
1:A:383:SER:C	1:A:384:ILE:HD12	2.25	0.56
1:A:177:GLN:O	1:A:178:SER:C	2.44	0.56
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.41	0.56
1:A:411:VAL:HG12	1:A:454:VAL:CG1	2.35	0.55
1:A:411:VAL:CB	1:A:454:VAL:HG11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:CG2	1:A:250:GLN:HG3	2.36	0.55
1:A:979:GLY:O	1:A:983:ILE:HG13	2.06	0.55
1:A:648:VAL:O	1:A:648:VAL:HG12	2.06	0.55
1:A:788:ILE:HG23	1:A:789:PRO:CD	2.36	0.55
1:A:367:PHE:CD2	1:A:596:VAL:HG22	2.41	0.55
1:A:470:ALA:O	1:A:474:VAL:HG23	2.06	0.55
1:A:247:THR:HB	1:A:250:GLN:HG3	1.88	0.55
1:A:369:ILE:CD1	1:A:528:VAL:HB	2.37	0.55
1:A:128:LYS:O	1:A:151:VAL:HG13	2.06	0.55
1:A:381:GLU:O	1:A:397:LYS:HD2	2.07	0.55
1:A:313:ALA:O	1:A:317:THR:HG23	2.07	0.54
1:A:264:ILE:HG23	1:A:302:LEU:HD21	1.89	0.54
1:A:436:LYS:CG	1:A:443:THR:HG21	2.36	0.54
1:A:408:ASP:O	1:A:411:VAL:HG22	2.06	0.54
1:A:122:TYR:HE2	1:A:726:VAL:CG2	2.19	0.54
1:A:394:GLU:HG3	1:A:396:LEU:HD21	1.88	0.54
1:A:411:VAL:HA	1:A:454:VAL:HG21	1.89	0.54
1:A:801:GLY:O	1:A:805:THR:HG23	2.07	0.54
1:A:179:ILE:O	1:A:705:VAL:HG12	2.08	0.54
1:A:100:ALA:HB3	3:A:1002:PTY:H311	1.89	0.54
1:A:553:GLY:CA	1:A:631:THR:HG22	2.38	0.54
1:A:880:HIS:HA	1:A:884:GLU:CB	2.36	0.54
1:A:358:THR:O	1:A:359:ASN:HB3	2.08	0.54
1:A:575:GLU:OE1	1:A:575:GLU:HA	2.08	0.54
1:A:247:THR:HG23	1:A:249:LEU:H	1.73	0.54
1:A:519:GLU:H	1:A:519:GLU:CD	2.11	0.53
1:A:654:THR:CG2	1:A:657:GLU:H	2.20	0.53
1:A:384:ILE:HD12	1:A:384:ILE:N	2.23	0.53
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.43	0.53
1:A:22:THR:HG22	1:A:23:GLY:O	2.08	0.53
1:A:433:VAL:HG12	1:A:434:TYR:N	2.24	0.53
1:A:857:MET:O	1:A:858:TYR:CB	2.55	0.53
1:A:75:LEU:CD1	1:A:297:LYS:HB3	2.36	0.53
1:A:86:THR:O	1:A:89:VAL:HG22	2.08	0.53
1:A:363:VAL:HG11	1:A:597:VAL:HG13	1.90	0.53
1:A:363:VAL:HG22	1:A:599:MET:HB3	1.89	0.53
1:A:497:TYR:CD2	1:A:512:MET:HE3	2.44	0.53
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.89	0.53
1:A:757:MET:HG3	1:A:760:PHE:CZ	2.44	0.52
1:A:920:GLN:OE1	1:A:920:GLN:HA	2.07	0.52
1:A:147:PRO:HG3	1:A:226:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:GLY:C	1:A:631:THR:HG22	2.30	0.52
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.90	0.52
1:A:311:LEU:CD1	1:A:764:LEU:HD12	2.33	0.52
1:A:106:VAL:HG13	1:A:107:TRP:H	1.75	0.52
1:A:457:THR:O	1:A:459:VAL:HG13	2.09	0.52
1:A:272:TRP:CZ3	1:A:273:LEU:HD23	2.45	0.52
1:A:421:ASN:OD1	1:A:423:SER:N	2.43	0.52
1:A:311:LEU:O	1:A:315:ILE:HG13	2.09	0.52
1:A:48:SER:OG	1:A:51:GLU:HG3	2.10	0.52
1:A:896:PRO:O	1:A:899:MET:HB2	2.09	0.52
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.92	0.52
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.90	0.52
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.40	0.52
1:A:389:TYR:CE2	1:A:436:LYS:HB2	2.44	0.52
1:A:758:LYS:HG3	1:A:828:LEU:HD21	1.93	0.52
1:A:737:ASP:C	1:A:739:ASN:H	2.13	0.51
1:A:920:GLN:HG3	1:A:924:ARG:NH1	2.25	0.51
1:A:482:GLU:OE1	1:A:573:ARG:NH1	2.43	0.51
1:A:865:VAL:O	1:A:865:VAL:HG22	2.09	0.51
1:A:18:VAL:HG23	1:A:24:LEU:HD23	1.91	0.51
1:A:244:GLN:CB	5:A:1101:HOH:O	2.58	0.51
1:A:973:ILE:O	1:A:976:PRO:HD2	2.10	0.51
1:A:23:GLY:HA2	1:A:150:ILE:HD13	1.92	0.51
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.40	0.51
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.92	0.51
1:A:389:TYR:CA	1:A:447:THR:HG21	2.41	0.51
1:A:612:GLN:O	1:A:615:ARG:HB2	2.11	0.51
1:A:77:TRP:O	1:A:78:PHE:HD1	1.94	0.51
1:A:102:ALA:O	1:A:106:VAL:HG12	2.11	0.50
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.44	0.50
1:A:338:SER:C	1:A:340:GLU:N	2.65	0.50
1:A:765:ILE:HG21	2:A:1001:1HT:H19	1.93	0.50
1:A:389:TYR:HA	1:A:447:THR:HG21	1.92	0.50
1:A:500:PRO:HG2	1:A:509:GLY:HA2	1.94	0.50
1:A:76:ALA:C	1:A:88:PHE:HE1	2.15	0.50
1:A:192:GLU:OE2	1:A:580:ASP:HA	2.12	0.50
1:A:680:GLU:HG3	1:A:683:HIS:CE1	2.46	0.50
1:A:512:MET:HB3	1:A:567:ARG:HB3	1.92	0.50
1:A:24:LEU:HG	1:A:149:ASP:CA	2.41	0.50
1:A:580:ASP:O	1:A:582:SER:N	2.45	0.50
1:A:200:VAL:HG21	1:A:489:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:HD22	1:A:466:GLU:HG3	1.94	0.50
1:A:391:PRO:HD2	1:A:434:TYR:CD2	2.46	0.50
1:A:367:PHE:C	1:A:367:PHE:CD1	2.84	0.49
1:A:23:GLY:HA3	1:A:130:TYR:O	2.12	0.49
1:A:411:VAL:HG12	1:A:454:VAL:HG11	1.94	0.49
1:A:497:TYR:HD2	1:A:512:MET:HE3	1.77	0.49
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.94	0.49
1:A:770:GLY:HA3	1:A:844:VAL:HG22	1.93	0.49
1:A:615:ARG:HG2	1:A:615:ARG:NH1	2.28	0.49
1:A:855:TRP:CE3	1:A:896:PRO:HD3	2.47	0.49
1:A:70:CYS:O	1:A:71:ILE:C	2.51	0.49
1:A:968:LEU:O	1:A:972:LYS:HG3	2.11	0.49
1:A:720:MET:HB3	1:A:738:ASP:OD1	2.12	0.49
1:A:756:ASN:OD1	1:A:810:ASN:HB2	2.13	0.49
1:A:467:ARG:HG3	1:A:467:ARG:O	2.12	0.49
1:A:411:VAL:HB	1:A:454:VAL:HG11	1.94	0.49
1:A:28:GLN:HG2	1:A:31:ARG:NH2	2.28	0.49
1:A:267:ILE:CD1	2:A:1001:1HT:H2	2.38	0.48
1:A:795:VAL:HA	1:A:799:THR:HB	1.94	0.48
1:A:478:LEU:HD22	1:A:479:MET:HG2	1.95	0.48
1:A:148:GLY:O	1:A:222:ILE:HG13	2.13	0.48
1:A:538:THR:HB	1:A:540:PRO:HD2	1.94	0.48
1:A:615:ARG:HG2	1:A:615:ARG:HH11	1.78	0.48
1:A:163:ILE:HB	1:A:208:LEU:HB2	1.95	0.48
1:A:39:ASN:HB2	1:A:226:THR:HB	1.94	0.48
1:A:527:TYR:HD2	1:A:592:THR:CG2	2.25	0.48
1:A:628:ASN:CB	1:A:678:ARG:HH21	2.25	0.48
1:A:950:VAL:HG12	1:A:950:VAL:O	2.14	0.48
1:A:748:GLU:CA	1:A:817:MET:HE3	2.39	0.48
1:A:394:GLU:CD	1:A:396:LEU:HD21	2.34	0.48
1:A:100:ALA:CB	3:A:1002:PTY:H311	2.43	0.48
1:A:345:THR:HG22	1:A:716:ILE:HD13	1.94	0.48
1:A:192:GLU:CD	1:A:580:ASP:HA	2.34	0.48
1:A:863:PRO:CG	1:A:890:ILE:HG21	2.44	0.48
1:A:869:GLN:HB3	1:A:872:HIS:ND1	2.28	0.48
1:A:25:THR:OG1	1:A:28:GLN:HG3	2.13	0.48
1:A:500:PRO:CG	1:A:509:GLY:HA2	2.43	0.48
1:A:203:ASP:OD1	1:A:489:ARG:HD3	2.14	0.47
1:A:421:ASN:OD1	1:A:442:GLU:HB3	2.14	0.47
1:A:407:PHE:O	1:A:411:VAL:HG13	2.13	0.47
1:A:152:GLU:HG3	1:A:152:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD1	1:A:60:LEU:N	2.45	0.47
1:A:755:ASN:O	1:A:758:LYS:HB3	2.15	0.47
1:A:77:TRP:HA	1:A:77:TRP:CE3	2.50	0.47
1:A:462:LEU:HD13	1:A:466:GLU:HG3	1.96	0.47
1:A:767:SER:O	1:A:771:GLU:HG3	2.14	0.47
1:A:285:GLY:HA3	1:A:288:TRP:CD1	2.49	0.47
1:A:424:SER:O	1:A:437:VAL:HB	2.15	0.47
1:A:48:SER:N	1:A:51:GLU:OE1	2.44	0.47
1:A:966:GLN:O	1:A:969:MET:HB3	2.14	0.47
1:A:969:MET:HA	1:A:969:MET:CE	2.42	0.47
1:A:294:TYR:O	1:A:297:LYS:HG2	2.15	0.47
1:A:969:MET:CE	1:A:972:LYS:HB2	2.45	0.47
1:A:577:VAL:HG21	1:A:583:ARG:HH11	1.79	0.47
1:A:733:MET:HE1	1:A:746:ALA:HB1	1.96	0.47
1:A:417:CYS:SG	1:A:564:LEU:HD11	2.55	0.47
1:A:761:ILE:O	1:A:765:ILE:HG12	2.15	0.47
1:A:662:PRO:O	1:A:664:ALA:N	2.48	0.47
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.95	0.47
1:A:314:VAL:HG13	1:A:805:THR:HG22	1.96	0.47
1:A:993:GLU:CD	1:A:993:GLU:H	2.16	0.47
1:A:749:GLU:O	1:A:753:ILE:HG12	2.15	0.46
1:A:627:ASP:O	1:A:677:ALA:HB1	2.15	0.46
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.98	0.46
1:A:949:TYR:O	1:A:951:ASP:N	2.48	0.46
1:A:907:ILE:HG12	1:A:974:SER:HB2	1.97	0.46
1:A:179:ILE:HG13	1:A:180:LEU:H	1.79	0.46
1:A:52:LEU:HD11	1:A:109:GLU:OE2	2.16	0.46
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.73	0.46
1:A:941:MET:O	1:A:944:HIS:HB3	2.16	0.46
1:A:146:VAL:HG13	1:A:147:PRO:CD	2.45	0.46
1:A:558:THR:HB	1:A:635:ILE:CD1	2.46	0.46
1:A:380:ASN:O	1:A:382:PHE:CE1	2.69	0.46
1:A:483:PHE:CE1	1:A:578:LEU:HD22	2.48	0.46
1:A:402:ILE:HG22	1:A:403:ARG:N	2.29	0.46
1:A:926:PRO:HG2	1:A:929:VAL:HG23	1.97	0.46
1:A:658:PHE:CZ	1:A:666:GLN:HG2	2.51	0.46
1:A:636:CYS:SG	1:A:675:CYS:HB2	2.55	0.46
1:A:270:ALA:O	1:A:274:ILE:CG1	2.60	0.45
1:A:530:VAL:O	1:A:530:VAL:HG23	2.16	0.45
1:A:40:GLU:CD	1:A:143:ARG:HE	2.20	0.45
1:A:106:VAL:HG13	1:A:107:TRP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HG	1:A:446:THR:HG21	1.98	0.45
1:A:44:GLU:HG3	1:A:117:GLU:OE2	2.16	0.45
1:A:24:LEU:CD1	1:A:149:ASP:HB3	2.46	0.45
1:A:392:GLU:O	1:A:451:LYS:HD3	2.17	0.45
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.47	0.45
1:A:394:GLU:CG	1:A:396:LEU:HD21	2.47	0.45
1:A:870:LEU:HD12	1:A:891:PHE:CE1	2.48	0.45
1:A:412:GLU:OE2	1:A:529:ARG:NE	2.46	0.45
1:A:527:TYR:HB2	1:A:592:THR:HG22	0.56	0.45
1:A:338:SER:O	1:A:340:GLU:N	2.50	0.45
1:A:39:ASN:CB	1:A:226:THR:HB	2.47	0.45
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.99	0.45
1:A:193:PRO:HA	1:A:206:ASN:HD22	1.80	0.45
1:A:901:LEU:HD13	1:A:959:LEU:HD21	1.99	0.45
1:A:358:THR:CG2	1:A:360:GLN:HG3	2.47	0.45
1:A:173:LEU:HD22	1:A:219:ALA:HB2	1.99	0.44
1:A:44:GLU:N	1:A:44:GLU:CD	2.70	0.44
1:A:122:TYR:HE2	1:A:726:VAL:HG23	1.81	0.44
1:A:748:GLU:CG	1:A:817:MET:HE3	2.42	0.44
1:A:791:GLN:HB3	1:A:901:LEU:HD11	1.97	0.44
1:A:668:GLU:HG3	1:A:672:ARG:CZ	2.47	0.44
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.48	0.44
1:A:771:GLU:O	1:A:774:CYS:HB3	2.18	0.44
1:A:247:THR:CB	1:A:250:GLN:HG3	2.48	0.44
1:A:104:VAL:HG21	3:A:1002:PTY:HC11	1.99	0.44
1:A:496:VAL:HG23	1:A:496:VAL:O	2.17	0.44
1:A:166:LEU:HG	1:A:221:GLY:HA2	2.00	0.44
1:A:491:ARG:CB	1:A:585:MET:HG3	2.48	0.44
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.76	0.44
1:A:971:LEU:CD2	1:A:975:LEU:HD11	2.47	0.44
1:A:949:TYR:O	1:A:950:VAL:C	2.56	0.44
1:A:836:ARG:HG2	1:A:984:LEU:HD13	1.99	0.44
1:A:423:SER:OG	1:A:442:GLU:HB2	2.18	0.44
1:A:898:THR:HG21	1:A:960:LYS:O	2.17	0.44
1:A:1:MET:CB	1:A:225:THR:HG22	2.37	0.44
1:A:103:ILE:O	1:A:106:VAL:HG13	2.18	0.44
1:A:865:VAL:HG23	1:A:868:HIS:CE1	2.53	0.44
1:A:606:GLU:O	1:A:741:SER:HB3	2.18	0.44
1:A:152:GLU:HB3	1:A:220:LEU:HD12	1.99	0.44
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.77	0.44
1:A:527:TYR:CG	1:A:592:THR:CG2	2.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:ASP:O	1:A:890:ILE:HG13	2.18	0.44
1:A:95:LEU:O	1:A:99:ILE:HG12	2.17	0.44
1:A:868:HIS:C	1:A:868:HIS:ND1	2.72	0.44
1:A:202:GLN:OE1	1:A:489:ARG:HD2	2.17	0.44
1:A:14:ALA:O	1:A:17:GLY:N	2.51	0.44
1:A:877:THR:O	1:A:880:HIS:ND1	2.51	0.43
1:A:415:THR:HG22	1:A:475:ILE:HD13	2.00	0.43
1:A:297:LYS:HA	1:A:300:VAL:HG22	2.00	0.43
1:A:586:GLU:OE1	1:A:586:GLU:N	2.50	0.43
1:A:394:GLU:OE1	1:A:401:PRO:HB3	2.18	0.43
1:A:122:TYR:HE2	1:A:726:VAL:HG21	1.83	0.43
1:A:608:MET:SD	1:A:639:ILE:HA	2.58	0.43
1:A:668:GLU:O	1:A:671:ARG:HG2	2.18	0.43
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.49	0.43
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.48	0.43
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.54	0.43
1:A:524:ARG:HD2	1:A:588:GLU:O	2.18	0.43
1:A:247:THR:CG2	1:A:340:GLU:OE1	2.65	0.43
1:A:555:GLY:O	1:A:557:ASP:N	2.51	0.43
1:A:886:LEU:C	1:A:886:LEU:HD12	2.38	0.43
1:A:258:GLU:O	1:A:261:SER:HB3	2.18	0.43
1:A:737:ASP:C	1:A:739:ASN:N	2.72	0.43
1:A:737:ASP:O	1:A:739:ASN:N	2.51	0.43
1:A:352:LYS:HE2	1:A:357:THR:HG21	2.01	0.43
1:A:285:GLY:O	1:A:288:TRP:HD1	2.01	0.43
1:A:550:LYS:O	1:A:554:THR:HB	2.18	0.43
1:A:617:ALA:HB1	1:A:751:ARG:NH1	2.33	0.43
1:A:691:LEU:O	1:A:696:GLU:HB2	2.19	0.43
1:A:528:VAL:O	1:A:528:VAL:HG23	2.18	0.43
1:A:890:ILE:O	1:A:893:ALA:CB	2.67	0.42
1:A:355:THR:CG2	1:A:720:MET:SD	3.07	0.42
1:A:19:SER:OG	1:A:22:THR:HB	2.19	0.42
1:A:974:SER:C	1:A:976:PRO:HD2	2.39	0.42
1:A:420:CYS:SG	1:A:515:LYS:HE2	2.60	0.42
1:A:754:TYR:O	1:A:758:LYS:HB2	2.19	0.42
1:A:371:LYS:O	1:A:377:CYS:HA	2.18	0.42
1:A:349:CYS:HA	1:A:622:ILE:O	2.18	0.42
1:A:150:ILE:HD12	1:A:150:ILE:N	2.34	0.42
1:A:500:PRO:O	1:A:501:ALA:CB	2.66	0.42
1:A:969:MET:HE2	1:A:972:LYS:HB2	2.00	0.42
1:A:916:LEU:HD23	1:A:916:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:HD11	1:A:797:LEU:CD1	2.34	0.42
1:A:291:GLY:O	1:A:294:TYR:HB3	2.20	0.42
1:A:748:GLU:CB	1:A:817:MET:HE3	2.49	0.42
1:A:951:ASP:O	1:A:952:PRO:C	2.58	0.42
1:A:485:LEU:HD12	1:A:495:SER:OG	2.19	0.42
1:A:336:LEU:HB2	1:A:337:PRO:HD3	2.01	0.42
1:A:411:VAL:CG1	1:A:454:VAL:HG11	2.50	0.42
1:A:76:ALA:HB1	1:A:88:PHE:HD1	1.82	0.42
1:A:657:GLU:O	1:A:661:LEU:HG	2.20	0.42
1:A:61:LEU:HD23	1:A:64:ILE:HD12	2.02	0.42
1:A:192:GLU:CD	1:A:580:ASP:CB	2.87	0.42
1:A:515:LYS:O	1:A:515:LYS:HG3	2.19	0.42
1:A:404:SER:OG	1:A:452:MET:HB2	2.19	0.42
1:A:629:LYS:O	1:A:633:ILE:HG13	2.20	0.42
1:A:916:LEU:HB3	1:A:925:MET:HE1	2.00	0.42
1:A:59:ASP:OD1	1:A:61:LEU:N	2.53	0.41
1:A:128:LYS:HE3	1:A:128:LYS:HB2	1.88	0.41
1:A:365:LYS:HB3	1:A:552:TRP:CZ3	2.55	0.41
1:A:10:GLU:O	1:A:13:LEU:N	2.53	0.41
1:A:756:ASN:HB3	1:A:808:GLY:HA2	2.00	0.41
1:A:593:PHE:CZ	1:A:595:GLY:HA2	2.55	0.41
1:A:449:VAL:HG11	1:A:472:ASN:OD1	2.20	0.41
1:A:800:ASP:C	1:A:803:PRO:HD2	2.41	0.41
1:A:90:GLU:HB3	1:A:91:PRO:HD3	2.02	0.41
1:A:691:LEU:CB	1:A:698:THR:HG21	2.50	0.41
1:A:289:ILE:O	1:A:293:ILE:HG12	2.20	0.41
1:A:253:LEU:C	1:A:253:LEU:HD23	2.40	0.41
1:A:857:MET:HB2	1:A:866:THR:HA	2.02	0.41
1:A:901:LEU:O	1:A:901:LEU:HD23	2.20	0.41
1:A:642:PHE:HD1	1:A:646:GLU:OE2	2.04	0.41
1:A:319:LEU:HB3	1:A:336:LEU:HB3	2.02	0.41
1:A:460:ARG:O	1:A:460:ARG:HD3	2.20	0.41
1:A:153:VAL:CB	1:A:214:ILE:HD11	2.50	0.41
1:A:452:MET:O	1:A:454:VAL:N	2.53	0.41
1:A:178:SER:O	1:A:182:GLY:N	2.51	0.41
1:A:834:PHE:CD1	1:A:834:PHE:C	2.94	0.41
1:A:748:GLU:OE2	1:A:817:MET:HG3	2.20	0.41
1:A:25:THR:HA	1:A:132:ALA:HB3	2.02	0.41
1:A:992:LEU:HD12	1:A:993:GLU:HG2	2.03	0.41
1:A:146:VAL:CG1	1:A:147:PRO:HD2	2.50	0.41
1:A:90:GLU:N	1:A:91:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:C	1:A:340:GLU:H	2.23	0.41
1:A:455:PHE:O	1:A:456:ASN:HB2	2.20	0.41
1:A:75:LEU:HD11	1:A:297:LYS:N	2.36	0.41
1:A:669:ALA:O	1:A:672:ARG:HG2	2.21	0.41
1:A:692:GLN:C	1:A:694:TYR:H	2.24	0.41
1:A:433:VAL:CG1	1:A:434:TYR:N	2.83	0.41
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.51	0.41
1:A:105:GLY:CA	3:A:1002:PTY:HC21	2.51	0.41
1:A:924:ARG:O	1:A:926:PRO:HD3	2.21	0.41
1:A:363:VAL:HG13	1:A:597:VAL:HG13	2.03	0.40
1:A:367:PHE:CE1	1:A:379:LEU:CD2	3.05	0.40
1:A:916:LEU:HD21	1:A:933:LEU:HD22	2.03	0.40
1:A:637:ARG:NH1	1:A:643:GLY:O	2.54	0.40
1:A:247:THR:HG22	1:A:250:GLN:HG3	2.02	0.40
1:A:580:ASP:C	1:A:582:SER:N	2.73	0.40
1:A:683:HIS:O	1:A:684:LYS:C	2.57	0.40
1:A:174:ARG:HA	1:A:187:VAL:O	2.21	0.40
1:A:802:LEU:HB3	1:A:936:SER:HB2	2.02	0.40
1:A:77:TRP:HE3	1:A:77:TRP:HA	1.85	0.40
1:A:811:PRO:HA	1:A:812:PRO:HD3	1.71	0.40
1:A:635:ILE:O	1:A:639:ILE:HG12	2.21	0.40
1:A:192:GLU:OE2	1:A:580:ASP:CA	2.70	0.40
1:A:654:THR:HG23	1:A:656:ARG:N	2.35	0.40
1:A:271:VAL:HA	1:A:274:ILE:HG12	2.04	0.40
1:A:907:ILE:HD11	1:A:974:SER:HA	2.03	0.40
1:A:703:ASP:OD1	1:A:704:GLY:N	2.55	0.40
1:A:957:PHE:O	1:A:958:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	992/994 (100%)	865 (87%)	106 (11%)	21 (2%)	9	46

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	THR
1	A	950	VAL
1	A	453	ASN
1	A	501	ALA
1	A	581	SER
1	A	606	GLU
1	A	663	LEU
1	A	869	GLN
1	A	285	GLY
1	A	457	THR
1	A	556	ARG
1	A	178	SER
1	A	520	GLY
1	A	738	ASP
1	A	951	ASP
1	A	81	GLY
1	A	160	PRO
1	A	470	ALA
1	A	605	LYS
1	A	864	GLY
1	A	975	LEU

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%)	817 (97%)	23 (3%)	52	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	49	LEU
1	A	101	ASN
1	A	135	LYS
1	A	207	MET
1	A	247	THR
1	A	298	ILE
1	A	360	GLN
1	A	364	CYS
1	A	367	PHE
1	A	375	ASP
1	A	396	LEU
1	A	411	VAL
1	A	490	ASP
1	A	596	VAL
1	A	606	GLU
1	A	666	GLN
1	A	844	VAL
1	A	868	HIS
1	A	869	GLN
1	A	925	MET
1	A	969	MET
1	A	993	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	990	ASN

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 3 ligands modelled in this entry, 1 is 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	1HT	A	1001	-	47,53,53	3.11	19 (40%)	48,78,78	3.58	26 (54%)
3	PTY	A	1002	-	22,23,49	1.79	2 (9%)	23,28,54	1.79	4 (17%)

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	1HT	A	1001	-	-	0/41/107/107	0/3/3/3
3	PTY	A	1002	-	-	0/27/27/53	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	1HT	OBG-CBX	-6.54	1.36	1.48
2	A	1001	1HT	OBD-CBT	-6.43	1.34	1.44
2	A	1001	1HT	OBC-CBR	-5.60	1.36	1.46
2	A	1001	1HT	OBF-CBU	-5.56	1.37	1.46
2	A	1001	1HT	OBE-CBS	-5.37	1.34	1.44
2	A	1001	1HT	CAG-CBN	-4.00	1.43	1.50
2	A	1001	1HT	CBY-CBU	-3.87	1.47	1.53
2	A	1001	1HT	OBH-CBY	-2.74	1.40	1.46
2	A	1001	1HT	OAP-CBW	-2.35	1.38	1.42
2	A	1001	1HT	CBV-CBT	-2.29	1.51	1.54
2	A	1001	1HT	OBH-CBM	2.40	1.41	1.33
2	A	1001	1HT	OBC-CBK	2.46	1.41	1.34
2	A	1001	1HT	CBO-CBJ	3.20	1.62	1.50
2	A	1001	1HT	CAF-CBJ	3.30	1.59	1.50
3	A	1002	PTY	O4-C30	3.49	1.43	1.33
2	A	1001	1HT	OBE-CBO	3.54	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	1HT	CAQ-CBJ	4.37	1.60	1.30
2	A	1001	1HT	OBF-CBP	4.63	1.42	1.35
2	A	1001	1HT	OAO-CBP	6.69	1.36	1.20
3	A	1002	PTY	O30-C30	7.01	1.43	1.22
2	A	1001	1HT	CBN-CBQ	9.38	1.54	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	1HT	OBF-CBP-OAO	-11.80	104.43	121.62
2	A	1001	1HT	OAO-CBP-CBW	-9.98	119.08	128.26
2	A	1001	1HT	CAG-CBN-CBQ	-9.95	103.88	129.97
2	A	1001	1HT	OBF-CBU-CBY	-5.99	100.44	104.23
3	A	1002	PTY	O4-C30-O30	-5.83	108.45	123.49
2	A	1001	1HT	OBH-CBM-OAM	-4.64	115.81	125.03
2	A	1001	1HT	OBF-CBP-CBW	-4.24	103.85	110.14
2	A	1001	1HT	CAG-CBN-CBS	-4.17	116.10	121.51
3	A	1002	PTY	O30-C30-C31	-3.91	108.09	123.72
2	A	1001	1HT	CAF-CBJ-CAQ	-3.49	110.55	123.55
2	A	1001	1HT	OAM-CBM-CAZ	-2.70	112.93	123.72
3	A	1002	PTY	C6-O7-C8	-2.62	111.60	117.89
2	A	1001	1HT	OBC-CBK-OAK	-2.58	116.75	123.67
2	A	1001	1HT	OAP-CBW-CAH	-2.51	104.88	109.41
2	A	1001	1HT	OBE-CBO-OAN	-2.49	118.32	123.30
2	A	1001	1HT	OBG-CBI-OAJ	-2.46	118.53	123.59
2	A	1001	1HT	OBC-CBR-CBY	-2.32	102.04	108.34
2	A	1001	1HT	OAN-CBO-CBJ	-2.29	117.66	125.17
2	A	1001	1HT	CAA-CAQ-CBJ	-2.27	116.05	127.86
2	A	1001	1HT	OBH-CBY-CBR	-2.14	103.63	108.43
2	A	1001	1HT	OAJ-CBI-CAE	-2.00	117.44	124.85
2	A	1001	1HT	OBG-CBI-CAE	2.16	115.41	110.73
2	A	1001	1HT	OBC-CBR-CBB	2.20	111.03	107.03
2	A	1001	1HT	OBD-CBL-CBA	2.29	116.51	111.53
3	A	1002	PTY	O7-C8-C11	2.43	119.75	110.96
2	A	1001	1HT	OBH-CBM-CAZ	2.61	116.08	110.68
2	A	1001	1HT	CBX-OBG-CBI	3.50	129.08	121.90
2	A	1001	1HT	OBE-CBO-CBJ	3.66	121.16	111.67
2	A	1001	1HT	CAI-CBX-CBB	3.87	118.42	110.32
2	A	1001	1HT	CBY-OBH-CBM	4.71	131.51	119.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	1HT	8	0
3	A	1002	PTY	4	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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	994/994 (100%)	-0.02	39 (3%)	43	28	30, 91, 164, 257	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	SER	6.0
1	A	504	SER	5.7
1	A	46	GLY	5.3
1	A	81	GLY	5.3
1	A	506	ALA	4.7
1	A	47	LYS	4.0
1	A	50	TRP	3.9
1	A	507	ALA	3.8
1	A	878	GLU	3.8
1	A	48	SER	3.6
1	A	951	ASP	3.6
1	A	888	CYS	3.4
1	A	508	VAL	3.2
1	A	428	ASN	3.2
1	A	435	GLU	3.2
1	A	430	THR	3.1
1	A	505	ARG	3.0
1	A	994	GLY	3.0
1	A	796	ASN	2.9
1	A	420	CYS	2.9
1	A	767	SER	2.9
1	A	284	HIS	2.8
1	A	109	GLU	2.7
1	A	768	ASN	2.7
1	A	280	ASN	2.6
1	A	80	GLU	2.5
1	A	876	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	881	PRO	2.3
1	A	285	GLY	2.3
1	A	183	GLU	2.3
1	A	766	SER	2.2
1	A	31	ARG	2.2
1	A	106	VAL	2.2
1	A	877	THR	2.2
1	A	509	GLY	2.2
1	A	434	TYR	2.1
1	A	429	GLU	2.1
1	A	924	ARG	2.0
1	A	883	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	PTY	A	1002	24/50	0.73	0.44	4.66	114,124,132,133	0
2	1HT	A	1001	51/51	0.85	0.41	2.22	152,152,152,152	0
4	K	A	1003	1/1	0.94	0.15	-1.67	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.