Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 – 06:17 am GMT

PDB ID	:	2VJC
Title	:	Torpedo Californica Acetylcholinesterase In Complex With A Non Hydrolysable Substrate Analogue, 4-Oxo-N,N,N- Trimethylpentanaminium - Orthorhombic space group - Dataset A at 150K
Authors	:	Colletier, J.P.; Bourgeois, D.; Fournier, D.; Silman, I.; Sussman, J.L.; Weik, M.
Deposited on	:	2007-12-09
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

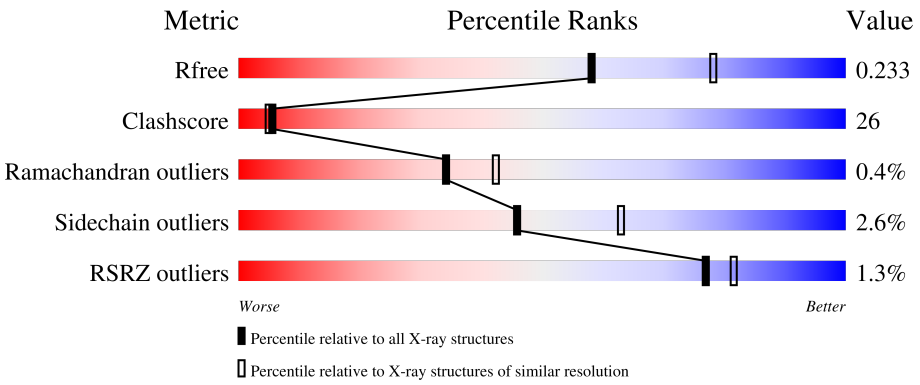
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

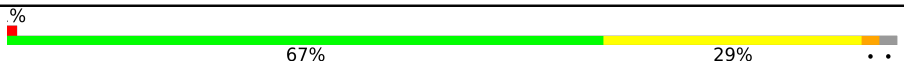
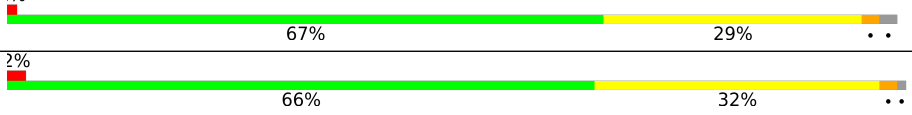
The reported resolution of this entry is 2.30 Å.

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	537	
1	B	537	

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
5	PGE	B	1537	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10185 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.

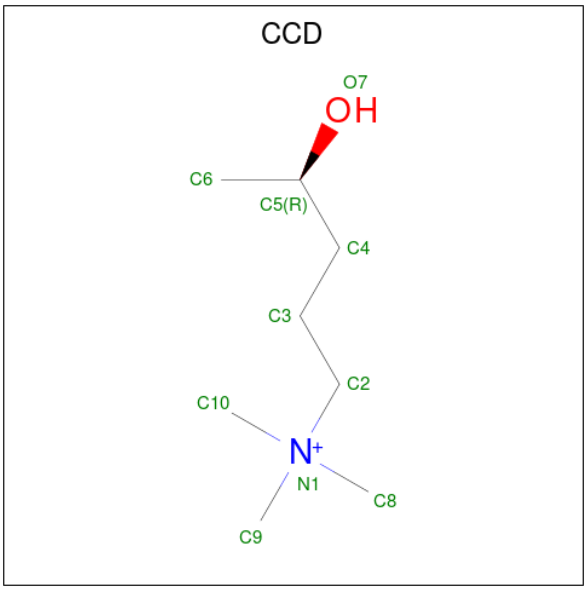
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	528	4210	2702	713	773	22	0	0	0
1	B	532	4244	2721	720	781	22	0	0	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

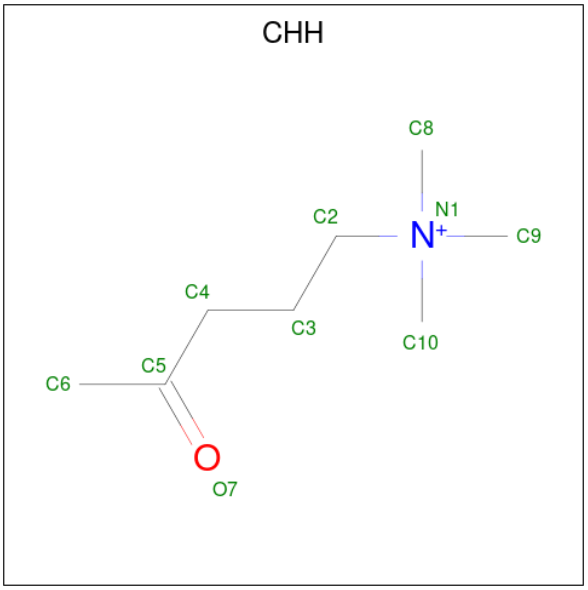
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	3	3	3	0	0
2	B	1	1	1	0	0

- Molecule 3 is (4R)-4-HYDROXY-N,N,N-TRIMETHYLPENTAN-1-AMINIUM (three-letter code: CCD) (formula: $C_8H_{20}NO$).



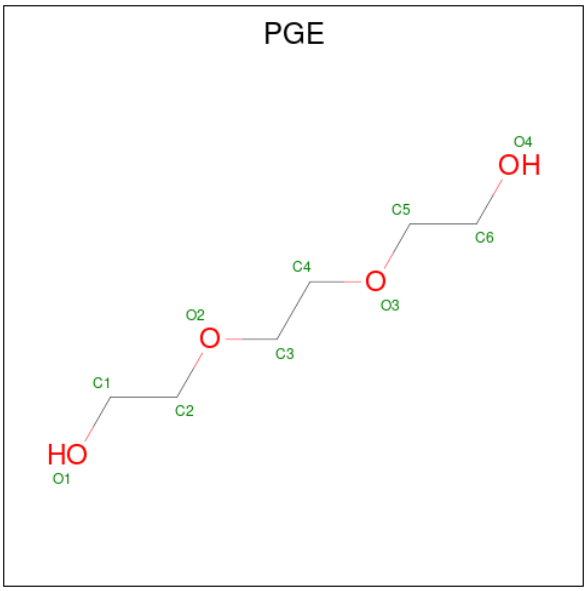
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	8	1	1	0	0
			Total	C	N	O		
3	B	1	10	8	1	1	0	0

- Molecule 4 is N,N,N-TRIMETHYL-4-OXOPENTAN-1-AMINIUM (three-letter code: CHH) (formula: $C_8H_{18}NO$).



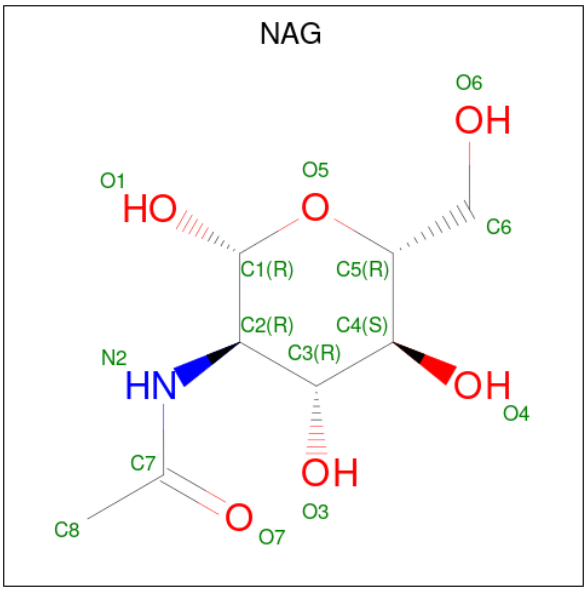
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	10	8	1	1	0	0
			Total	C	N	O		
4	B	1	10	8	1	1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	10	6	4	0	0
			Total	C	O		
5	A	1	10	6	4	0	0
			Total	C	O		
5	B	1	10	6	4	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0

- Molecule 7 is water.

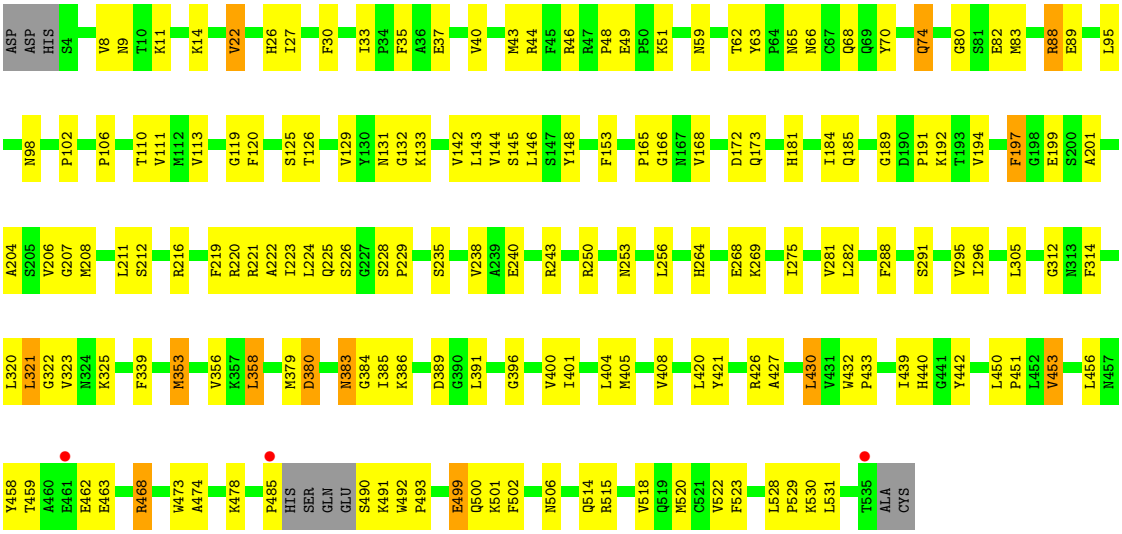
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	858	858	858	0	0
7	B	743	743	743	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

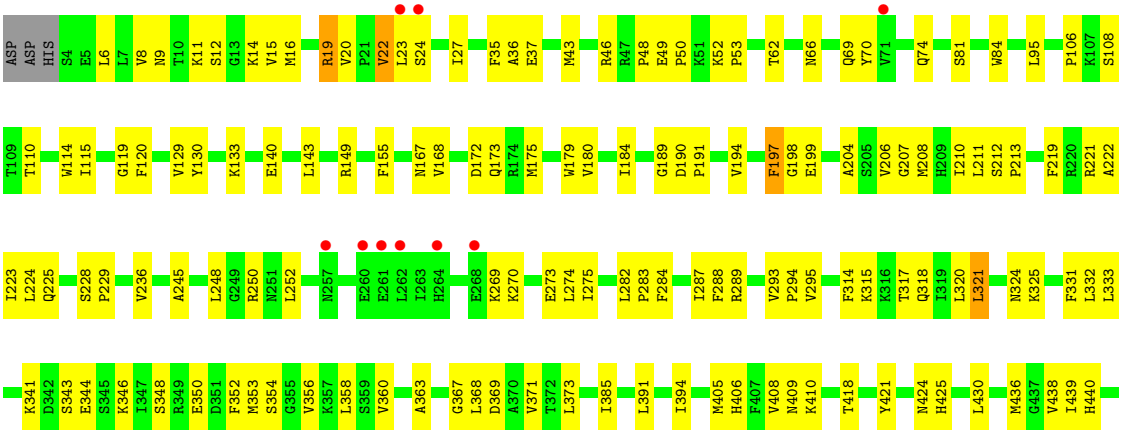
• Molecule 1: ACETYLCHOLINESTERASE

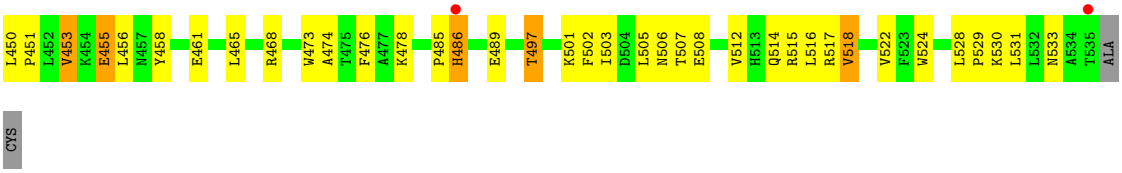
Chain A:



• Molecule 1: ACETYLCHOLINESTERASE

Chain B:




L450
P451
L452
V453
K454
E455
L456
N457
Y458
E461
L465
R468
W473
A474
T475
F476
A477
K478
P485
H486
E489
T497
K501
F502
I503
D504
L505
N506
T507
E508
V512
H513
Q514
R515
L516
R517
V518
V522
F523
W524
L528
P529
K530
L531
L532
N533
A534
T535
ALA

CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.83Å 107.49Å 151.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.92 – 2.30 45.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.92-2.30) 99.8 (45.91-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.238 0.188 , 0.233	Depositor DCC
R_{free} test set	3815 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10185	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3129e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CCD, CL, NAG, CHH, PGE

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	0.35	0/4331	0.59	0/5879
1	B	0.34	0/4367	0.59	0/5929
All	All	0.34	0/8698	0.59	0/11808

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4210	0	4068	192	0
1	B	4244	0	4095	232	0
2	A	3	0	0	1	0
2	B	1	0	0	0	0
3	A	10	0	19	5	0
3	B	10	0	19	2	0
4	A	10	0	18	0	0
4	B	10	0	18	0	0
5	A	20	0	28	1	0
5	B	10	0	14	2	0
6	A	28	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	26	1	0
7	A	858	0	0	124	0
7	B	743	0	0	157	0
All	All	10185	0	8331	436	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 26.

All (436) 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:194:VAL:HB	7:A:2456:HOH:O	1.62	0.96
1:A:191:PRO:HB2	7:A:2393:HOH:O	1.69	0.92
1:B:198:GLY:HA2	7:B:2204:HOH:O	1.69	0.91
1:B:206:VAL:HG11	7:B:2346:HOH:O	1.70	0.91
1:B:194:VAL:HG12	7:B:2318:HOH:O	1.72	0.89
1:B:194:VAL:HB	7:B:2319:HOH:O	1.73	0.89
1:A:95:LEU:HD22	7:A:2348:HOH:O	1.72	0.87
1:A:219:PHE:HA	7:A:2456:HOH:O	1.75	0.87
1:B:115:ILE:HB	7:B:2329:HOH:O	1.73	0.87
1:B:245:ALA:HA	7:B:2370:HOH:O	1.76	0.86
1:B:356:VAL:HB	7:B:2507:HOH:O	1.73	0.86
1:B:331:PHE:HB3	7:B:2418:HOH:O	1.76	0.85
1:A:172:ASP:HB3	7:A:2348:HOH:O	1.77	0.84
1:B:317:THR:HG22	7:B:2444:HOH:O	1.77	0.84
1:A:165:PRO:HG2	7:A:2371:HOH:O	1.78	0.84
3:A:1537:CCD:H93	7:A:2442:HOH:O	1.77	0.83
1:A:68:GLN:HB2	7:A:2181:HOH:O	1.77	0.82
1:A:168:VAL:HG13	7:A:2371:HOH:O	1.79	0.82
1:A:404:LEU:HD21	7:A:2582:HOH:O	1.78	0.82
1:A:194:VAL:HG13	7:A:2290:HOH:O	1.79	0.82
1:B:19:ARG:NH2	1:B:19:ARG:HB2	1.95	0.81
1:B:503:ILE:HG23	7:B:2670:HOH:O	1.79	0.81
1:A:295:VAL:HB	7:A:2473:HOH:O	1.80	0.81
1:B:66:ASN:HB2	7:B:2157:HOH:O	1.78	0.81
1:B:143:LEU:HG	7:B:2253:HOH:O	1.80	0.80
1:B:514:GLN:HA	7:B:2662:HOH:O	1.81	0.80
1:B:506:ASN:HB3	7:B:2673:HOH:O	1.80	0.80
1:A:453:VAL:HG22	1:A:456:LEU:HG	1.64	0.80
1:A:514:GLN:HA	7:A:2781:HOH:O	1.81	0.79
1:A:89:GLU:HG2	7:A:2243:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:HG3	7:B:2568:HOH:O	1.82	0.79
1:B:421:TYR:HA	7:B:2671:HOH:O	1.81	0.79
1:A:235:SER:HB2	7:A:2470:HOH:O	1.83	0.78
1:B:358:LEU:HB3	7:B:2416:HOH:O	1.83	0.78
1:A:40:VAL:HG13	7:A:2251:HOH:O	1.84	0.78
1:A:194:VAL:HG11	7:A:2218:HOH:O	1.83	0.77
1:B:194:VAL:HG13	1:B:219:PHE:HA	1.65	0.77
1:A:493:PRO:HB2	7:A:2773:HOH:O	1.83	0.77
1:B:15:VAL:HB	7:B:2010:HOH:O	1.86	0.76
1:B:184:ILE:HG23	7:B:2303:HOH:O	1.84	0.76
1:A:88:ARG:NH1	1:A:88:ARG:HB3	2.01	0.75
1:B:194:VAL:CG1	1:B:219:PHE:HA	2.17	0.75
1:A:192:LYS:HG3	7:A:2426:HOH:O	1.84	0.75
1:B:250:ARG:HD3	7:B:2167:HOH:O	1.86	0.75
2:A:1536:CL:CL	7:A:2061:HOH:O	2.42	0.74
1:B:48:PRO:HB2	1:B:175:MET:HE1	1.70	0.74
1:B:515:ARG:HB3	1:B:518:VAL:CG1	2.18	0.74
1:A:386:LYS:HA	7:A:2674:HOH:O	1.88	0.74
1:B:19:ARG:HD2	7:B:2030:HOH:O	1.88	0.73
1:B:507:THR:HG23	7:B:2675:HOH:O	1.88	0.72
1:B:95:LEU:HG	7:B:2175:HOH:O	1.90	0.72
1:B:6:LEU:HD23	7:B:2049:HOH:O	1.90	0.72
1:B:184:ILE:HG13	7:B:2303:HOH:O	1.89	0.72
1:A:113:VAL:HG13	7:A:2347:HOH:O	1.89	0.71
1:A:11:LYS:HE3	7:A:2400:HOH:O	1.89	0.71
1:B:332:LEU:HA	7:B:2458:HOH:O	1.90	0.70
1:B:198:GLY:HA3	7:B:2329:HOH:O	1.92	0.70
1:B:353:MET:O	1:B:356:VAL:HG22	1.91	0.70
1:B:46:ARG:HD2	7:B:2073:HOH:O	1.91	0.69
1:A:145:SER:HB2	7:A:2345:HOH:O	1.91	0.69
1:B:70:TYR:HB2	7:B:2406:HOH:O	1.90	0.69
1:B:48:PRO:HB2	1:B:175:MET:CE	2.23	0.69
1:A:226:SER:HB3	7:A:2591:HOH:O	1.92	0.69
1:A:102:PRO:HG2	1:A:106:PRO:HD3	1.74	0.68
1:B:512:VAL:HG13	7:B:2669:HOH:O	1.93	0.68
1:A:281:VAL:HG23	7:A:2548:HOH:O	1.91	0.68
1:A:405:MET:O	1:A:408:VAL:HG12	1.93	0.68
1:B:287:ILE:HG23	7:B:2416:HOH:O	1.91	0.68
1:A:321:LEU:HG	7:A:2582:HOH:O	1.94	0.67
1:A:383:ASN:C	1:A:383:ASN:HD22	1.96	0.67
1:B:287:ILE:HB	7:B:2418:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:HG2	7:B:2041:HOH:O	1.93	0.67
1:B:436:MET:HE2	7:B:2456:HOH:O	1.94	0.67
1:B:35:PHE:HB3	7:B:2055:HOH:O	1.94	0.67
1:B:501:LYS:HA	7:B:2662:HOH:O	1.93	0.67
1:A:83:MET:HE2	7:A:2224:HOH:O	1.94	0.67
1:B:394:ILE:HD12	7:B:2563:HOH:O	1.95	0.67
1:B:110:THR:OG1	1:B:478:LYS:HG2	1.95	0.66
1:B:515:ARG:HB3	1:B:518:VAL:HG13	1.76	0.66
1:B:149:ARG:HG2	7:B:2099:HOH:O	1.94	0.66
1:B:206:VAL:HG12	7:B:2330:HOH:O	1.95	0.66
1:B:439:ILE:HG23	7:B:2456:HOH:O	1.96	0.66
1:A:70:TYR:HB2	7:A:2526:HOH:O	1.96	0.66
1:B:385:ILE:HG13	7:B:2553:HOH:O	1.95	0.65
1:B:27:ILE:HD11	1:B:133:LYS:HB2	1.78	0.65
1:B:318:GLN:HB3	7:B:2579:HOH:O	1.96	0.65
1:B:502:PHE:HB2	7:B:2671:HOH:O	1.97	0.65
1:A:385:ILE:HG22	7:A:2666:HOH:O	1.95	0.65
1:B:506:ASN:HB2	7:B:2678:HOH:O	1.97	0.65
1:A:132:GLY:HA3	1:A:143:LEU:HD23	1.79	0.64
1:A:240:GLU:CD	1:A:243:ARG:HH12	2.00	0.64
1:A:468:ARG:HD2	7:A:2378:HOH:O	1.96	0.64
1:B:468:ARG:HD2	7:B:2625:HOH:O	1.98	0.64
1:A:88:ARG:HD2	1:A:126:THR:HG21	1.78	0.64
1:A:400:VAL:HG11	7:A:2591:HOH:O	1.97	0.63
1:A:44:ARG:HB2	7:A:2252:HOH:O	1.99	0.63
1:A:474:ALA:O	1:A:478:LYS:HG2	1.98	0.63
1:B:69:GLN:HA	7:B:2122:HOH:O	1.98	0.63
1:A:125:SER:HB2	7:A:2345:HOH:O	1.98	0.63
1:A:144:VAL:HG12	7:A:2347:HOH:O	2.00	0.62
1:A:427:ALA:HB2	7:A:2702:HOH:O	2.00	0.62
1:A:110:THR:OG1	1:A:478:LYS:HB3	1.99	0.62
1:A:228:SER:HB3	7:A:2460:HOH:O	1.99	0.62
5:B:1537:PGE:H1	5:B:1537:PGE:H4	1.80	0.62
1:B:19:ARG:HB2	1:B:19:ARG:HH21	1.63	0.62
1:B:37:GLU:OE2	1:B:52:LYS:HG2	2.00	0.61
1:B:207:GLY:HA3	1:B:229:PRO:HD3	1.80	0.61
1:B:287:ILE:N	7:B:2416:HOH:O	2.34	0.61
1:B:391:LEU:HA	7:B:2563:HOH:O	1.99	0.61
1:A:49:GLU:HG3	7:A:2138:HOH:O	2.00	0.61
1:B:507:THR:N	7:B:2675:HOH:O	2.34	0.61
1:A:506:ASN:HB2	7:A:2791:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PRO:HG2	7:A:2426:HOH:O	2.01	0.60
1:B:289:ARG:HB3	7:B:2371:HOH:O	2.01	0.60
1:B:368:LEU:HD23	7:B:2526:HOH:O	2.00	0.60
1:A:253:ASN:HB3	7:A:2497:HOH:O	2.01	0.60
1:A:502:PHE:HD2	7:A:2781:HOH:O	1.84	0.60
1:A:82:GLU:HG2	7:A:2102:HOH:O	2.00	0.60
1:B:405:MET:HA	1:B:408:VAL:HG12	1.82	0.60
1:A:59:ASN:HA	7:A:2039:HOH:O	2.01	0.60
1:B:224:LEU:HD12	7:B:2346:HOH:O	2.01	0.60
1:A:325:LYS:HE2	7:A:2589:HOH:O	2.02	0.60
1:A:43:MET:HG2	7:A:2126:HOH:O	2.01	0.59
1:B:155:PHE:HA	7:B:2261:HOH:O	2.01	0.59
1:B:206:VAL:HG23	7:B:2329:HOH:O	2.02	0.59
1:B:508:GLU:HG3	7:B:2676:HOH:O	2.03	0.59
1:A:88:ARG:HB3	1:A:88:ARG:CZ	2.34	0.58
1:A:74:GLN:HG2	7:A:2204:HOH:O	2.03	0.58
1:A:282:LEU:HD23	7:A:2548:HOH:O	2.03	0.58
1:A:458:TYR:HB3	7:A:2737:HOH:O	2.03	0.58
1:A:518:VAL:O	1:A:522:VAL:HG23	2.04	0.58
1:B:343:SER:HB3	7:B:2485:HOH:O	2.04	0.58
1:B:315:LYS:HG2	7:B:2444:HOH:O	2.03	0.58
1:A:66:ASN:N	7:A:2174:HOH:O	2.36	0.58
1:A:501:LYS:HA	7:A:2781:HOH:O	2.02	0.58
1:B:353:MET:HG3	7:B:2085:HOH:O	2.02	0.58
1:A:88:ARG:HG3	7:A:2174:HOH:O	2.04	0.58
1:A:430:LEU:CD1	1:A:432:TRP:H	2.17	0.58
1:A:148:TYR:HA	7:A:2348:HOH:O	2.03	0.57
1:A:204:ALA:O	1:A:208:MET:HG3	2.03	0.57
1:B:406:HIS:CD2	7:B:2568:HOH:O	2.56	0.57
1:B:8:VAL:HB	7:B:2010:HOH:O	2.02	0.57
1:B:106:PRO:HB2	7:B:2309:HOH:O	2.05	0.57
7:A:2644:HOH:O	1:B:530:LYS:HD3	2.04	0.57
1:B:348:SER:HA	7:B:2547:HOH:O	2.05	0.56
1:B:191:PRO:HA	7:B:2319:HOH:O	2.06	0.56
1:A:220:ARG:N	7:A:2456:HOH:O	2.32	0.56
1:B:502:PHE:HD1	7:B:2671:HOH:O	1.88	0.56
1:B:221:ARG:HD3	1:B:318:GLN:OE1	2.07	0.55
1:A:26:HIS:HB2	7:A:2052:HOH:O	2.06	0.55
1:B:324:ASN:ND2	7:B:2450:HOH:O	2.39	0.55
1:B:252:LEU:HD22	7:B:2391:HOH:O	2.07	0.55
1:B:344:GLU:OE2	1:B:346:LYS:HE3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HD3	7:A:2058:HOH:O	2.05	0.55
1:A:305:LEU:HD13	7:A:2463:HOH:O	2.05	0.55
1:B:287:ILE:HG21	7:B:2458:HOH:O	2.06	0.55
1:B:269:LYS:HD2	7:B:2391:HOH:O	2.05	0.55
1:B:81:SER:HA	7:B:2461:HOH:O	2.07	0.55
1:A:88:ARG:HA	7:A:2232:HOH:O	2.05	0.55
1:B:223:ILE:N	7:B:2346:HOH:O	2.40	0.55
1:A:98:ASN:ND2	7:A:2268:HOH:O	2.39	0.55
1:B:367:GLY:O	1:B:371:VAL:HG23	2.07	0.55
1:B:320:LEU:HG	7:B:2581:HOH:O	2.06	0.55
1:B:455:GLU:CD	1:B:455:GLU:H	2.10	0.55
1:B:189:GLY:CA	7:B:2303:HOH:O	2.54	0.55
1:B:211:LEU:HD23	1:B:314:PHE:HB3	1.89	0.55
1:B:369:ASP:HB3	7:B:2528:HOH:O	2.07	0.54
1:A:83:MET:HE3	1:A:129:VAL:HG11	1.90	0.54
1:A:426:ARG:HD2	7:A:2703:HOH:O	2.06	0.54
1:B:197:PHE:HB3	1:B:223:ILE:HB	1.90	0.54
1:B:273:GLU:HB3	7:B:2391:HOH:O	2.07	0.54
1:B:465:LEU:HD22	7:B:2675:HOH:O	2.08	0.54
1:B:468:ARG:HD3	7:B:2281:HOH:O	2.07	0.54
6:B:1541:NAG:H62	7:B:2735:HOH:O	2.07	0.54
1:B:391:LEU:HD12	7:B:2563:HOH:O	2.08	0.54
1:B:518:VAL:O	1:B:522:VAL:HG23	2.08	0.54
1:A:173:GLN:NE2	7:A:2379:HOH:O	2.41	0.54
1:A:216:ARG:HD2	7:A:2448:HOH:O	2.06	0.54
1:A:62:THR:HA	7:A:2162:HOH:O	2.08	0.53
1:A:132:GLY:CA	1:A:143:LEU:HD23	2.38	0.53
5:B:1537:PGE:H62	5:B:1537:PGE:H3	1.89	0.53
1:A:113:VAL:HG23	7:A:2290:HOH:O	2.07	0.53
1:A:453:VAL:CG2	1:A:456:LEU:HG	2.36	0.53
1:B:515:ARG:HB3	1:B:518:VAL:HG11	1.88	0.53
1:A:111:VAL:HG21	1:A:184:ILE:HG12	1.91	0.53
1:B:283:PRO:HB3	7:B:2366:HOH:O	2.09	0.53
1:B:46:ARG:HD3	7:B:2074:HOH:O	2.08	0.53
1:A:264:HIS:HB3	7:A:2270:HOH:O	2.08	0.53
1:B:354:SER:O	1:B:358:LEU:HD13	2.08	0.53
6:A:1541:NAG:H4	7:A:2846:HOH:O	2.08	0.53
1:B:274:LEU:HD12	7:B:2395:HOH:O	2.09	0.53
1:B:275:ILE:HG12	7:B:2122:HOH:O	2.08	0.53
1:B:350:GLU:HG2	7:B:2503:HOH:O	2.09	0.53
1:B:287:ILE:HG12	7:B:2416:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:THR:HG22	7:B:2101:HOH:O	2.09	0.52
1:A:430:LEU:HD12	1:A:432:TRP:H	1.74	0.52
1:B:119:GLY:O	1:B:120:PHE:HB2	2.10	0.52
1:A:264:HIS:O	1:A:268:GLU:HG2	2.09	0.52
1:B:321:LEU:H	1:B:321:LEU:HD23	1.75	0.52
1:B:27:ILE:HD11	1:B:133:LYS:CB	2.39	0.52
1:B:204:ALA:O	1:B:208:MET:HG3	2.10	0.52
1:B:19:ARG:HB2	1:B:19:ARG:CZ	2.40	0.51
6:A:1541:NAG:H61	7:A:2839:HOH:O	2.10	0.51
1:B:270:LYS:HB2	1:B:273:GLU:HG3	1.91	0.51
1:A:321:LEU:HD23	1:A:321:LEU:H	1.76	0.51
1:B:36:ALA:CB	1:B:175:MET:HE3	2.41	0.51
1:B:425:HIS:N	7:B:2673:HOH:O	2.44	0.51
1:B:223:ILE:C	7:B:2346:HOH:O	2.48	0.51
1:A:420:LEU:HD13	7:A:2302:HOH:O	2.10	0.51
3:A:1537:CCD:H63	7:A:2300:HOH:O	2.11	0.51
1:A:379:MET:HG2	7:B:2689:HOH:O	2.11	0.51
1:A:463:GLU:N	7:A:2737:HOH:O	2.44	0.51
1:A:515:ARG:HD2	7:B:2542:HOH:O	2.11	0.51
1:A:462:GLU:HB2	7:A:2737:HOH:O	2.10	0.50
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.94	0.50
1:B:179:TRP:HB2	7:B:2056:HOH:O	2.12	0.50
1:A:322:GLY:N	7:A:2582:HOH:O	2.44	0.50
1:A:35:PHE:HZ	7:A:2348:HOH:O	1.94	0.50
1:B:108:SER:HB3	7:B:2196:HOH:O	2.11	0.50
1:B:197:PHE:CB	1:B:223:ILE:HB	2.41	0.50
1:A:442:TYR:HB3	7:A:2718:HOH:O	2.11	0.50
1:A:499:GLU:HG3	7:A:2779:HOH:O	2.12	0.50
1:B:478:LYS:NZ	7:B:2637:HOH:O	2.43	0.50
6:A:1541:NAG:H83	6:A:1541:NAG:O3	2.11	0.50
1:A:250:ARG:HG3	7:A:2257:HOH:O	2.11	0.49
1:B:189:GLY:C	7:B:2303:HOH:O	2.49	0.49
1:B:502:PHE:HD2	7:B:2662:HOH:O	1.93	0.49
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.94	0.49
1:A:379:MET:HE3	7:B:2689:HOH:O	2.11	0.49
1:B:27:ILE:HG22	7:B:2046:HOH:O	2.11	0.49
1:B:140:GLU:HB3	7:B:2246:HOH:O	2.13	0.49
1:B:248:LEU:HB2	7:B:2370:HOH:O	2.12	0.49
1:B:531:LEU:HD23	1:B:531:LEU:C	2.32	0.49
1:B:516:LEU:HD12	1:B:517:ARG:HG3	1.95	0.49
1:B:224:LEU:CD1	7:B:2346:HOH:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ILE:HA	7:B:2557:HOH:O	2.12	0.49
1:A:485:PRO:HA	7:A:2771:HOH:O	2.13	0.49
1:B:43:MET:HE1	7:B:2027:HOH:O	2.13	0.49
1:A:451:PRO:HB3	7:A:2737:HOH:O	2.12	0.48
1:B:410:LYS:CG	7:B:2568:HOH:O	2.51	0.48
1:A:321:LEU:HD23	1:A:321:LEU:N	2.28	0.48
1:A:400:VAL:HG21	7:A:2591:HOH:O	2.11	0.48
1:B:222:ALA:HB1	7:B:2346:HOH:O	2.13	0.48
1:B:461:GLU:HB3	7:B:2620:HOH:O	2.12	0.48
1:A:119:GLY:O	1:A:120:PHE:HB2	2.14	0.48
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.43	0.48
1:A:238:VAL:HG13	7:A:2473:HOH:O	2.13	0.48
1:A:353:MET:HG2	7:A:2621:HOH:O	2.14	0.48
1:A:450:LEU:O	1:A:453:VAL:HG13	2.13	0.48
3:A:1537:CCD:H21	7:A:2369:HOH:O	2.13	0.48
1:A:396:GLY:HA3	7:A:2676:HOH:O	2.14	0.48
1:A:408:VAL:HB	7:A:2302:HOH:O	2.11	0.48
1:A:389:ASP:HB2	7:A:2674:HOH:O	2.13	0.48
1:A:63:TYR:CD1	1:A:126:THR:HG22	2.48	0.48
1:A:83:MET:CE	1:A:129:VAL:HG11	2.44	0.48
1:B:450:LEU:N	1:B:451:PRO:CD	2.77	0.48
1:B:22:VAL:O	1:B:22:VAL:HG13	2.13	0.48
1:B:168:VAL:HG22	7:B:2261:HOH:O	2.13	0.47
1:B:486:HIS:HB3	7:B:2650:HOH:O	2.14	0.47
1:B:11:LYS:HD2	7:B:2019:HOH:O	2.13	0.47
1:A:131:ASN:OD1	1:A:133:LYS:HG2	2.14	0.47
1:A:323:VAL:HG21	1:A:401:ILE:HG12	1.96	0.47
1:B:269:LYS:HB2	1:B:274:LEU:HD11	1.96	0.47
1:A:185:GLN:HA	1:A:189:GLY:O	2.14	0.47
1:B:270:LYS:HE3	7:B:2387:HOH:O	2.15	0.47
1:B:346:LYS:HG2	7:B:2557:HOH:O	2.13	0.47
1:A:8:VAL:HG13	7:A:2416:HOH:O	2.14	0.47
7:A:2648:HOH:O	1:B:373:LEU:HD11	2.13	0.47
1:A:269:LYS:HG3	7:A:2491:HOH:O	2.14	0.47
1:A:491:LYS:HE2	7:A:2398:HOH:O	2.13	0.47
1:B:84:TRP:CE3	3:B:1539:CCD:H91	2.49	0.47
1:A:530:LYS:HE3	7:B:2529:HOH:O	2.13	0.47
5:A:1540:PGE:H4	7:A:2560:HOH:O	2.13	0.47
1:B:49:GLU:HG3	1:B:50:PRO:HD2	1.96	0.47
1:A:238:VAL:HG11	7:A:2553:HOH:O	2.14	0.46
1:A:22:VAL:HG11	1:A:27:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASN:HD22	1:A:384:GLY:N	2.12	0.46
1:A:181:HIS:CD2	7:A:2393:HOH:O	2.68	0.46
1:B:333:LEU:HD22	7:B:2474:HOH:O	2.16	0.46
1:A:243:ARG:NH1	1:A:243:ARG:HB3	2.30	0.46
1:A:432:TRP:HB3	1:A:433:PRO:HD2	1.97	0.46
1:B:129:VAL:HG13	1:B:130:TYR:CD1	2.51	0.46
1:B:197:PHE:N	7:B:2327:HOH:O	2.48	0.46
1:A:65:ASN:OD1	1:A:89:GLU:HB3	2.15	0.46
1:A:427:ALA:HB3	1:A:430:LEU:HD23	1.97	0.46
1:B:114:TRP:CE3	7:B:2204:HOH:O	2.68	0.46
1:B:341:LYS:HG3	7:B:2474:HOH:O	2.15	0.46
1:B:282:LEU:HD22	7:B:2371:HOH:O	2.15	0.46
1:B:405:MET:O	1:B:408:VAL:HG12	2.16	0.46
1:A:501:LYS:HE2	7:A:2809:HOH:O	2.16	0.46
1:B:173:GLN:NE2	7:B:2283:HOH:O	2.49	0.46
1:A:291:SER:HA	7:A:2548:HOH:O	2.16	0.45
1:A:396:GLY:HA3	7:A:2680:HOH:O	2.17	0.45
1:B:20:VAL:CG2	1:B:27:ILE:HG13	2.46	0.45
1:B:155:PHE:HZ	7:B:2283:HOH:O	1.98	0.45
1:B:184:ILE:C	7:B:2303:HOH:O	2.53	0.45
1:B:502:PHE:HD2	7:B:2661:HOH:O	1.99	0.45
1:B:352:PHE:HD2	1:B:353:MET:CE	2.30	0.45
1:B:497:THR:HG21	7:B:2575:HOH:O	2.15	0.45
1:A:153:PHE:CD2	7:A:2181:HOH:O	2.55	0.45
1:B:321:LEU:HD23	1:B:321:LEU:N	2.32	0.45
1:B:438:VAL:HG12	7:B:2450:HOH:O	2.17	0.45
1:B:485:PRO:HA	7:B:2648:HOH:O	2.17	0.45
1:A:275:ILE:HG23	7:A:2526:HOH:O	2.16	0.45
1:A:320:LEU:HG	7:A:2581:HOH:O	2.16	0.45
1:A:51:LYS:HB3	7:A:2026:HOH:O	2.16	0.45
1:A:142:VAL:HG11	1:A:184:ILE:HD11	1.99	0.45
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.99	0.45
1:B:9:ASN:HA	1:B:14:LYS:HA	1.98	0.45
1:B:486:HIS:HB2	7:B:2649:HOH:O	2.16	0.45
1:B:503:ILE:N	7:B:2671:HOH:O	2.49	0.45
1:A:119:GLY:H	3:A:1537:CCD:HO7	1.62	0.45
1:A:520:MET:O	1:A:523:PHE:HB3	2.16	0.45
1:B:293:VAL:HB	1:B:294:PRO:HD2	1.98	0.45
1:B:533:ASN:ND2	7:B:2714:HOH:O	2.49	0.45
1:A:353:MET:O	1:A:356:VAL:HG22	2.16	0.45
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:C	1:A:531:LEU:HD23	2.37	0.45
1:B:6:LEU:HD11	1:B:19:ARG:HH22	1.82	0.45
1:A:80:GLY:HA2	7:A:2716:HOH:O	2.16	0.45
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.17	0.45
1:B:180:VAL:O	1:B:184:ILE:HG22	2.16	0.45
1:A:380:ASP:HB3	7:A:2658:HOH:O	2.17	0.44
1:B:210:ILE:HD12	7:B:2330:HOH:O	2.16	0.44
1:B:224:LEU:HD12	1:B:224:LEU:N	2.31	0.44
1:A:199:GLU:HA	1:A:225:GLN:O	2.17	0.44
1:A:383:ASN:C	1:A:383:ASN:ND2	2.68	0.44
1:A:166:GLY:N	7:A:2371:HOH:O	2.49	0.44
1:A:219:PHE:CA	7:A:2456:HOH:O	2.48	0.44
1:A:240:GLU:HA	7:A:2479:HOH:O	2.16	0.44
1:A:296:ILE:HG12	7:A:2470:HOH:O	2.16	0.44
1:B:346:LYS:HA	7:B:2557:HOH:O	2.17	0.44
1:A:220:ARG:NH1	7:A:2457:HOH:O	2.45	0.44
1:B:408:VAL:HG23	1:B:418:THR:HG21	1.99	0.44
1:B:224:LEU:HD11	7:B:2330:HOH:O	2.16	0.44
1:B:528:LEU:HB3	1:B:529:PRO:HD3	2.00	0.44
1:A:224:LEU:HD12	1:A:224:LEU:N	2.33	0.44
1:B:12:SER:HA	7:B:2021:HOH:O	2.17	0.44
1:B:514:GLN:NE2	7:B:2687:HOH:O	2.50	0.44
1:A:221:ARG:HB2	7:A:2441:HOH:O	2.17	0.44
1:A:88:ARG:HB3	1:A:88:ARG:HH11	1.79	0.44
1:A:197:PHE:HB3	1:A:223:ILE:HB	2.00	0.43
1:B:453:VAL:HG13	1:B:456:LEU:HG	2.00	0.43
1:A:11:LYS:CE	7:A:2400:HOH:O	2.60	0.43
1:A:439:ILE:HG22	1:A:440:HIS:N	2.33	0.43
1:A:111:VAL:HB	1:A:194:VAL:HG22	2.00	0.43
1:B:424:ASN:C	7:B:2673:HOH:O	2.55	0.43
1:A:453:VAL:HG22	1:A:453:VAL:O	2.19	0.43
1:B:405:MET:CA	1:B:408:VAL:HG12	2.48	0.43
1:A:40:VAL:HA	7:A:2252:HOH:O	2.18	0.43
1:B:36:ALA:HB2	1:B:175:MET:CE	2.48	0.43
1:A:228:SER:HB2	1:A:229:PRO:HD2	2.00	0.43
1:A:197:PHE:CB	1:A:223:ILE:HB	2.48	0.43
1:A:468:ARG:HD3	7:A:2746:HOH:O	2.18	0.43
1:B:48:PRO:HB3	1:B:172:ASP:OD1	2.19	0.43
1:B:352:PHE:HD2	1:B:353:MET:HE2	1.84	0.43
1:B:453:VAL:CG2	1:B:455:GLU:HG2	2.48	0.43
1:B:62:THR:HA	7:B:2101:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:HD21	1:A:14:LYS:HE2	1.84	0.42
1:A:485:PRO:HA	7:A:2763:HOH:O	2.19	0.42
1:B:199:GLU:HA	1:B:225:GLN:O	2.19	0.42
1:B:358:LEU:HG	7:B:2410:HOH:O	2.18	0.42
1:B:430:LEU:HD21	1:B:439:ILE:HD12	2.00	0.42
1:A:9:ASN:ND2	1:A:14:LYS:HE2	2.34	0.42
1:B:358:LEU:HD12	7:B:2410:HOH:O	2.18	0.42
1:A:358:LEU:HD13	7:A:2635:HOH:O	2.19	0.42
1:B:206:VAL:CG1	1:B:222:ALA:HB1	2.49	0.42
1:B:293:VAL:HB	1:B:294:PRO:CD	2.49	0.42
1:A:240:GLU:CD	1:A:243:ARG:NH1	2.71	0.42
1:B:115:ILE:N	7:B:2204:HOH:O	2.52	0.42
1:B:476:PHE:HE1	7:B:2579:HOH:O	2.02	0.42
1:A:256:LEU:HB3	7:A:2501:HOH:O	2.19	0.42
3:A:1537:CCD:H42	7:A:2300:HOH:O	2.19	0.42
1:B:315:LYS:C	7:B:2444:HOH:O	2.57	0.42
1:B:344:GLU:HA	7:B:2475:HOH:O	2.19	0.42
1:B:474:ALA:HB1	1:B:478:LYS:NZ	2.35	0.42
1:A:184:ILE:HG13	1:A:189:GLY:HA3	2.02	0.42
1:B:23:LEU:O	1:B:24:SER:HB2	2.20	0.42
1:B:408:VAL:HG13	1:B:409:ASN:N	2.35	0.42
1:A:421:TYR:HB3	1:A:492:TRP:CZ2	2.55	0.42
1:B:358:LEU:HD13	7:B:2506:HOH:O	2.20	0.42
1:B:358:LEU:HA	7:B:2410:HOH:O	2.18	0.42
1:B:440:HIS:NE2	3:B:1539:CCD:H41	2.35	0.42
1:A:142:VAL:HG11	7:A:2421:HOH:O	2.19	0.42
1:B:425:HIS:CG	7:B:2675:HOH:O	2.72	0.42
1:B:502:PHE:N	7:B:2662:HOH:O	2.53	0.42
1:A:282:LEU:HD13	7:A:2540:HOH:O	2.19	0.42
1:A:339:PHE:CZ	1:A:391:LEU:HD23	2.55	0.42
1:A:37:GLU:OE2	1:A:51:LYS:HD2	2.20	0.41
1:B:49:GLU:N	1:B:175:MET:HE1	2.35	0.41
1:A:430:LEU:HD12	1:A:432:TRP:HB2	2.03	0.41
1:B:503:ILE:N	7:B:2670:HOH:O	2.52	0.41
1:A:500:GLN:O	7:A:2781:HOH:O	2.21	0.41
1:B:74:GLN:HG2	7:B:2134:HOH:O	2.20	0.41
1:B:391:LEU:HA	1:B:391:LEU:HD12	1.87	0.41
1:B:478:LYS:HE3	7:B:2247:HOH:O	2.20	0.41
1:B:524:TRP:HB3	7:B:2703:HOH:O	2.18	0.41
1:B:115:ILE:HA	7:B:2206:HOH:O	2.20	0.41
1:B:518:VAL:HG13	7:B:2695:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:MET:CG	7:A:2621:HOH:O	2.66	0.41
1:B:275:ILE:HG23	7:B:2406:HOH:O	2.21	0.41
1:B:451:PRO:HA	1:B:458:TYR:CD1	2.55	0.41
1:B:207:GLY:HA2	7:B:2330:HOH:O	2.20	0.41
1:B:210:ILE:HD11	1:B:222:ALA:HB3	2.02	0.41
1:B:325:LYS:HE2	7:B:2452:HOH:O	2.21	0.41
1:B:360:VAL:HG12	1:B:363:ALA:HB2	2.02	0.41
1:B:391:LEU:CA	7:B:2563:HOH:O	2.65	0.41
1:B:530:LYS:HE2	1:B:530:LYS:HB3	1.92	0.41
1:B:52:LYS:HE2	1:B:52:LYS:HB3	1.92	0.41
1:B:53:PRO:HG3	7:B:2021:HOH:O	2.19	0.41
1:A:201:ALA:HB1	7:A:2349:HOH:O	2.20	0.41
1:A:212:SER:O	1:A:216:ARG:HG3	2.21	0.41
1:A:490:SER:N	7:A:2764:HOH:O	2.54	0.41
1:B:6:LEU:HD11	1:B:19:ARG:NH2	2.36	0.41
1:B:283:PRO:HG2	7:B:2369:HOH:O	2.20	0.41
1:A:30:PHE:HB3	1:A:33:ILE:HD11	2.03	0.41
1:A:48:PRO:HB3	1:A:172:ASP:OD1	2.21	0.41
1:A:321:LEU:N	1:A:321:LEU:CD2	2.84	0.41
1:A:321:LEU:O	1:A:420:LEU:HA	2.21	0.41
1:A:391:LEU:HD21	7:A:2314:HOH:O	2.21	0.41
1:A:440:HIS:CE1	7:A:2591:HOH:O	2.74	0.41
1:B:236:VAL:HG23	1:B:295:VAL:HG12	2.03	0.41
1:B:394:ILE:CD1	7:B:2563:HOH:O	2.61	0.41
1:B:461:GLU:CD	1:B:461:GLU:H	2.22	0.41
1:A:450:LEU:O	1:A:456:LEU:HD12	2.21	0.40
1:B:167:ASN:N	7:B:2261:HOH:O	2.54	0.40
1:B:486:HIS:N	7:B:2648:HOH:O	2.54	0.40
1:B:489:GLU:OE1	1:B:489:GLU:N	2.53	0.40
1:A:146:LEU:N	7:A:2347:HOH:O	2.55	0.40
1:B:190:ASP:HA	1:B:191:PRO:HD2	1.99	0.40
1:B:228:SER:HB2	1:B:229:PRO:HD2	2.03	0.40
1:A:220:ARG:HG3	1:A:221:ARG:HG3	2.03	0.40
1:A:478:LYS:HG2	1:A:478:LYS:H	1.72	0.40
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.56	0.40
1:A:339:PHE:CE2	1:A:391:LEU:HD23	2.57	0.40
1:B:212:SER:HA	1:B:213:PRO:HD3	1.93	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	524/537 (98%)	494 (94%)	28 (5%)	2 (0%)	34	42
1	B	530/537 (99%)	507 (96%)	21 (4%)	2 (0%)	34	42
All	All	1054/1074 (98%)	1001 (95%)	49 (5%)	4 (0%)	34	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ASP
1	B	486	HIS
1	A	22	VAL
1	B	22	VAL

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	461/469 (98%)	448 (97%)	13 (3%)	43	60
1	B	465/469 (99%)	454 (98%)	11 (2%)	49	66
All	All	926/938 (99%)	902 (97%)	24 (3%)	46	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	88	ARG

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Mol	Chain	Res	Type
1	A	197	PHE
1	A	288	PHE
1	A	321	LEU
1	A	353	MET
1	A	358	LEU
1	A	383	ASN
1	A	430	LEU
1	A	453	VAL
1	A	468	ARG
1	A	473	TRP
1	A	499	GLU
1	B	19	ARG
1	B	197	PHE
1	B	284	PHE
1	B	288	PHE
1	B	321	LEU
1	B	453	VAL
1	B	455	GLU
1	B	473	TRP
1	B	497	THR
1	B	505	LEU
1	B	518	VAL

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

Mol	Chain	Res	Type
1	A	9	ASN
1	A	68	GLN
1	A	383	ASN
1	A	514	GLN
1	B	68	GLN
1	B	74	GLN
1	B	181	HIS
1	B	257	ASN
1	B	457	ASN
1	B	500	GLN
1	B	514	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
5	PGE	A	1543	-	9,9,9	0.94	0	8,8,8	0.95	0
6	NAG	B	1540	1	14,14,15	0.49	0	17,19,21	0.74	1 (5%)
3	CCD	A	1537	1	9,9,9	0.59	0	11,12,12	1.44	2 (18%)
3	CCD	B	1539	1	9,9,9	0.63	0	11,12,12	1.26	0
5	PGE	B	1537	-	9,9,9	1.50	2 (22%)	8,8,8	1.66	3 (37%)
4	CHH	B	1536	-	9,9,9	1.98	1 (11%)	11,12,12	0.89	0
5	PGE	A	1540	-	9,9,9	0.88	0	8,8,8	1.26	1 (12%)
6	NAG	A	1541	1	14,14,15	0.46	0	17,19,21	0.65	0
4	CHH	A	1538	-	9,9,9	2.32	2 (22%)	11,12,12	0.82	0
6	NAG	A	1542	1	14,14,15	0.54	0	17,19,21	0.68	1 (5%)
6	NAG	B	1541	1	14,14,15	0.57	0	17,19,21	0.67	0

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
5	PGE	A	1543	-	-	1/7/7/7	-
6	NAG	B	1540	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CCD	A	1537	1	-	0/7/7/7	-
3	CCD	B	1539	1	-	0/7/7/7	-
5	PGE	B	1537	-	-	5/7/7/7	-
4	CHH	B	1536	-	-	3/7/7/7	-
5	PGE	A	1540	-	-	1/7/7/7	-
6	NAG	A	1541	1	-	4/6/23/26	0/1/1/1
4	CHH	A	1538	-	-	2/7/7/7	-
6	NAG	A	1542	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1541	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1538	CHH	O7-C5	6.14	1.45	1.21
4	B	1536	CHH	O7-C5	5.48	1.42	1.21
4	A	1538	CHH	C4-C5	2.06	1.56	1.50
5	B	1537	PGE	O2-C2	2.04	1.50	1.42
5	B	1537	PGE	O2-C3	2.03	1.50	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1540	PGE	O3-C4-C3	2.82	123.13	110.39
5	B	1537	PGE	C3-O2-C2	2.59	124.50	113.29
5	B	1537	PGE	O3-C5-C6	2.43	120.75	110.07
3	A	1537	CCD	O7-C5-C4	2.24	120.51	109.80
3	A	1537	CCD	C10-N1-C9	-2.23	103.24	108.97
6	B	1540	NAG	C2-N2-C7	-2.22	119.74	122.90
5	B	1537	PGE	O3-C4-C3	2.10	119.85	110.39
6	A	1542	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1536	CHH	C2-C3-C4-C5
6	A	1541	NAG	C8-C7-N2-C2
6	A	1541	NAG	O7-C7-N2-C2
6	B	1540	NAG	O7-C7-N2-C2
6	B	1540	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	1542	NAG	O5-C5-C6-O6
6	A	1542	NAG	C4-C5-C6-O6
4	B	1536	CHH	N1-C2-C3-C4
6	A	1542	NAG	C8-C7-N2-C2
6	A	1542	NAG	O7-C7-N2-C2
4	A	1538	CHH	C2-C3-C4-C5
5	B	1537	PGE	C4-C3-O2-C2
6	A	1541	NAG	C4-C5-C6-O6
4	B	1536	CHH	C3-C4-C5-O7
5	B	1537	PGE	C6-C5-O3-C4
5	A	1540	PGE	C3-C4-O3-C5
5	B	1537	PGE	C1-C2-O2-C3
5	A	1543	PGE	C6-C5-O3-C4
5	B	1537	PGE	C3-C4-O3-C5
6	A	1541	NAG	O5-C5-C6-O6
4	A	1538	CHH	N1-C2-C3-C4
5	B	1537	PGE	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1537	CCD	5	0
3	B	1539	CCD	2	0
5	B	1537	PGE	2	0
5	A	1540	PGE	1	0
6	A	1541	NAG	3	0
6	B	1541	NAG	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 (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	528/537 (98%)	-0.21	3 (0%)	89	92	21, 29, 45, 59	0
1	B	532/537 (99%)	-0.08	11 (2%)	63	70	21, 29, 45, 72	0
All	All	1060/1074 (98%)	-0.14	14 (1%)	77	81	21, 29, 45, 72	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	HIS	5.1
1	B	535	THR	4.4
1	B	257	ASN	4.1
1	B	264	HIS	3.1
1	B	261	GLU	2.9
1	B	260	GLU	2.8
1	A	485	PRO	2.7
1	B	23	LEU	2.6
1	A	461	GLU	2.6
1	B	262	LEU	2.3
1	B	268	GLU	2.3
1	A	535	THR	2.1
1	B	24	SER	2.1
1	B	71	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	B	1537	10/10	0.58	0.23	82,83,86,86	0
2	CL	A	1544	1/1	0.69	0.13	78,78,78,78	0
5	PGE	A	1540	10/10	0.73	0.36	77,78,78,78	0
5	PGE	A	1543	10/10	0.74	0.37	77,78,79,79	0
6	NAG	A	1541	14/15	0.79	0.24	54,57,59,59	0
6	NAG	A	1542	14/15	0.79	0.14	47,49,54,56	0
2	CL	A	1539	1/1	0.86	0.09	59,59,59,59	0
4	CHH	A	1538	10/10	0.87	0.51	83,83,84,84	0
6	NAG	B	1541	14/15	0.87	0.12	36,41,45,49	0
6	NAG	B	1540	14/15	0.88	0.15	53,56,57,59	0
4	CHH	B	1536	10/10	0.89	0.63	81,81,82,82	0
3	CCD	B	1539	10/10	0.89	0.25	26,32,33,33	0
3	CCD	A	1537	10/10	0.90	0.20	28,32,34,34	0
2	CL	B	1538	1/1	0.91	0.07	59,59,59,59	0
2	CL	A	1536	1/1	0.95	0.05	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.