



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 AM GMT

PDB ID : 2IW3
Title : ELONGATION FACTOR 3 IN COMPLEX WITH ADP
Authors : Andersen, C.B.F.; Becker, T.; Blau, M.; Anand, M.; Halic, M.; Balar, B.; Mielke, T.; Boesen, T.; Pedersen, J.S.; Spahn, C.M.T.; Kinzy, T.G.; Andersen, G.R.; Beckmann, R.
Deposited on : 2006-06-26
Resolution : 2.40 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

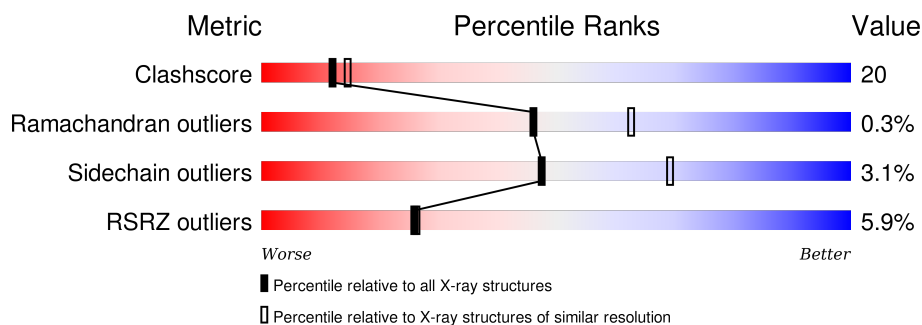
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	986	<div> <div>7%</div> <div>65%</div> <div>32%</div> <div>..</div> </div>
1	B	986	<div> <div>4%</div> <div>73%</div> <div>25%</div> <div>..</div> </div>

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	ADP	B	1977	-	-	-	X
3	SO4	A	1974	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1976	-	-	X	X
3	SO4	A	1977	-	-	X	X
3	SO4	B	1979	-	-	X	X
3	SO4	B	1980	-	-	-	X
3	SO4	B	1982	-	-	-	X
3	SO4	B	1983	-	-	-	X

2 Entry composition [i](#)

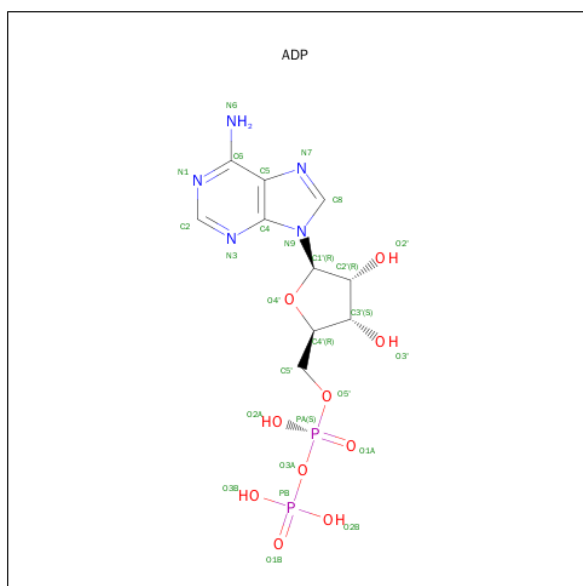
There are 4 unique types of molecules in this entry. The entry contains 16312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ELONGATION FACTOR 3A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	973	Total	C	N	O	S	Se	0	0	1
			7579	4790	1297	1455	15	22			
1	B	981	Total	C	N	O	S	Se	0	0	1
			7647	4829	1316	1465	15	22			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

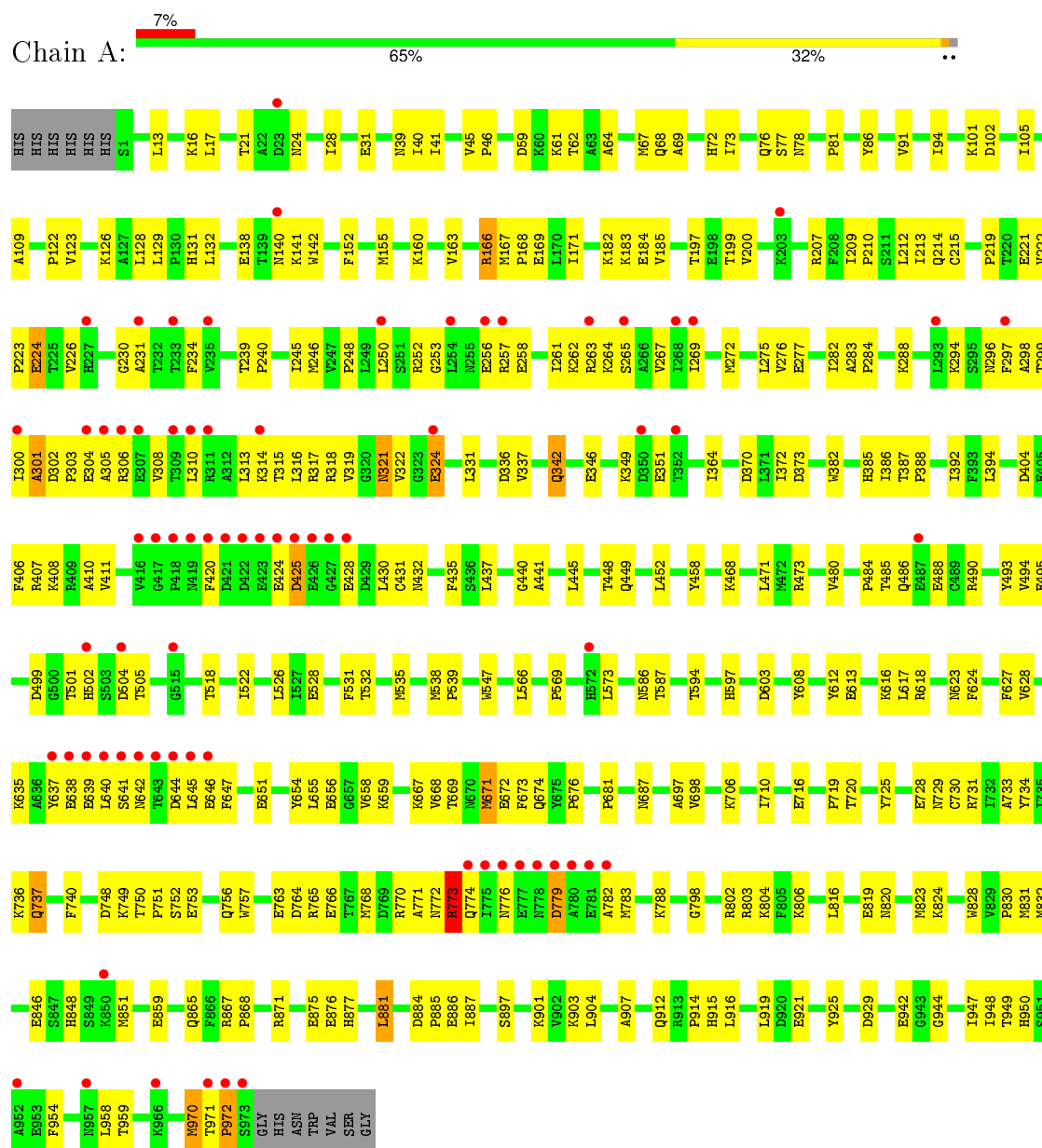
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	413	Total 413	O 413	0	0
4	B	554	Total 554	O 554	0	0

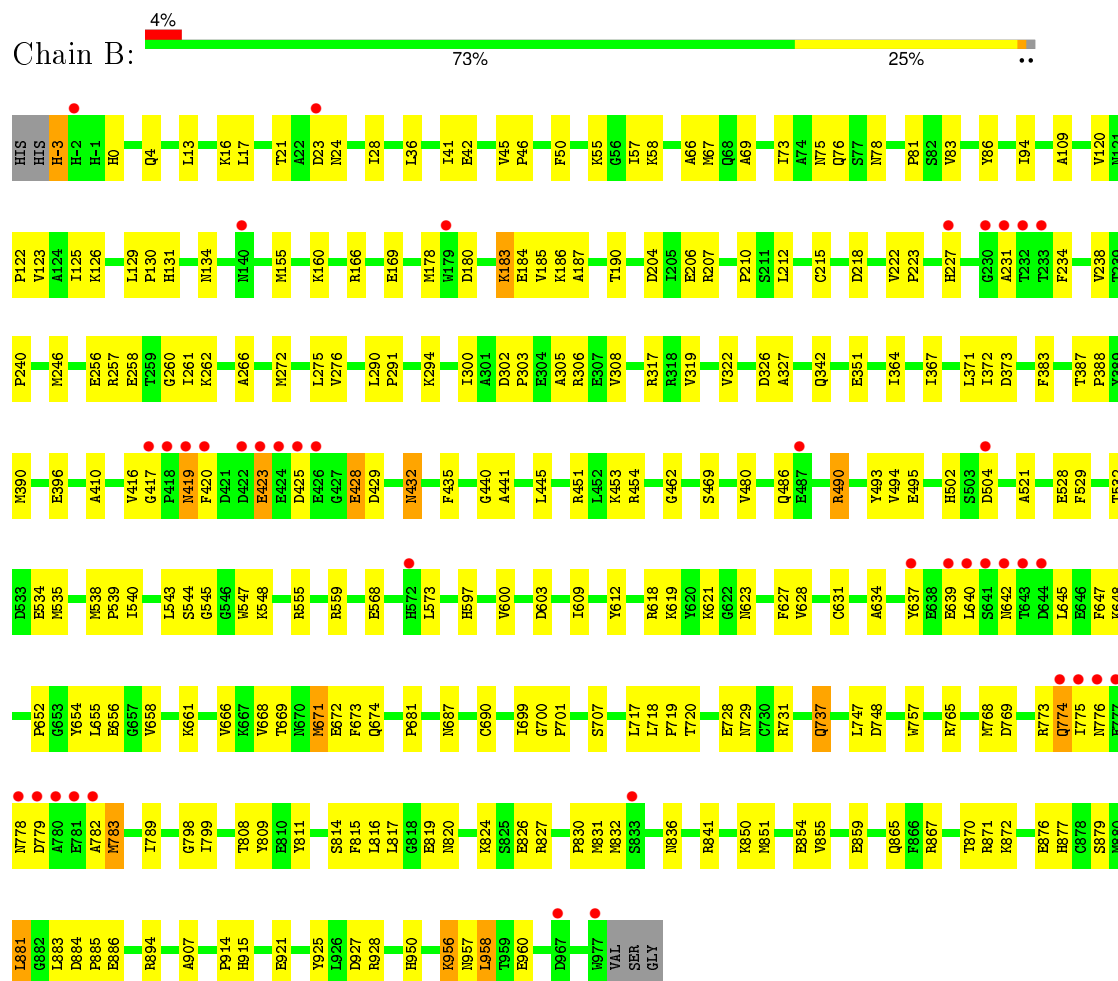
3 Residue-property plots

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: ELONGATION FACTOR 3A



• Molecule 1: ELONGATION FACTOR 3A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.80Å 107.70Å 209.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40 19.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.00-2.40) 99.4 (19.83-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.242 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 87433 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16312	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO4, ADP

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	0.33	0/7695	0.59	2/10390 (0.0%)
1	B	0.37	1/7768 (0.0%)	0.61	1/10489 (0.0%)
All	All	0.35	1/15463 (0.0%)	0.60	3/20879 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	ALA	C-O	5.12	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	GLU	N-CA-C	-5.78	95.38	111.00
1	A	425	ASP	N-CA-C	-5.44	96.32	111.00
1	A	773	ARG	N-CA-C	-5.11	97.22	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	7579	0	7627	340	0
1	B	7647	0	7676	282	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	12	0	0
2	B	27	0	12	6	0
3	A	25	0	0	7	0
3	B	40	0	0	5	0
4	A	413	0	0	105	0
4	B	554	0	0	76	0
All	All	16312	0	15327	609	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 20.

All (609) 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:B:420:PHE:CZ	1:B:621:LYS:HB2	1.94	1.03
1:B:731:ARG:H	1:B:915:HIS:HD2	1.04	1.01
1:B:798:GLY:HA2	1:B:851:MSE:HE1	1.44	0.98
1:A:528:GLU:HG3	1:B:867:ARG:HH12	1.29	0.98
1:A:67:MSE:HE1	1:A:109:ALA:HA	1.46	0.97
1:A:867:ARG:NH1	1:B:528:GLU:HG3	1.80	0.95
1:B:67:MSE:CE	1:B:94:ILE:HG23	1.99	0.93
1:A:445:LEU:HD22	4:A:2262:HOH:O	1.67	0.93
1:A:67:MSE:CE	1:A:94:ILE:HG23	1.99	0.93
1:B:246:MSE:HA	1:B:246:MSE:HE2	1.51	0.90
1:A:246:MSE:HE2	1:A:246:MSE:HA	1.54	0.90
1:A:61:LYS:HG3	1:A:62:THR:HG23	1.54	0.88
1:B:717:LEU:HD23	4:B:2398:HOH:O	1.74	0.87
1:A:452:LEU:HB2	4:A:2191:HOH:O	1.74	0.87
1:A:736:LYS:HE3	4:A:2395:HOH:O	1.75	0.86
1:A:67:MSE:HE3	1:A:94:ILE:HG23	1.57	0.86
1:B:67:MSE:HE1	1:B:94:ILE:HG23	1.55	0.86
1:B:731:ARG:H	1:B:915:HIS:CD2	1.94	0.85
1:B:372:ILE:HD11	1:B:410:ALA:HB1	1.57	0.85
1:A:129:LEU:HD13	1:A:155:MSE:HE1	1.57	0.85
1:A:313:LEU:HD22	4:A:2138:HOH:O	1.77	0.85
1:A:823:MSE:HB2	4:A:2347:HOH:O	1.75	0.85
1:A:428:GLU:HA	4:A:2190:HOH:O	1.76	0.84
1:B:731:ARG:HH12	1:B:865:GLN:HE21	1.26	0.84
1:A:67:MSE:CE	1:A:109:ALA:HA	2.07	0.84
1:B:634:ALA:HA	1:B:637:TYR:CE1	2.13	0.83
1:A:297:PHE:CE1	1:A:310:LEU:HB2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLU:HB2	2:B:1977:ADP:H5'1	1.61	0.82
1:B:532:THR:HG22	1:B:535:MSE:HG3	1.60	0.82
1:A:779:ASP:HB3	1:A:782:ALA:HB3	1.59	0.82
1:A:300:ILE:HB	4:A:2140:HOH:O	1.80	0.81
1:A:763:GLU:HA	4:A:2393:HOH:O	1.80	0.81
1:A:528:GLU:HG3	1:B:867:ARG:NH1	1.96	0.81
1:A:731:ARG:H	1:A:915:HIS:HD2	1.27	0.81
1:B:420:PHE:CE1	1:B:621:LYS:HB2	2.15	0.81
1:B:773:ARG:HB3	4:B:2445:HOH:O	1.79	0.81
1:B:486:GLN:HB3	1:B:490:ARG:NH1	1.96	0.80
1:A:299:THR:HB	4:A:2142:HOH:O	1.83	0.79
1:B:445:LEU:HB3	4:B:2349:HOH:O	1.82	0.78
1:A:300:ILE:HG13	4:A:2142:HOH:O	1.84	0.78
1:A:628:VAL:HA	4:A:2264:HOH:O	1.81	0.78
1:B:234:PHE:HB2	4:B:2152:HOH:O	1.82	0.78
1:A:372:ILE:HD11	1:A:410:ALA:HB1	1.63	0.78
1:A:970:MSE:HE3	1:A:972:PRO:HD3	1.65	0.78
1:A:710:ILE:HG21	4:A:2014:HOH:O	1.82	0.78
1:B:396:GLU:HB2	2:B:1977:ADP:C5'	2.15	0.77
1:A:215:CYS:HB3	4:A:2123:HOH:O	1.85	0.77
1:A:803:ARG:HG2	4:A:2338:HOH:O	1.84	0.77
1:A:947:ILE:HG21	1:A:954:PHE:HE2	1.48	0.76
1:A:720:THR:HB	4:A:2280:HOH:O	1.85	0.76
1:A:91:VAL:HG11	4:A:2056:HOH:O	1.85	0.76
1:A:731:ARG:HH12	1:A:865:GLN:HE21	1.30	0.76
1:B:67:MSE:HE1	1:B:109:ALA:HA	1.67	0.76
1:A:305:ALA:HB3	4:A:2153:HOH:O	1.84	0.76
1:A:867:ARG:HH12	1:B:528:GLU:HG3	1.47	0.75
1:B:212:LEU:HD22	1:B:246:MSE:HE1	1.69	0.75
1:B:535:MSE:HE1	1:B:547:TRP:CD2	2.22	0.75
1:B:212:LEU:CD2	1:B:246:MSE:HE1	2.17	0.75
1:A:671:MSE:HE3	1:A:719:PRO:HB3	1.69	0.75
1:B:634:ALA:HA	1:B:637:TYR:HE1	1.52	0.75
1:A:569:PRO:HD3	4:A:2254:HOH:O	1.86	0.74
1:B:67:MSE:CE	1:B:109:ALA:HA	2.17	0.74
1:B:420:PHE:CZ	4:B:2263:HOH:O	2.40	0.74
1:A:430:LEU:HB2	4:A:2191:HOH:O	1.88	0.74
1:A:637:TYR:HA	4:A:2265:HOH:O	1.87	0.74
3:A:1976:SO4:O2	1:B:871:ARG:NH2	2.21	0.74
1:B:779:ASP:CG	1:B:782:ALA:HB3	2.09	0.73
1:B:134:ASN:HB3	4:B:2100:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASN:HA	4:A:2142:HOH:O	1.89	0.73
1:A:276:VAL:HB	1:A:319:VAL:HG11	1.71	0.73
1:B:416:VAL:HG23	1:B:417:GLY:H	1.52	0.73
1:A:535:MSE:HE1	1:A:547:TRP:CD2	2.23	0.72
1:B:66:ALA:HB3	4:B:2052:HOH:O	1.88	0.72
1:A:779:ASP:CB	1:A:782:ALA:HB3	2.20	0.72
1:A:67:MSE:HE1	1:A:94:ILE:HG23	1.70	0.71
1:A:535:MSE:HA	1:A:538:MSE:HE3	1.71	0.71
1:B:212:LEU:CD1	1:B:246:MSE:HE1	2.21	0.71
1:A:140:ASN:OD1	1:A:141:LYS:HD2	1.91	0.70
1:B:490:ARG:HD3	4:B:2317:HOH:O	1.90	0.70
1:A:31:GLU:OE2	1:A:676:PRO:HD2	1.91	0.70
1:A:64:ALA:HB2	4:A:2040:HOH:O	1.91	0.70
1:B:728:GLU:H	1:B:728:GLU:CD	1.93	0.70
1:B:699:ILE:HG22	1:B:700:GLY:N	2.07	0.70
1:B:212:LEU:HD13	1:B:246:MSE:HE1	1.74	0.70
1:A:306:ARG:HG2	4:A:2140:HOH:O	1.92	0.70
1:A:729:ASN:N	3:A:1977:SO4:O2	2.24	0.69
1:A:200:VAL:CG2	1:A:245:ILE:HD12	2.22	0.69
1:A:617:LEU:HB2	4:A:2197:HOH:O	1.92	0.69
1:B:419:ASN:ND2	1:B:420:PHE:H	1.90	0.69
1:B:775:ILE:O	1:B:775:ILE:HG22	1.93	0.69
1:A:617:LEU:HG	4:A:2262:HOH:O	1.93	0.69
1:B:0:HIS:O	1:B:4:GLN:HG3	1.92	0.68
1:B:420:PHE:HZ	1:B:621:LYS:HD2	1.59	0.68
1:A:67:MSE:HE1	1:A:109:ALA:CA	2.24	0.68
1:A:597:HIS:HD2	1:A:638:GLU:O	1.76	0.68
1:A:468:LYS:HA	4:A:2205:HOH:O	1.93	0.67
1:B:67:MSE:HE3	1:B:94:ILE:HG23	1.74	0.67
1:B:731:ARG:HB2	4:B:2517:HOH:O	1.93	0.67
1:A:706:LYS:O	1:A:710:ILE:HG12	1.94	0.67
1:A:13:LEU:O	1:A:28:ILE:HD11	1.95	0.67
1:B:57:ILE:HA	4:B:2052:HOH:O	1.94	0.67
1:B:429:ASP:OD1	1:B:453:LYS:HE3	1.95	0.67
1:B:798:GLY:HA2	1:B:851:MSE:CE	2.22	0.66
1:A:731:ARG:H	1:A:915:HIS:CD2	2.09	0.66
1:B:212:LEU:HD13	1:B:246:MSE:CE	2.26	0.66
1:B:950:HIS:HB3	2:B:1977:ADP:O1B	1.95	0.66
1:A:624:PHE:CZ	1:A:639:GLU:HG3	2.30	0.66
1:B:371:LEU:HA	4:B:2240:HOH:O	1.96	0.66
1:A:672:GLU:HG2	4:A:2280:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ASN:HD22	1:B:645:LEU:HD12	1.61	0.66
1:B:699:ILE:HG22	1:B:700:GLY:H	1.60	0.65
1:B:631:CYS:HB3	4:B:2357:HOH:O	1.95	0.65
1:A:566:LEU:HD13	4:A:2253:HOH:O	1.96	0.65
1:B:420:PHE:CZ	1:B:621:LYS:HD2	2.31	0.65
1:A:667:LYS:HG2	1:A:725:TYR:CD2	2.32	0.65
1:B:276:VAL:HB	1:B:319:VAL:HG11	1.79	0.65
1:A:76:GLN:HB2	1:A:774:GLN:HE21	1.61	0.65
1:B:486:GLN:HB3	1:B:490:ARG:HH12	1.61	0.64
1:A:970:MSE:HG2	1:A:971:THR:N	2.11	0.64
1:A:618:ARG:HG2	4:A:2260:HOH:O	1.97	0.64
1:B:67:MSE:HE3	1:B:94:ILE:HG12	1.80	0.64
1:A:698:VAL:HG12	1:A:706:LYS:HE3	1.79	0.64
1:B:671:MSE:HE1	1:B:673:PHE:HB2	1.79	0.64
1:A:420:PHE:HE2	1:A:425:ASP:OD2	1.79	0.64
1:B:671:MSE:HE2	1:B:672:GLU:O	1.98	0.64
1:A:658:VAL:HG23	4:A:2290:HOH:O	1.97	0.64
1:A:392:ILE:HG23	4:A:2016:HOH:O	1.97	0.64
1:A:132:LEU:HD13	4:A:2074:HOH:O	1.96	0.64
1:A:868:PRO:HB3	4:A:2375:HOH:O	1.96	0.64
1:A:669:THR:HA	1:A:687:ASN:OD1	1.98	0.64
1:A:41:ILE:HD12	1:A:46:PRO:HD3	1.80	0.64
1:A:671:MSE:HE1	1:A:673:PHE:HB2	1.79	0.64
1:B:180:ASP:O	1:B:186:LYS:HE3	1.96	0.64
1:B:881:LEU:HD13	1:B:907:ALA:HA	1.78	0.64
1:B:535:MSE:HA	1:B:538:MSE:HG2	1.80	0.63
1:A:828:TRP:HB2	4:A:2352:HOH:O	1.97	0.63
1:A:820:ASN:HB3	4:A:2347:HOH:O	1.97	0.63
1:A:547:TRP:NE1	3:A:1974:SO4:O4	2.32	0.63
1:A:256:GLU:HG3	1:A:257:ARG:H	1.62	0.63
1:A:317:ARG:HG2	1:A:322:VAL:HG21	1.80	0.63
1:A:324:GLU:H	1:A:324:GLU:CD	2.01	0.63
4:A:2097:HOH:O	1:B:210:PRO:HG2	1.98	0.63
1:A:448:THR:HG21	4:A:2262:HOH:O	1.98	0.63
1:B:707:SER:HB2	4:B:2396:HOH:O	1.97	0.63
1:A:641:SER:HA	1:A:887:ILE:HD11	1.82	0.62
1:B:776:ASN:HB3	1:B:779:ASP:HB2	1.81	0.62
1:B:317:ARG:HG2	1:B:322:VAL:HG21	1.81	0.62
1:A:535:MSE:O	1:A:538:MSE:HG2	1.99	0.62
1:A:471:LEU:HB3	4:A:2205:HOH:O	1.97	0.62
1:A:779:ASP:HB3	1:A:782:ALA:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ASP:HB3	4:B:2127:HOH:O	2.00	0.62
1:A:736:LYS:NZ	4:A:2296:HOH:O	2.30	0.62
1:B:884:ASP:HB2	4:B:2497:HOH:O	1.98	0.62
1:B:538:MSE:HB2	1:B:539:PRO:HD2	1.82	0.62
1:B:827:ARG:HG3	1:B:827:ARG:HH11	1.63	0.62
1:B:671:MSE:HE3	1:B:719:PRO:HB3	1.83	0.61
1:A:783:MSE:HG3	1:A:848:HIS:CE1	2.35	0.61
1:B:654:TYR:CE2	1:B:656:GLU:HG2	2.35	0.61
1:A:603:ASP:HA	1:A:623:ASN:HB2	1.82	0.61
1:B:928:ARG:HH11	1:B:928:ARG:HB3	1.66	0.61
1:A:667:LYS:HG2	1:A:725:TYR:HD2	1.64	0.61
1:B:420:PHE:CE2	4:B:2263:HOH:O	2.53	0.61
1:A:276:VAL:HB	1:A:319:VAL:CG1	2.31	0.61
1:B:826:GLU:O	1:B:827:ARG:HG3	2.01	0.61
1:B:532:THR:HG22	1:B:535:MSE:CG	2.31	0.61
1:A:223:PRO:HG2	4:A:2111:HOH:O	1.99	0.61
1:A:62:THR:HG22	4:A:2002:HOH:O	2.01	0.61
1:B:532:THR:CG2	1:B:535:MSE:HG3	2.29	0.60
1:B:661:LYS:HD2	4:B:2532:HOH:O	2.01	0.60
1:A:871:ARG:O	1:A:875:GLU:HG3	2.00	0.60
1:A:734:TYR:CE2	1:A:736:LYS:HD2	2.36	0.60
1:B:532:THR:HG23	1:B:535:MSE:H	1.66	0.60
1:A:947:ILE:HG21	1:A:954:PHE:CE2	2.34	0.60
1:B:544:SER:O	1:B:548:LYS:HG3	2.00	0.60
1:A:671:MSE:HE2	1:A:672:GLU:C	2.21	0.60
1:B:728:GLU:OE1	1:B:728:GLU:N	2.28	0.60
1:A:816:LEU:HD23	1:A:830:PRO:HA	1.84	0.60
1:A:867:ARG:HH11	1:B:528:GLU:HG3	1.66	0.60
1:A:617:LEU:HD12	4:A:2197:HOH:O	2.01	0.60
1:B:720:THR:HG22	4:B:2378:HOH:O	2.01	0.59
1:A:698:VAL:HG11	1:A:710:ILE:HD11	1.84	0.59
1:A:129:LEU:CD1	1:A:155:MSE:HE1	2.29	0.59
1:B:877:HIS:HE1	1:B:907:ALA:O	1.85	0.59
1:B:779:ASP:OD1	1:B:782:ALA:HB3	2.02	0.59
1:A:253:GLY:HA2	4:A:2125:HOH:O	2.02	0.59
1:B:17:LEU:CA	1:B:28:ILE:HD13	2.33	0.59
1:A:407:ARG:O	1:A:411:VAL:HG23	2.02	0.59
1:A:200:VAL:HG21	1:A:245:ILE:HD12	1.85	0.59
1:B:545:GLY:N	3:B:1985:SO4:O1	2.28	0.59
1:A:262:LYS:HG3	4:A:2126:HOH:O	2.02	0.59
1:A:272:MSE:HA	4:A:2131:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:LEU:O	1:B:658:VAL:HG22	2.03	0.59
1:B:774:GLN:O	1:B:774:GLN:HG2	2.01	0.59
1:B:628:VAL:HA	4:B:2357:HOH:O	2.02	0.58
1:A:733:ALA:HB2	1:A:914:PRO:HG3	1.85	0.58
1:A:222:VAL:O	1:A:226:VAL:HG23	2.04	0.58
1:B:731:ARG:N	1:B:915:HIS:HD2	1.89	0.58
1:A:21:THR:HG22	1:A:24:ASN:ND2	2.19	0.58
1:A:437:LEU:HD12	4:A:2208:HOH:O	2.03	0.58
1:A:269:ILE:HD11	4:A:2121:HOH:O	2.03	0.58
1:B:618:ARG:NH2	3:B:1981:SO4:O2	2.37	0.58
1:B:256:GLU:HG3	4:B:2163:HOH:O	2.04	0.58
1:B:234:PHE:HB3	1:B:275:LEU:HD12	1.85	0.58
1:A:667:LYS:HE2	1:A:725:TYR:CD2	2.39	0.58
1:B:669:THR:HA	1:B:687:ASN:OD1	2.04	0.57
1:A:881:LEU:HD13	1:A:907:ALA:HA	1.86	0.57
1:A:122:PRO:HB3	4:A:2078:HOH:O	2.03	0.57
1:A:265:SER:O	1:A:269:ILE:HG13	2.03	0.57
1:B:57:ILE:HG12	4:B:2052:HOH:O	2.05	0.57
1:A:617:LEU:N	4:A:2262:HOH:O	2.37	0.57
1:B:655:LEU:HB2	1:B:658:VAL:HG21	1.87	0.57
1:A:406:PHE:HE2	4:A:2176:HOH:O	1.88	0.57
1:B:960:GLU:HB2	4:B:2546:HOH:O	2.05	0.57
1:A:59:ASP:OD1	1:A:61:LYS:HE2	2.05	0.57
1:B:647:PHE:HB2	1:B:881:LEU:HA	1.87	0.57
1:A:252:ARG:NH2	4:A:2124:HOH:O	2.35	0.57
1:B:13:LEU:O	1:B:28:ILE:HD11	2.05	0.56
1:A:763:GLU:HB3	1:A:768:MSE:HE3	1.86	0.56
1:A:763:GLU:OE1	1:A:768:MSE:HE3	2.06	0.56
1:B:731:ARG:HH12	1:B:865:GLN:NE2	1.98	0.56
1:A:448:THR:HG23	4:A:2197:HOH:O	2.04	0.56
1:A:212:LEU:HD21	1:A:246:MSE:HE1	1.88	0.56
1:B:718:LEU:HD12	1:B:719:PRO:HD2	1.87	0.56
1:A:674:GLN:HB2	1:A:681:PRO:HB3	1.88	0.56
1:A:757:TRP:CH2	1:A:765:ARG:HD2	2.39	0.56
1:B:658:VAL:HG23	1:B:658:VAL:O	2.06	0.56
1:B:867:ARG:NE	4:B:2488:HOH:O	2.38	0.56
1:A:219:PRO:O	1:A:222:VAL:HG23	2.06	0.56
1:A:645:LEU:H	1:A:903:LYS:NZ	2.04	0.56
1:A:776:ASN:HB3	1:A:779:ASP:OD2	2.06	0.56
1:A:912:GLN:NE2	4:A:2393:HOH:O	2.39	0.56
1:B:327:ALA:HB3	4:B:2201:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLN:HB2	1:A:774:GLN:NE2	2.20	0.55
1:A:183:LYS:HD2	1:B:218:ASP:OD2	2.07	0.55
1:B:429:ASP:OD1	1:B:453:LYS:CE	2.54	0.55
1:A:230:GLY:HA3	1:A:264:LYS:HE3	1.87	0.55
1:A:200:VAL:HG22	1:A:245:ILE:HD12	1.87	0.55
1:B:535:MSE:HE1	1:B:547:TRP:CG	2.42	0.55
1:B:17:LEU:HA	1:B:28:ILE:HD13	1.89	0.55
1:B:639:GLU:OE2	1:B:645:LEU:HD21	2.07	0.55
1:A:167:MSE:CE	1:A:171:ILE:HD11	2.37	0.55
1:B:160:LYS:HE2	4:B:2132:HOH:O	2.06	0.55
1:A:851:MSE:HE2	4:A:2332:HOH:O	2.07	0.55
1:A:221:GLU:CG	1:B:187:ALA:HB1	2.37	0.55
1:B:276:VAL:HB	1:B:319:VAL:CG1	2.35	0.54
1:B:122:PRO:HA	4:B:2088:HOH:O	2.07	0.54
1:B:81:PRO:HD3	4:B:2411:HOH:O	2.07	0.54
1:A:612:TYR:HE1	4:A:2205:HOH:O	1.90	0.54
1:A:613:GLU:HB2	4:A:2260:HOH:O	2.06	0.54
1:A:647:PHE:HB2	1:A:881:LEU:HA	1.89	0.54
1:B:535:MSE:O	1:B:538:MSE:HG2	2.06	0.54
1:A:234:PHE:HB3	1:A:275:LEU:HD12	1.90	0.54
1:A:231:ALA:HB2	1:B:778:ASN:OD1	2.08	0.54
1:B:166:ARG:NH2	1:B:373:ASP:OD2	2.40	0.54
1:B:223:PRO:O	1:B:227:HIS:CD2	2.60	0.54
1:B:775:ILE:HG13	4:B:2446:HOH:O	2.06	0.54
1:B:416:VAL:HG23	1:B:417:GLY:N	2.22	0.54
1:A:221:GLU:HG2	1:B:187:ALA:HB1	1.88	0.54
1:A:299:THR:HG22	1:A:299:THR:O	2.07	0.54
1:A:671:MSE:HE2	1:A:672:GLU:O	2.07	0.54
1:A:916:LEU:HD23	1:A:944:GLY:HA3	1.88	0.54
1:A:182:LYS:HD2	1:A:184:GLU:OE1	2.08	0.54
1:B:67:MSE:HG3	4:B:2052:HOH:O	2.08	0.54
1:A:499:ASP:OD2	1:A:501:THR:HG23	2.08	0.54
1:A:919:LEU:HD12	1:A:919:LEU:N	2.23	0.54
1:A:306:ARG:HD3	4:A:2152:HOH:O	2.06	0.54
1:A:67:MSE:HE3	1:A:94:ILE:CG2	2.36	0.54
1:A:903:LYS:HE2	4:A:2271:HOH:O	2.07	0.54
1:A:387:THR:N	1:A:388:PRO:HD2	2.23	0.54
1:A:486:GLN:HB3	1:A:490:ARG:HH11	1.73	0.53
1:A:518:THR:O	1:A:522:ILE:HG13	2.08	0.53
1:A:594:THR:HG23	4:A:2254:HOH:O	2.08	0.53
1:B:600:VAL:HG11	1:B:886:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:MSE:HE3	1:A:163:VAL:HG22	1.91	0.53
1:B:-3:HIS:HB2	4:B:2005:HOH:O	2.07	0.53
1:A:532:THR:CG2	1:A:535:MSE:HG3	2.38	0.53
1:B:294:LYS:CE	1:B:326:ASP:OD2	2.56	0.53
1:B:234:PHE:HA	4:B:2151:HOH:O	2.07	0.53
1:A:263:ARG:O	1:A:267:VAL:HG23	2.09	0.53
1:B:420:PHE:HZ	4:B:2263:HOH:O	1.81	0.53
1:A:616:LYS:HB2	4:A:2260:HOH:O	2.07	0.53
1:B:956:LYS:O	1:B:957:ASN:HB2	2.09	0.53
1:A:294:LYS:HA	4:A:2138:HOH:O	2.09	0.53
1:A:616:LYS:NZ	3:A:1975:SO4:O3	2.29	0.53
1:B:246:MSE:HE2	1:B:246:MSE:CA	2.33	0.53
1:A:816:LEU:HD13	4:A:2352:HOH:O	2.08	0.53
1:A:257:ARG:HG3	1:A:258:GLU:HG3	1.89	0.53
1:A:296:ASN:C	1:A:298:ALA:H	2.13	0.52
1:A:764:ASP:OD1	1:A:766:GLU:HB2	2.09	0.52
1:A:132:LEU:HG	4:A:2056:HOH:O	2.09	0.52
1:B:871:ARG:HD2	4:B:2494:HOH:O	2.09	0.52
1:B:642:ASN:ND2	1:B:645:LEU:HD12	2.24	0.52
1:A:40:ILE:HG13	1:A:41:ILE:HG13	1.90	0.52
1:A:138:GLU:HG3	4:A:2063:HOH:O	2.09	0.52
1:A:641:SER:HA	1:A:887:ILE:CD1	2.40	0.52
1:A:346:GLU:OE1	1:A:349:LYS:HD3	2.09	0.52
1:A:635:LYS:HA	1:A:642:ASN:OD1	2.09	0.52
1:B:817:LEU:HD13	4:B:2453:HOH:O	2.09	0.52
1:A:72:HIS:CE1	1:A:773:ARG:HD3	2.44	0.52
1:B:45:VAL:HG11	1:B:86:TYR:CE2	2.45	0.52
1:B:867:ARG:CZ	4:B:2488:HOH:O	2.57	0.52
1:B:950:HIS:ND1	2:B:1977:ADP:O1B	2.43	0.52
1:B:206:GLU:HG2	4:B:2135:HOH:O	2.09	0.52
1:B:789:ILE:HD12	1:B:815:PHE:CZ	2.45	0.52
1:A:219:PRO:HG3	4:A:2109:HOH:O	2.10	0.51
1:A:283:ALA:HB3	1:A:331:LEU:HD21	1.92	0.51
1:A:485:THR:OG1	1:A:488:GLU:HG3	2.10	0.51
1:A:668:VAL:CG1	1:A:671:MSE:HB2	2.39	0.51
1:B:258:GLU:HG2	1:B:260:GLY:H	1.75	0.51
1:A:788:LYS:HD2	1:A:788:LYS:N	2.26	0.51
1:A:318:ARG:NH2	1:A:424:GLU:OE1	2.43	0.51
1:B:246:MSE:HA	1:B:246:MSE:CE	2.33	0.51
1:A:431:CYS:N	4:A:2191:HOH:O	2.44	0.51
1:B:543:LEU:HD12	4:B:2310:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PRO:O	1:A:214:GLN:HG2	2.10	0.51
1:B:799:ILE:HG22	1:B:855:VAL:HG21	1.91	0.51
1:A:624:PHE:O	1:A:627:PHE:HB3	2.11	0.51
1:B:603:ASP:HA	1:B:623:ASN:HB2	1.92	0.51
1:B:666:VAL:HB	1:B:690:CYS:HB2	1.93	0.51
1:A:212:LEU:HD13	1:A:245:ILE:HG22	1.92	0.51
1:A:78:ASN:ND2	1:A:736:LYS:HZ3	2.08	0.51
1:A:78:ASN:HD21	1:A:736:LYS:NZ	2.09	0.51
1:B:877:HIS:HD2	4:B:2486:HOH:O	1.94	0.51
1:A:302:ASP:OD2	1:A:304:GLU:HB3	2.10	0.51
1:A:131:HIS:HB2	4:A:2056:HOH:O	2.09	0.51
1:A:224:GLU:HB2	4:A:2111:HOH:O	2.10	0.51
1:A:752:SER:O	1:A:756:GLN:HG3	2.11	0.51
1:A:246:MSE:HA	1:A:246:MSE:CE	2.34	0.51
1:A:17:LEU:CA	1:A:28:ILE:HD13	2.41	0.51
1:A:645:LEU:H	1:A:903:LYS:HZ3	1.57	0.51
1:A:819:GLU:HG2	4:A:2343:HOH:O	2.10	0.51
1:B:129:LEU:HB3	1:B:130:PRO:HD3	1.92	0.51
1:A:197:THR:O	1:A:200:VAL:HG23	2.11	0.51
1:B:445:LEU:HD22	4:B:2349:HOH:O	2.11	0.51
1:A:824:LYS:HB3	1:B:306:ARG:HH12	1.75	0.51
1:A:78:ASN:ND2	1:A:736:LYS:NZ	2.58	0.50
1:B:532:THR:CG2	1:B:535:MSE:H	2.24	0.50
1:A:404:ASP:O	1:A:408:LYS:HG3	2.11	0.50
1:B:183:LYS:H	1:B:183:LYS:HD3	1.77	0.50
1:B:222:VAL:HB	1:B:223:PRO:HD3	1.92	0.50
1:B:809:TYR:OH	3:B:1979:SO4:O4	2.23	0.50
1:B:671:MSE:HE2	1:B:672:GLU:C	2.31	0.50
1:B:396:GLU:HB2	2:B:1977:ADP:H5'2	1.91	0.50
1:B:256:GLU:O	1:B:262:LYS:HE3	2.11	0.50
1:B:568:GLU:OE1	1:B:597:HIS:ND1	2.41	0.50
1:A:386:ILE:HD13	4:A:2176:HOH:O	2.11	0.50
1:A:385:HIS:HA	4:A:2183:HOH:O	2.11	0.50
1:B:266:ALA:HB3	1:B:308:VAL:HG12	1.93	0.50
1:B:779:ASP:OD2	1:B:782:ALA:HB3	2.11	0.50
1:A:667:LYS:CG	1:A:725:TYR:HB3	2.42	0.50
1:B:634:ALA:HA	1:B:637:TYR:CD1	2.46	0.50
1:A:17:LEU:N	1:A:28:ILE:HD13	2.26	0.50
1:B:50:PHE:HZ	1:B:83:VAL:HG13	1.77	0.50
1:B:387:THR:N	1:B:388:PRO:HD2	2.26	0.50
1:A:166:ARG:NH2	1:A:373:ASP:OD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:PHE:HB3	1:B:619:LYS:O	2.11	0.50
1:A:167:MSE:HE1	1:A:171:ILE:HD11	1.93	0.50
1:A:710:ILE:HD12	1:A:948:ILE:HD11	1.94	0.49
1:A:222:VAL:N	1:A:223:PRO:HD2	2.27	0.49
1:A:656:GLU:HG3	4:A:2275:HOH:O	2.13	0.49
1:B:757:TRP:CH2	1:B:765:ARG:HD2	2.47	0.49
1:A:45:VAL:HG11	1:A:86:TYR:CE2	2.47	0.49
1:B:914:PRO:HA	4:B:2517:HOH:O	2.13	0.49
1:B:775:ILE:HB	4:B:2445:HOH:O	2.12	0.49
1:A:719:PRO:HG2	1:A:806:LYS:HD3	1.93	0.49
1:A:737:GLN:HA	1:A:740:PHE:HD2	1.78	0.49
1:A:640:LEU:HD11	1:A:884:ASP:OD2	2.13	0.49
1:A:798:GLY:HA2	1:A:851:MSE:HE1	1.94	0.49
1:B:699:ILE:CG2	1:B:700:GLY:N	2.76	0.49
1:B:58:LYS:O	1:B:58:LYS:HG2	2.12	0.49
1:A:651:GLU:OE2	1:A:942:GLU:HG3	2.13	0.48
1:A:382:TRP:CD2	1:A:407:ARG:HB2	2.48	0.48
1:B:674:GLN:HB2	1:B:681:PRO:HA	1.95	0.48
1:A:306:ARG:N	4:A:2153:HOH:O	2.46	0.48
1:B:445:LEU:HD21	1:B:612:TYR:CE2	2.48	0.48
1:A:624:PHE:CE1	1:A:639:GLU:HG3	2.48	0.48
1:A:261:ILE:HG13	4:A:2128:HOH:O	2.13	0.48
1:A:123:VAL:HG13	1:A:370:ASP:OD2	2.13	0.48
1:A:494:VAL:HG12	1:A:495:GLU:HG3	1.94	0.48
1:B:120:VAL:HG23	4:B:2088:HOH:O	2.13	0.48
1:B:294:LYS:HE2	1:B:326:ASP:OD2	2.13	0.48
1:B:372:ILE:HD11	1:B:410:ALA:CB	2.39	0.48
1:B:303:PRO:HG2	4:B:2189:HOH:O	2.13	0.48
1:B:775:ILE:HD11	4:B:2081:HOH:O	2.14	0.48
1:A:655:LEU:HB3	4:A:2290:HOH:O	2.13	0.48
1:A:250:LEU:HD13	1:A:269:ILE:HG12	1.96	0.48
1:A:667:LYS:HE2	1:A:725:TYR:CG	2.49	0.47
1:B:204:ASP:HB3	4:B:2151:HOH:O	2.14	0.47
1:A:877:HIS:HE1	1:A:907:ALA:O	1.96	0.47
1:B:223:PRO:HB3	1:B:261:ILE:CD1	2.45	0.47
1:A:440:GLY:O	1:A:441:ALA:HB3	2.14	0.47
1:A:802:ARG:HB3	1:A:859:GLU:HG3	1.95	0.47
1:A:736:LYS:NZ	1:A:770:ARG:HD2	2.28	0.47
1:A:535:MSE:HE1	1:A:547:TRP:CG	2.50	0.47
1:B:240:PRO:HD2	4:B:2156:HOH:O	2.14	0.47
1:B:78:ASN:HA	4:B:2064:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:ARG:HG2	4:B:2055:HOH:O	2.15	0.47
1:B:773:ARG:HA	4:B:2055:HOH:O	2.15	0.47
1:A:535:MSE:HA	1:A:538:MSE:HG2	1.97	0.47
1:B:827:ARG:NH1	1:B:827:ARG:HG3	2.28	0.47
1:B:540:ILE:HB	4:B:2310:HOH:O	2.15	0.47
1:B:432:ASN:HB2	4:B:2264:HOH:O	2.14	0.47
1:A:647:PHE:HB3	4:A:2271:HOH:O	2.15	0.47
1:B:816:LEU:HD23	1:B:830:PRO:HA	1.96	0.47
1:B:768:MSE:HE2	4:B:2432:HOH:O	2.13	0.47
1:B:769:ASP:HA	4:B:2443:HOH:O	2.15	0.47
1:B:419:ASN:HD22	1:B:420:PHE:H	1.61	0.47
1:B:425:ASP:OD2	4:B:2263:HOH:O	2.20	0.47
1:B:819:GLU:O	1:B:826:GLU:HA	2.15	0.47
1:A:262:LYS:HB3	4:A:2141:HOH:O	2.15	0.47
1:B:765:ARG:NH2	4:B:2433:HOH:O	2.45	0.47
1:A:667:LYS:HG3	1:A:725:TYR:HB3	1.96	0.47
1:B:42:GLU:HG3	4:B:2004:HOH:O	2.14	0.47
1:A:538:MSE:HB2	1:A:539:PRO:HD2	1.96	0.47
1:A:897:SER:C	4:A:2389:HOH:O	2.53	0.47
1:A:105:ILE:HG12	4:A:2040:HOH:O	2.14	0.47
1:B:701:PRO:HG3	4:B:2007:HOH:O	2.14	0.47
1:A:160:LYS:HG3	1:A:199:THR:HG22	1.97	0.47
1:A:324:GLU:N	1:A:324:GLU:CD	2.68	0.46
1:B:428:GLU:OE2	1:B:454:ARG:NE	2.46	0.46
1:B:820:ASN:HB2	1:B:826:GLU:HA	1.97	0.46
1:B:16:LYS:HB3	1:B:28:ILE:HD12	1.96	0.46
1:A:728:GLU:O	1:A:729:ASN:HB2	2.16	0.46
1:B:69:ALA:O	1:B:73:ILE:HG13	2.15	0.46
1:B:371:LEU:HD23	4:B:2240:HOH:O	2.16	0.46
1:B:67:MSE:HE1	1:B:109:ALA:CA	2.43	0.46
1:A:535:MSE:HG2	1:A:538:MSE:HE3	1.97	0.46
1:A:750:THR:OG1	1:A:753:GLU:HG3	2.16	0.46
1:A:803:ARG:N	4:A:2338:HOH:O	2.49	0.46
1:B:808:THR:OG1	1:B:809:TYR:N	2.46	0.46
1:A:256:GLU:HG2	1:A:261:ILE:HD13	1.97	0.46
1:A:566:LEU:HD22	4:A:2253:HOH:O	2.14	0.46
1:A:916:LEU:CD2	1:A:944:GLY:HA3	2.46	0.46
1:A:654:TYR:CE2	1:B:521:ALA:HB2	2.51	0.46
1:A:473:ARG:NH2	4:A:2206:HOH:O	2.49	0.46
1:A:152:PHE:N	4:A:2074:HOH:O	2.49	0.46
1:A:77:SER:H	1:A:774:GLN:HE22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:MSE:HG2	1:A:971:THR:H	1.80	0.46
1:A:253:GLY:O	1:A:256:GLU:HB2	2.16	0.46
1:B:654:TYR:HE2	1:B:656:GLU:HG2	1.78	0.46
1:B:435:PHE:CD1	1:B:480:VAL:HG13	2.50	0.46
1:A:448:THR:CG2	4:A:2197:HOH:O	2.61	0.46
1:A:697:ALA:HB2	1:A:959:THR:HG21	1.97	0.46
1:A:250:LEU:O	1:A:253:GLY:N	2.47	0.45
1:B:451:ARG:NH1	4:B:2274:HOH:O	2.50	0.45
1:B:811:TYR:HE2	1:B:841:ARG:HB2	1.81	0.45
1:A:731:ARG:HH12	1:A:865:GLN:NE2	2.07	0.45
1:A:586:ASN:ND2	3:A:1976:SO4:O3	2.45	0.45
1:A:831:MSE:O	1:A:832:MSE:HE2	2.16	0.45
1:B:364:ILE:HD13	1:B:390:MSE:HG2	1.99	0.45
1:B:737:GLN:HG2	4:B:2105:HOH:O	2.16	0.45
1:A:78:ASN:HD21	1:A:736:LYS:HZ1	1.62	0.45
1:B:462:GLY:CA	1:B:637:TYR:HE2	2.30	0.45
1:B:921:GLU:OE2	1:B:950:HIS:HD2	2.00	0.45
1:B:0:HIS:HB3	4:B:2392:HOH:O	2.16	0.45
1:A:304:GLU:OE2	1:A:304:GLU:HA	2.16	0.45
1:B:125:ILE:HG23	1:B:126:LYS:N	2.32	0.45
1:A:304:GLU:O	1:A:308:VAL:HG23	2.16	0.45
1:B:420:PHE:CZ	1:B:621:LYS:CB	2.84	0.45
1:B:535:MSE:HA	1:B:538:MSE:HE3	1.99	0.45
1:B:728:GLU:O	1:B:729:ASN:HB2	2.16	0.45
1:B:178:MSE:HE3	1:B:190:THR:OG1	2.16	0.45
1:B:609:ILE:HG13	1:B:627:PHE:HB2	1.98	0.45
1:B:652:PRO:HB3	1:B:914:PRO:O	2.17	0.45
1:B:76:GLN:HG3	1:B:775:ILE:HD11	1.99	0.45
1:A:716:GLU:HG3	1:A:771:ALA:HB2	1.97	0.45
1:B:824:LYS:HB3	1:B:824:LYS:HE2	1.65	0.45
1:B:814:SER:HA	1:B:836:ASN:OD1	2.17	0.45
1:A:342:GLN:HB3	1:A:342:GLN:HE21	1.66	0.45
1:B:820:ASN:O	1:B:826:GLU:HB2	2.16	0.45
1:A:212:LEU:CD1	1:A:246:MSE:HE3	2.46	0.45
1:A:948:ILE:HG21	4:A:2012:HOH:O	2.16	0.45
1:A:773:ARG:NH1	1:A:846:GLU:OE1	2.46	0.45
1:A:69:ALA:O	1:A:73:ILE:HG13	2.16	0.45
1:A:306:ARG:HG3	4:A:2153:HOH:O	2.16	0.44
1:B:451:ARG:CD	4:B:2274:HOH:O	2.65	0.44
1:B:773:ARG:NH1	4:B:2445:HOH:O	2.49	0.44
1:B:17:LEU:N	1:B:28:ILE:CD1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD13	1:A:246:MSE:HE3	1.99	0.44
1:B:185:VAL:HG12	4:B:2127:HOH:O	2.18	0.44
1:A:310:LEU:HD21	1:A:314:LYS:HE3	1.98	0.44
1:B:75:ASN:HB2	4:B:2446:HOH:O	2.17	0.44
1:B:317:ARG:HA	1:B:322:VAL:HG13	1.99	0.44
1:B:884:ASP:HA	1:B:885:PRO:HD3	1.85	0.44
1:A:949:THR:OG1	1:A:950:HIS:N	2.50	0.44
1:B:184:GLU:OE1	1:B:184:GLU:N	2.50	0.44
1:A:128:LEU:HD12	4:A:2056:HOH:O	2.18	0.44
1:A:737:GLN:HB3	1:A:925:TYR:CD2	2.52	0.44
1:A:277:GLU:HG3	4:A:2135:HOH:O	2.17	0.44
1:B:494:VAL:HG12	1:B:495:GLU:HG3	1.98	0.44
1:A:16:LYS:HB3	1:A:28:ILE:HD12	2.00	0.44
1:B:637:TYR:HB2	4:B:2360:HOH:O	2.17	0.44
1:A:710:ILE:HD12	1:A:948:ILE:CD1	2.48	0.44
1:B:16:LYS:CG	1:B:28:ILE:HD12	2.47	0.44
1:B:423:GLU:N	4:B:2274:HOH:O	2.51	0.44
1:A:321:ASN:O	1:A:321:ASN:ND2	2.51	0.44
1:A:296:ASN:C	1:A:298:ALA:N	2.71	0.44
1:B:775:ILE:O	1:B:775:ILE:CG2	2.65	0.44
1:A:765:ARG:HD3	4:A:2317:HOH:O	2.18	0.44
1:A:749:LYS:HB3	1:A:753:GLU:HB2	1.99	0.44
1:B:921:GLU:OE2	1:B:950:HIS:CD2	2.71	0.43
1:B:773:ARG:O	1:B:775:ILE:N	2.51	0.43
1:B:699:ILE:CG2	1:B:700:GLY:H	2.28	0.43
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.81	0.43
1:A:532:THR:HG22	1:A:535:MSE:HG3	2.01	0.43
1:B:950:HIS:CB	2:B:1977:ADP:O1B	2.66	0.43
1:B:306:ARG:CZ	4:B:2191:HOH:O	2.67	0.43
1:B:729:ASN:N	3:B:1979:SO4:O3	2.34	0.43
1:B:36:LEU:HG	1:B:83:VAL:HG21	1.99	0.43
1:B:747:LEU:HB3	1:B:894:ARG:HB2	2.01	0.43
1:A:209:ILE:O	1:A:213:ILE:HG13	2.19	0.43
1:A:751:PRO:HB3	1:A:904:LEU:HD13	2.00	0.43
1:B:212:LEU:HD13	1:B:246:MSE:HE3	2.01	0.43
1:A:212:LEU:CD2	1:A:246:MSE:HE1	2.48	0.43
1:A:256:GLU:CG	1:A:257:ARG:H	2.32	0.43
1:A:212:LEU:CD1	1:A:246:MSE:CE	2.97	0.43
1:B:302:ASP:O	1:B:306:ARG:HG3	2.19	0.43
1:B:451:ARG:NE	4:B:2264:HOH:O	2.51	0.43
1:A:248:PRO:HG2	4:A:2120:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:VAL:HG21	1:B:272:MSE:O	2.19	0.43
1:A:646:GLU:C	4:A:2271:HOH:O	2.58	0.42
1:A:337:VAL:HG23	4:A:2163:HOH:O	2.19	0.42
1:A:867:ARG:CZ	4:A:2372:HOH:O	2.67	0.42
1:B:67:MSE:HE3	1:B:94:ILE:CG2	2.48	0.42
1:A:182:LYS:HB3	1:A:185:VAL:HG23	2.01	0.42
1:A:587:THR:OG1	1:B:870:THR:HG22	2.19	0.42
1:A:223:PRO:HB3	1:A:261:ILE:HD13	2.00	0.42
1:A:318:ARG:NE	1:A:424:GLU:OE2	2.52	0.42
1:A:67:MSE:HE1	1:A:109:ALA:CB	2.49	0.42
1:A:313:LEU:HD21	1:A:317:ARG:NH2	2.33	0.42
1:A:282:ILE:O	1:A:282:ILE:HG13	2.19	0.42
1:A:200:VAL:CG2	1:A:245:ILE:CD1	2.96	0.42
1:B:41:ILE:HD12	1:B:46:PRO:HD3	2.00	0.42
1:A:364:ILE:HG23	4:A:2176:HOH:O	2.19	0.42
1:A:640:LEU:HD21	1:A:886:GLU:HB2	2.01	0.42
1:A:81:PRO:HG2	4:A:2031:HOH:O	2.18	0.42
1:A:59:ASP:CG	1:A:61:LYS:HG2	2.40	0.42
1:A:772:ASN:O	1:A:774:GLN:OE1	2.36	0.42
1:B:186:LYS:N	4:B:2127:HOH:O	2.52	0.42
1:A:526:LEU:O	1:A:531:PHE:HB2	2.20	0.42
1:A:505:THR:O	1:A:539:PRO:HA	2.20	0.42
1:A:351:GLU:HG2	1:A:394:LEU:HD21	2.02	0.42
1:B:21:THR:HG23	1:B:23:ASP:HB2	2.01	0.42
1:A:239:THR:HB	1:A:240:PRO:CD	2.50	0.42
1:B:462:GLY:N	1:B:637:TYR:HE2	2.17	0.42
1:A:921:GLU:CD	1:A:949:THR:HA	2.41	0.42
1:A:435:PHE:CD1	1:A:480:VAL:HG13	2.55	0.42
1:A:315:THR:O	1:A:319:VAL:HG23	2.20	0.42
1:A:167:MSE:N	1:A:168:PRO:HD2	2.35	0.42
1:B:597:HIS:H	1:B:597:HIS:HD1	1.68	0.42
1:B:123:VAL:HG12	1:B:367:ILE:HG23	2.02	0.42
1:A:39:ASN:ND2	4:A:2012:HOH:O	2.51	0.41
1:B:647:PHE:C	1:B:648:LYS:HD3	2.41	0.41
1:A:303:PRO:HG3	1:B:826:GLU:OE2	2.20	0.41
1:A:901:LYS:HD2	4:A:2389:HOH:O	2.19	0.41
1:B:879:SER:HA	1:B:883:LEU:O	2.20	0.41
1:A:804:LYS:HG2	3:A:1977:SO4:O3	2.20	0.41
1:A:658:VAL:HA	4:A:2276:HOH:O	2.19	0.41
1:A:234:PHE:HB2	4:A:2131:HOH:O	2.20	0.41
1:A:671:MSE:HE3	1:A:719:PRO:CB	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:VAL:CG1	1:B:671:MSE:HB2	2.50	0.41
1:A:420:PHE:CZ	1:A:425:ASP:OD1	2.73	0.41
1:A:644:ASP:O	1:A:645:LEU:HD23	2.21	0.41
1:A:877:HIS:HD2	4:A:2374:HOH:O	2.02	0.41
1:A:68:GLN:O	1:A:72:HIS:HD2	2.03	0.41
1:B:291:PRO:HG2	4:B:2185:HOH:O	2.20	0.41
1:A:730:CYS:HA	1:A:915:HIS:CD2	2.56	0.41
1:B:647:PHE:O	1:B:648:LYS:HD3	2.20	0.41
1:B:957:ASN:HA	1:B:957:ASN:HD22	1.68	0.41
1:B:850:LYS:O	1:B:854:GLU:HG3	2.21	0.41
1:A:142:TRP:HD1	4:A:2065:HOH:O	2.03	0.41
1:B:290:LEU:N	1:B:291:PRO:HD2	2.36	0.41
1:B:383:PHE:CD1	1:B:927:ASP:HB3	2.56	0.41
1:B:737:GLN:HB3	1:B:925:TYR:CD2	2.55	0.41
1:A:306:ARG:NH2	4:A:2143:HOH:O	2.53	0.41
1:A:547:TRP:CD1	3:A:1974:SO4:O4	2.74	0.41
1:B:300:ILE:HG21	1:B:305:ALA:HB3	2.03	0.41
1:B:950:HIS:HB2	4:B:2533:HOH:O	2.21	0.41
1:A:301:ALA:O	1:A:302:ASP:C	2.59	0.41
1:A:126:LYS:NZ	1:A:373:ASP:OD2	2.39	0.41
1:B:131:HIS:HA	3:B:1983:SO4:O1	2.21	0.41
1:B:867:ARG:NH2	4:B:2488:HOH:O	2.54	0.41
1:A:239:THR:HB	1:A:240:PRO:HD2	2.03	0.41
1:B:419:ASN:ND2	1:B:420:PHE:N	2.64	0.40
1:B:419:ASN:HD22	1:B:420:PHE:N	2.19	0.40
1:A:67:MSE:HE2	1:A:109:ALA:HA	2.00	0.40
1:A:430:LEU:O	1:A:484:PRO:HG2	2.21	0.40
1:A:17:LEU:HA	1:A:28:ILE:HD13	2.02	0.40
1:A:252:ARG:CZ	4:A:2109:HOH:O	2.68	0.40
1:A:502:HIS:C	1:A:504:ASP:H	2.23	0.40
1:B:502:HIS:C	1:B:504:ASP:H	2.24	0.40
1:A:105:ILE:CG1	4:A:2040:HOH:O	2.68	0.40
1:A:458:TYR:CD1	1:A:608:TYR:HB2	2.57	0.40
1:B:440:GLY:O	1:B:441:ALA:HB3	2.21	0.40
1:A:234:PHE:CZ	1:A:272:MSE:HB2	2.57	0.40
1:B:55:LYS:NZ	4:B:2044:HOH:O	2.53	0.40
1:B:779:ASP:O	1:B:783:MSE:HG2	2.21	0.40
1:A:234:PHE:CB	1:A:275:LEU:HD12	2.52	0.40
1:A:283:ALA:HB3	1:A:284:PRO:CD	2.51	0.40
1:B:21:THR:HG22	1:B:24:ASN:ND2	2.37	0.40
1:A:102:ASP:OD2	1:A:105:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LYS:HA	1:A:264:LYS:HD2	1.98	0.40
1:B:207:ARG:HA	4:B:2135:HOH:O	2.20	0.40
1:A:884:ASP:HA	1:A:885:PRO:HD3	1.92	0.40
1:B:824:LYS:HA	4:B:2470:HOH:O	2.22	0.40
1:B:555:ARG:HH21	1:B:559:ARG:NH2	2.20	0.40
1:B:831:MSE:C	1:B:832:MSE:HE2	2.42	0.40
1:A:207:ARG:NH1	4:A:2104:HOH:O	2.55	0.40
1:B:958:LEU:HA	1:B:958:LEU:HD23	1.95	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	971/986 (98%)	927 (96%)	42 (4%)	2 (0%)	52	69
1	B	979/986 (99%)	945 (96%)	31 (3%)	3 (0%)	46	63
All	All	1950/1972 (99%)	1872 (96%)	73 (4%)	5 (0%)	46	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	640	LEU
1	B	774	GLN
1	B	423	GLU
1	A	301	ALA
1	A	972	PRO

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	831/821 (101%)	806 (97%)	25 (3%)	48	70
1	B	838/821 (102%)	812 (97%)	26 (3%)	47	69
All	All	1669/1642 (102%)	1618 (97%)	51 (3%)	47	69

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	166	ARG
1	A	169	GLU
1	A	224	GLU
1	A	288	LYS
1	A	316	LEU
1	A	321	ASN
1	A	324	GLU
1	A	336	ASP
1	A	342	GLN
1	A	432	ASN
1	A	449	GLN
1	A	493	TYR
1	A	573	LEU
1	A	659	LYS
1	A	671	MSE
1	A	737	GLN
1	A	748	ASP
1	A	773	ARG
1	A	779	ASP
1	A	876	GLU
1	A	881	LEU
1	A	929	ASP
1	A	958	LEU
1	A	970	MSE
1	B	-3	HIS
1	B	155	MSE

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Mol	Chain	Res	Type
1	B	169	GLU
1	B	183	LYS
1	B	215	CYS
1	B	257	ARG
1	B	342	GLN
1	B	351	GLU
1	B	419	ASN
1	B	432	ASN
1	B	469	SER
1	B	490	ARG
1	B	493	TYR
1	B	529	PHE
1	B	534	GLU
1	B	573	LEU
1	B	671	MSE
1	B	737	GLN
1	B	748	ASP
1	B	783	MSE
1	B	859	GLU
1	B	872	LYS
1	B	876	GLU
1	B	881	LEU
1	B	956	LYS
1	B	958	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	78	ASN
1	A	97	ASN
1	A	271	ASN
1	A	321	ASN
1	A	342	GLN
1	A	413	ASN
1	A	432	ASN
1	A	496	HIS
1	A	597	HIS
1	A	604	ASN
1	A	611	ASN
1	A	711	ASN
1	A	729	ASN

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Mol	Chain	Res	Type
1	A	756	GLN
1	A	848	HIS
1	A	865	GLN
1	A	877	HIS
1	A	915	HIS
1	A	924	ASN
1	B	5	GLN
1	B	97	ASN
1	B	227	HIS
1	B	271	ASN
1	B	321	ASN
1	B	342	GLN
1	B	413	ASN
1	B	419	ASN
1	B	604	ASN
1	B	611	ASN
1	B	642	ASN
1	B	711	ASN
1	B	729	ASN
1	B	756	GLN
1	B	784	ASN
1	B	848	HIS
1	B	865	GLN
1	B	877	HIS
1	B	915	HIS
1	B	924	ASN
1	B	957	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	1973	-	22,29,29	1.17	2 (9%)	27,45,45	2.45	4 (14%)
3	SO4	A	1974	-	4,4,4	0.90	0	6,6,6	0.35	0
3	SO4	A	1975	-	4,4,4	0.91	0	6,6,6	0.35	0
3	SO4	A	1976	-	4,4,4	0.91	0	6,6,6	0.35	0
3	SO4	A	1977	-	4,4,4	0.92	0	6,6,6	0.09	0
3	SO4	A	1978	-	4,4,4	0.90	0	6,6,6	0.35	0
2	ADP	B	1977	-	22,29,29	1.18	2 (9%)	27,45,45	2.57	3 (11%)
3	SO4	B	1978	-	4,4,4	0.90	0	6,6,6	0.08	0
3	SO4	B	1979	-	4,4,4	0.91	0	6,6,6	0.36	0
3	SO4	B	1980	-	4,4,4	0.90	0	6,6,6	0.09	0
3	SO4	B	1981	-	4,4,4	0.90	0	6,6,6	0.09	0
3	SO4	B	1982	-	4,4,4	0.90	0	6,6,6	0.08	0
3	SO4	B	1983	-	4,4,4	0.91	0	6,6,6	0.08	0
3	SO4	B	1984	-	4,4,4	0.91	0	6,6,6	0.36	0
3	SO4	B	1985	-	4,4,4	0.90	0	6,6,6	0.09	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
2	ADP	A	1973	-	-	0/12/32/32	0/3/3/3
3	SO4	A	1974	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1975	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1976	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1977	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1978	-	-	0/0/0/0	0/0/0/0
2	ADP	B	1977	-	-	0/12/32/32	0/3/3/3
3	SO4	B	1978	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1979	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	1980	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1981	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1982	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1983	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1984	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1985	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1977	ADP	O4'-C1'	2.11	1.43	1.41
2	A	1973	ADP	O4'-C1'	2.16	1.43	1.41
2	B	1977	ADP	PB-O1B	3.09	1.61	1.51
2	A	1973	ADP	PB-O1B	3.13	1.61	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1977	ADP	N3-C2-N1	-9.76	121.42	128.89
2	A	1973	ADP	N3-C2-N1	-9.70	121.47	128.89
2	B	1977	ADP	C4'-O4'-C1'	-6.84	102.21	109.72
2	A	1973	ADP	C4'-O4'-C1'	-5.71	103.45	109.72
2	B	1977	ADP	PA-O3A-PB	-3.74	120.12	132.67
2	A	1973	ADP	PA-O3A-PB	-3.58	120.68	132.67
2	A	1973	ADP	C4-C5-N7	-2.17	107.49	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1974	SO4	2	0
3	A	1975	SO4	1	0
3	A	1976	SO4	2	0
3	A	1977	SO4	2	0
2	B	1977	ADP	6	0
3	B	1979	SO4	2	0
3	B	1981	SO4	1	0
3	B	1983	SO4	1	0
3	B	1985	SO4	1	0

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, 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	951/986 (96%)	0.22	73 (7%) 16 16	22, 44, 82, 108	0
1	B	959/986 (97%)	-0.10	40 (4%) 40 41	17, 33, 63, 106	0
All	All	1910/1972 (96%)	0.06	113 (5%) 26 26	17, 39, 75, 108	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	778	ASN	11.5
1	B	640	LEU	11.2
1	A	779	ASP	9.1
1	A	424	GLU	7.5
1	A	643	THR	7.4
1	B	779	ASP	7.0
1	B	776	ASN	6.9
1	A	423	GLU	6.8
1	A	957	ASN	6.6
1	A	422	ASP	6.6
1	B	641	SER	6.5
1	B	639	GLU	6.5
1	B	775	ILE	6.4
1	B	774	GLN	6.2
1	B	778	ASN	6.2
1	A	644	ASP	6.0
1	B	780	ALA	6.0
1	B	642	ASN	5.5
1	A	973	SER	5.5
1	A	637	TYR	5.5
1	A	777	GLU	5.4
1	A	645	LEU	5.4
1	A	426	GLU	5.2
1	B	420	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	5.0
1	B	423	GLU	5.0
1	B	426	GLU	4.9
1	B	424	GLU	4.8
1	A	638	GLU	4.7
1	A	776	ASN	4.5
1	B	-2	HIS	4.4
1	A	641	SER	4.4
1	A	782	ALA	4.4
1	B	643	THR	4.3
1	B	777	GLU	4.3
1	A	306	ARG	4.2
1	B	644	ASP	4.0
1	A	419	ASN	4.0
1	B	504	ASP	4.0
1	A	781	GLU	4.0
1	A	300	ILE	4.0
1	A	775	ILE	3.8
1	B	425	ASP	3.8
1	A	324	GLU	3.8
1	A	417	GLY	3.8
1	A	427	GLY	3.7
1	A	307	GLU	3.7
1	A	257	ARG	3.6
1	A	504	ASP	3.6
1	A	971	THR	3.5
1	A	642	ASN	3.5
1	B	781	GLU	3.5
1	A	774	GLN	3.5
1	B	977	TRP	3.5
1	A	646	GLU	3.4
1	A	352	THR	3.3
1	A	235	VAL	3.3
1	B	23	ASP	3.2
1	A	972	PRO	3.2
1	A	297	PHE	3.2
1	B	422	ASP	3.2
1	A	428	GLU	3.2
1	A	305	ALA	3.1
1	A	487	GLU	3.1
1	A	421	ASP	3.1
1	A	640	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	425	ASP	3.0
1	A	263	ARG	3.0
1	A	639	GLU	3.0
1	A	269	ILE	2.9
1	A	227	HIS	2.8
1	A	350	ASP	2.8
1	A	572	HIS	2.8
1	A	420	PHE	2.7
1	A	309	THR	2.7
1	B	572	HIS	2.7
1	A	311	ARG	2.7
1	A	268	ILE	2.7
1	B	782	ALA	2.7
1	A	23	ASP	2.6
1	B	419	ASN	2.6
1	B	637	TYR	2.6
1	A	265	SER	2.6
1	A	310	LEU	2.6
1	B	230	GLY	2.5
1	A	203	LYS	2.5
1	B	417	GLY	2.5
1	A	416	VAL	2.5
1	B	233	THR	2.5
1	A	952	ALA	2.4
1	B	179	TRP	2.4
1	A	140	ASN	2.4
1	A	515	GLY	2.3
1	A	314	LYS	2.3
1	B	967	ASP	2.3
1	A	418	PRO	2.3
1	A	966	LYS	2.3
1	A	850	LYS	2.2
1	A	502	HIS	2.2
1	A	293	LEU	2.2
1	A	304	GLU	2.2
1	A	254	LEU	2.2
1	A	250	LEU	2.2
1	B	418	PRO	2.2
1	B	227	HIS	2.2
1	B	140	ASN	2.2
1	A	231	ALA	2.1
1	A	780	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLU	2.1
1	B	487	GLU	2.1
1	A	233	THR	2.0
1	B	232	THR	2.0
1	B	833	SER	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	SO4	A	1974	5/5	0.95	0.41	6.38	80,81,81,81	0
3	SO4	A	1976	5/5	0.95	0.24	5.68	54,55,58,59	0
3	SO4	B	1980	5/5	0.93	0.28	3.71	73,73,74,74	0
2	ADP	B	1977	27/27	0.85	0.21	3.40	24,37,70,72	0
3	SO4	B	1982	5/5	0.97	0.18	3.35	63,63,63,65	0
3	SO4	B	1979	5/5	0.96	0.28	3.27	59,61,62,63	0
3	SO4	A	1977	5/5	0.93	0.33	2.32	83,83,84,85	0
3	SO4	B	1983	5/5	0.97	0.30	2.20	63,65,65,66	0
3	SO4	B	1978	5/5	0.95	0.17	1.59	55,56,57,59	0
2	ADP	A	1973	27/27	0.79	0.22	1.53	33,53,80,81	0
3	SO4	B	1984	5/5	0.99	0.10	-0.82	37,38,40,40	0
3	SO4	A	1978	5/5	0.98	0.10	-0.97	48,50,50,51	0
3	SO4	A	1975	5/5	0.91	0.25	-	83,84,84,85	0
3	SO4	B	1981	5/5	0.88	0.38	-	85,85,86,86	0
3	SO4	B	1985	5/5	0.90	0.51	-	73,73,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.