



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:27 PM UTC

PDB ID : 2IW3 / pdb_00002iw3
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

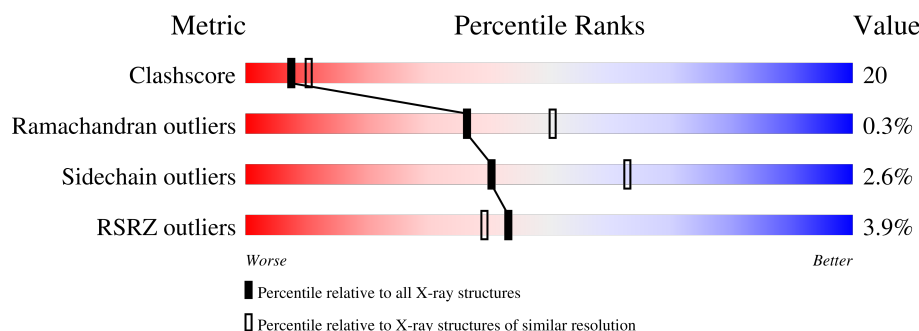
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. 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	5% 63% 33% ..
1	B	986	3% 71% 27% ..

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
3	SO4	A	1974	-	-	X	-
3	SO4	A	1976	-	-	X	-
3	SO4	A	1977	-	-	X	-
3	SO4	B	1979	-	-	X	-

2 Entry composition [i](#)

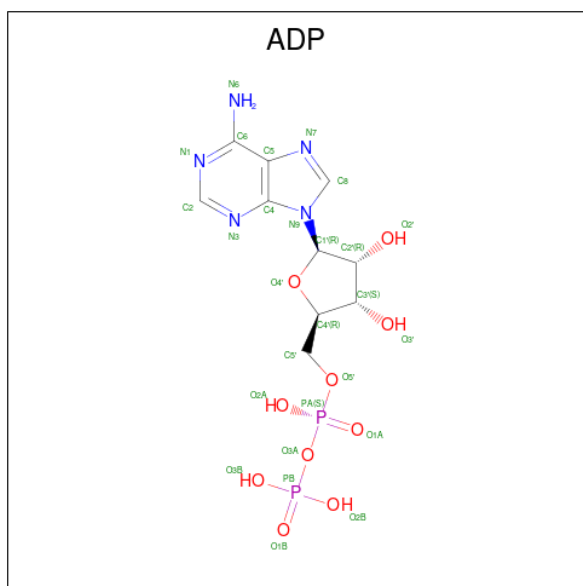
There are 4 unique types of molecules in this entry. The entry contains 16312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: 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		

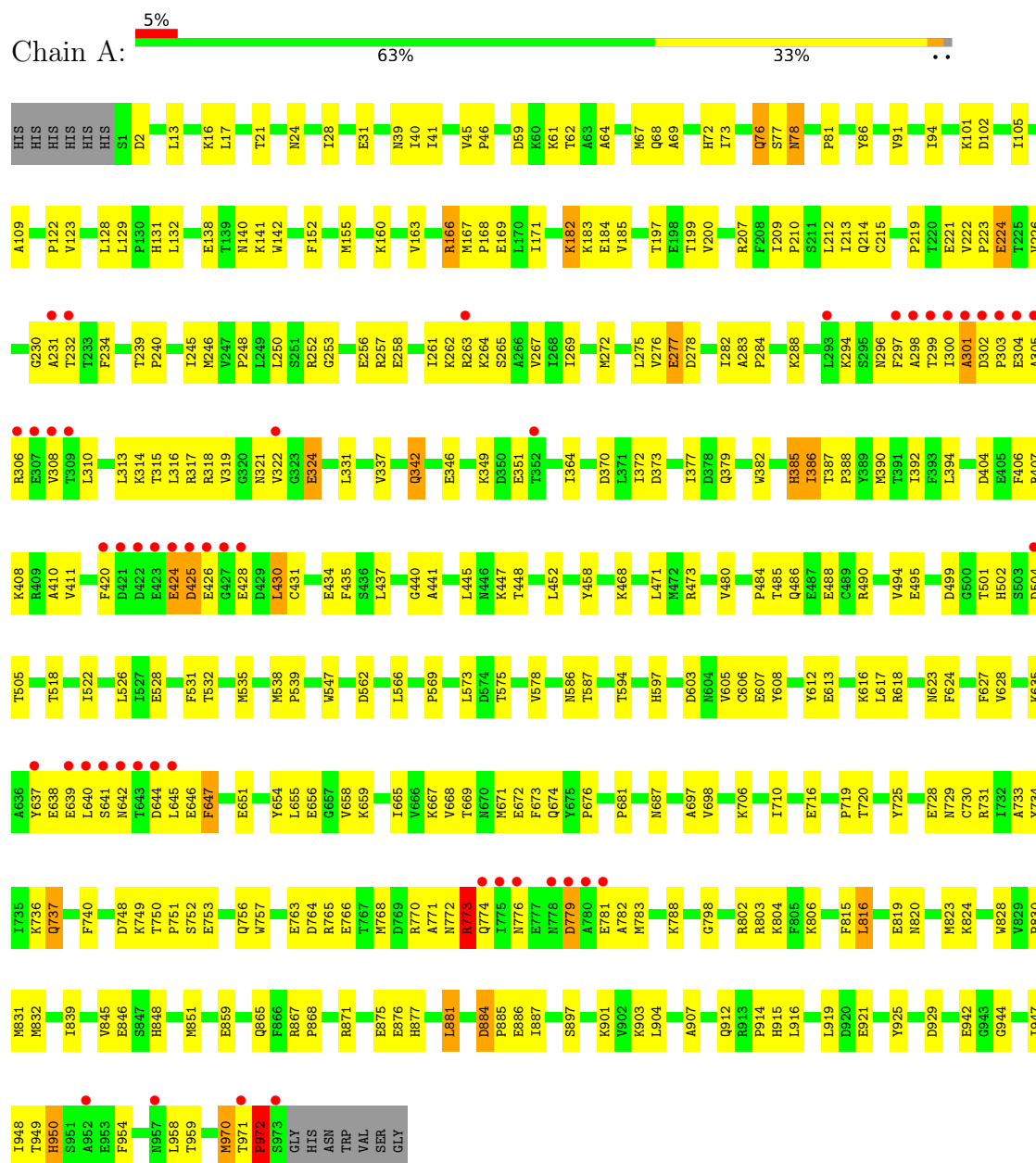
- Molecule 4 is water.

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

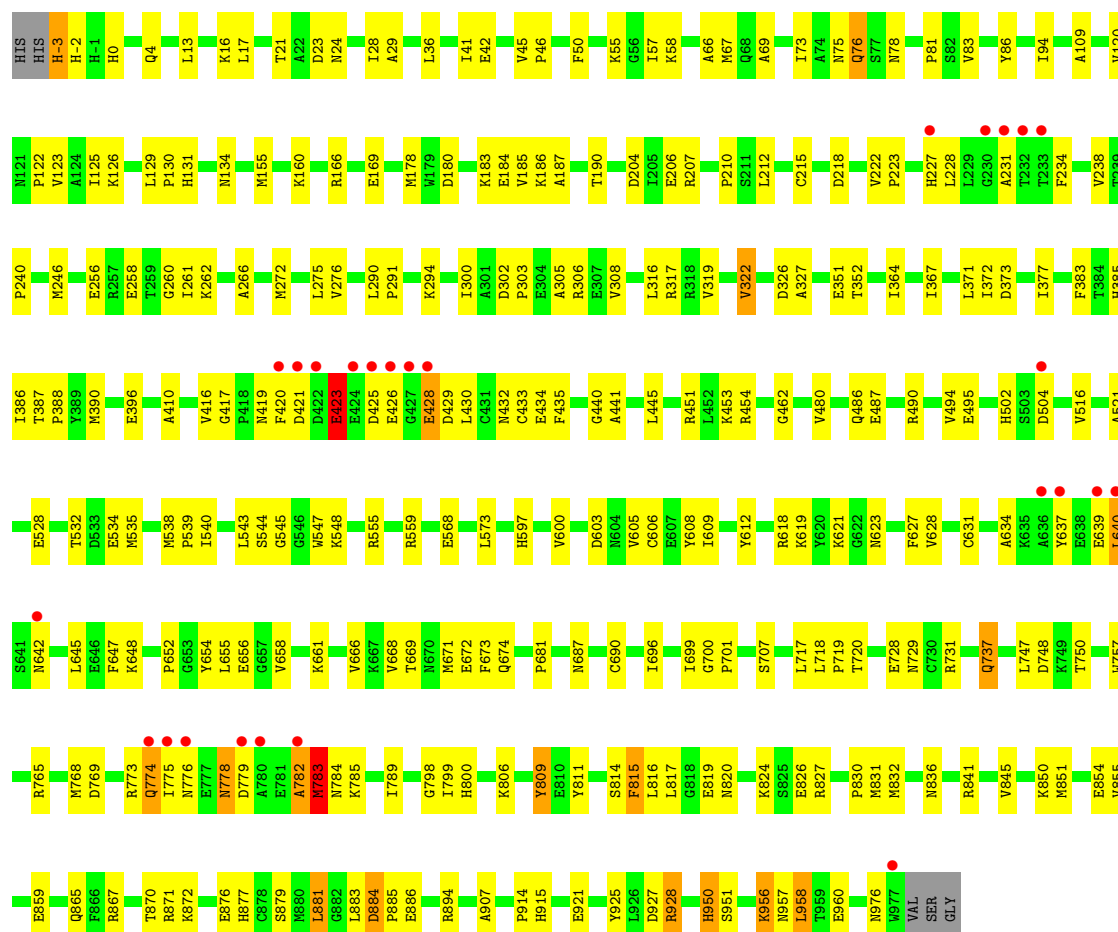
3 Residue-property plots [i](#)

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: 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 35.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.00-2.40) 99.2 (35.00-2.40)	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 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SO4

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	0.41	1/7695 (0.0%)	0.94	31/10390 (0.3%)
1	B	0.45	2/7768 (0.0%)	0.94	32/10489 (0.3%)
All	All	0.43	3/15463 (0.0%)	0.94	63/20879 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	ALA	C-O	6.84	1.33	1.24
1	A	972	PRO	C-N	-5.65	1.25	1.33
1	B	976	ASN	C-N	-5.34	1.25	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	GLU	N-CA-C	-10.23	95.38	110.52
1	B	386	ILE	N-CA-C	9.21	119.73	111.81
1	A	430	LEU	N-CA-C	-8.51	101.75	112.90
1	A	386	ILE	N-CA-C	7.92	118.62	111.81
1	A	773	ARG	N-CA-C	-7.87	97.22	109.25
1	B	784	ASN	N-CA-C	-7.75	104.75	112.97
1	B	783	MSE	N-CA-C	-7.71	103.61	113.16
1	B	605	VAL	N-CA-C	7.63	118.53	112.12
1	B	845	VAL	N-CA-C	7.59	119.28	110.62
1	A	605	VAL	N-CA-C	7.58	118.08	111.56
1	A	426	GLU	N-CA-C	7.31	120.71	108.20
1	B	815	PHE	N-CA-C	7.15	120.75	109.81
1	A	2	ASP	N-CA-C	-7.06	103.93	112.54
1	A	434	GLU	N-CA-C	-6.99	97.50	108.90
1	A	950	HIS	N-CA-C	-6.94	105.36	114.31
1	A	815	PHE	N-CA-C	6.86	119.84	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ASP	N-CA-C	-6.80	96.32	110.80
1	A	76	GLN	N-CA-C	6.49	120.46	112.54
1	B	950	HIS	N-CA-C	-6.34	105.48	113.72
1	B	377	ILE	N-CA-C	6.24	119.77	113.47
1	A	606	CYS	N-CA-C	6.22	119.49	110.28
1	B	884	ASP	CA-C-N	6.22	125.71	119.24
1	B	884	ASP	C-N-CA	6.22	125.71	119.24
1	B	426	GLU	N-CA-C	6.17	118.85	107.99
1	B	76	GLN	N-CA-C	6.14	119.88	112.38
1	A	377	ILE	N-CA-C	6.09	119.62	113.47
1	A	845	VAL	N-CA-C	5.98	117.44	110.62
1	B	696	ILE	N-CA-C	5.97	117.19	108.53
1	B	434	GLU	N-CA-C	-5.97	98.69	108.41
1	A	665	ILE	N-CA-C	-5.95	106.94	113.43
1	B	-2	HIS	N-CA-C	-5.93	99.33	109.24
1	B	640	LEU	N-CA-C	5.89	123.35	110.80
1	B	228	LEU	N-CA-C	5.86	117.67	111.28
1	A	379	GLN	N-CA-C	5.86	117.67	111.28
1	B	385	HIS	N-CA-C	5.72	120.40	112.45
1	A	385	HIS	N-CA-C	5.66	120.32	112.45
1	A	575	THR	N-CA-C	5.65	117.44	111.28
1	B	750	THR	N-CA-C	-5.64	102.80	110.36
1	B	800	HIS	N-CA-C	5.51	120.65	113.88
1	B	430	LEU	N-CA-C	-5.40	105.82	112.90
1	B	809	TYR	N-CA-C	5.37	117.98	109.50
1	B	433	CYS	N-CA-C	5.36	118.30	109.72
1	B	782	ALA	N-CA-C	-5.33	106.16	113.30
1	A	578	VAL	N-CA-C	-5.31	105.36	110.72
1	B	29	ALA	N-CA-C	-5.29	105.52	111.28
1	A	424	GLU	CA-C-N	5.26	131.59	121.54
1	A	424	GLU	C-N-CA	5.26	131.59	121.54
1	B	423	GLU	N-CA-C	5.25	121.99	110.80
1	A	816	LEU	N-CA-C	-5.23	100.38	108.90
1	B	951	SER	N-CA-C	5.20	116.79	108.41
1	B	606	CYS	N-CA-C	5.19	118.17	110.48
1	B	421	ASP	N-CA-C	5.19	117.43	109.07
1	A	278	ASP	CA-C-N	5.16	124.66	119.19
1	A	278	ASP	C-N-CA	5.16	124.66	119.19
1	A	647	PHE	N-CA-C	5.07	117.12	109.41
1	A	884	ASP	CA-C-N	5.07	124.51	119.24
1	A	884	ASP	C-N-CA	5.07	124.51	119.24
1	B	778	ASN	N-CA-C	-5.05	104.54	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	806	LYS	CB-CA-C	-5.04	110.78	116.63
1	A	607	GLU	N-CA-C	-5.04	107.52	113.97
1	A	562	ASP	N-CA-C	-5.01	107.71	113.88
1	A	839	ILE	CA-C-N	5.01	125.01	119.90
1	A	839	ILE	C-N-CA	5.01	125.01	119.90

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	350	0
1	B	7647	0	7676	288	0
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	110	0
4	B	554	0	0	76	0
All	All	16312	0	15327	624	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 (624) 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:A:445:LEU:HD22	4:A:2262:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MSE:CE	1:B:94:ILE:HG23	1.99	0.93
1:A:67:MSE:CE	1:A:94:ILE:HG23	1.99	0.93
1:A:246:MSE:HA	1:A:246:MSE:HE2	1.54	0.90
1:B:246:MSE:HE2	1:B:246:MSE:HA	1.51	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:A:129:LEU:HD13	1:A:155:MSE:HE1	1.57	0.85
1:B:372:ILE:HD11	1:B:410:ALA:HB1	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
1:B:396:GLU:HB2	2:B:1977:ADP:H5'1	1.61	0.82
1:A:779:ASP:HB3	1:A:782:ALA:HB3	1.59	0.82
1:B:532:THR:HG22	1:B:535:MSE:HG3	1.60	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:B:779:ASP:CG	1:B:782:ALA:HB3	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:728:GLU:CD	1:B:728:GLU:H	1.93	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:A:671:MSE:HE3	1:A:719:PRO:HB3	1.69	0.75
1:B:212:LEU:CD2	1:B:246:MSE:HE1	2.17	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:134:ASN:HB3	4:B:2100:HOH:O	1.87	0.73
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:A:31:GLU:OE2	1:A:676:PRO:HD2	1.91	0.70
1:B:490:ARG:HD3	4:B:2317:HOH:O	1.90	0.70
1:A:64:ALA:HB2	4:A:2040:HOH:O	1.91	0.70
1:B:699:ILE:HG22	1:B:700:GLY:N	2.07	0.70
1:A:306:ARG:HG2	4:A:2140:HOH:O	1.92	0.70
1:B:212:LEU:HD13	1:B:246:MSE:HE1	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:706:LYS:O	1:A:710:ILE:HG12	1.94	0.67
1:B:731:ARG:HB2	4:B:2517:HOH:O	1.93	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:A:324:GLU:CD	1:A:324:GLU:H	2.01	0.67
1:A:731:ARG:H	1:A:915:HIS:CD2	2.09	0.66
1:B:798:GLY:HA2	1:B:851:MSE:CE	2.22	0.66
1:A:624:PHE:CZ	1:A:639:GLU:HG3	2.30	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: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
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:A:671:MSE:HE2	1:A:672:GLU:C	2.21	0.65
1:A:618:ARG:HG2	4:A:2260:HOH:O	1.97	0.64
1:B:486:GLN:HB3	1:B:490:ARG:HH12	1.61	0.64
1:B:67:MSE:HE3	1:B:94:ILE:HG12	1.80	0.64
1:A:420:PHE:HE2	1:A:425:ASP:OD2	1.79	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:392:ILE:HG23	4:A:2016:HOH:O	1.97	0.64
1:A:658:VAL:HG23	4:A:2290:HOH:O	1.97	0.64
1:B:671:MSE:HE2	1:B:672:GLU:O	1.98	0.64
1:A:132:LEU:HD13	4:A:2074:HOH:O	1.96	0.64
1:A:669:THR:HA	1:A:687:ASN:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PRO:HB3	4:A:2375:HOH:O	1.96	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:A:970:MSE:HG2	1:A:971:THR:N	2.11	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:A:828:TRP:HB2	4:A:2352:HOH:O	1.97	0.63
1:B:535:MSE:HA	1:B:538:MSE:HG2	1.80	0.63
1:A:256:GLU:HG3	1:A:257:ARG:H	1.62	0.63
1:A:547:TRP:NE1	3:A:1974:SO4:O4	2.32	0.63
1:A:820:ASN:HB3	4:A:2347:HOH:O	1.97	0.63
1:A:317:ARG:HG2	1:A:322:VAL:HG21	1.80	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:317:ARG:HG2	1:B:322:VAL:HG21	1.81	0.62
1:B:776:ASN:HB3	1:B:779:ASP:HB2	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
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:A:603:ASP:HA	1:A:623:ASN:HB2	1.82	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:B:671:MSE:HE3	1:B:719:PRO:HB3	1.83	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:A:223:PRO:HG2	4:A:2111:HOH:O	1.99	0.61
1:B:532:THR:HG22	1:B:535:MSE:CG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:816:LEU:HD23	1:A:830:PRO:HA	1.84	0.60
1:B:728:GLU:OE1	1:B:728:GLU:N	2.28	0.60
1:A:617:LEU:HD12	4:A:2197:HOH:O	2.01	0.60
1:A:867:ARG:HH11	1:B:528:GLU:HG3	1.66	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:A:407:ARG:O	1:A:411:VAL:HG23	2.02	0.59
1:B:17:LEU:CA	1:B:28:ILE:HD13	2.33	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
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:A:21:THR:HG22	1:A:24:ASN:ND2	2.19	0.58
1:B:731:ARG:N	1:B:915:HIS:HD2	1.89	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:256:GLU:HG3	4:B:2163:HOH:O	2.04	0.58
1:B:618:ARG:NH2	3:B:1981:SO4:O2	2.37	0.58
1:A:667:LYS:HE2	1:A:725:TYR:CD2	2.39	0.58
1:B:234:PHE:HB3	1:B:275:LEU:HD12	1.85	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:A:296:ASN:C	1:A:298:ALA:H	2.13	0.57
1:B:57:ILE:HG12	4:B:2052:HOH:O	2.05	0.57
1:A:406:PHE:HE2	4:A:2176:HOH:O	1.88	0.57
1:A:617:LEU:N	4:A:2262:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:LEU:HB2	1:B:658:VAL:HG21	1.87	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:A:252:ARG:NH2	4:A:2124:HOH:O	2.35	0.57
1:B:647:PHE:HB2	1:B:881:LEU:HA	1.87	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:A:212:LEU:HD21	1:A:246:MSE:HE1	1.88	0.56
1:A:448:THR:HG23	4:A:2197:HOH:O	2.04	0.56
1:A:674:GLN:HB2	1:A:681:PRO:HB3	1.88	0.56
1:B:718:LEU:HD12	1:B:719:PRO:HD2	1.87	0.56
1:B:731:ARG:HH12	1:B:865:GLN:NE2	1.98	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: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:B:867:ARG:NE	4:B:2488:HOH:O	2.38	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
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:671:MSE:HE2	1:B:672:GLU:C	2.31	0.55
1:B:17:LEU:HA	1:B:28:ILE:HD13	1.89	0.55
1:B:535:MSE:HE1	1:B:547:TRP:CG	2.42	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:A:221:GLU:CG	1:B:187:ALA:HB1	2.37	0.55
1:A:851:MSE:HE2	4:A:2332:HOH:O	2.07	0.55
1:B:160:LYS:HE2	4:B:2132:HOH:O	2.06	0.55
1:B:81:PRO:HD3	4:B:2411:HOH:O	2.07	0.54
1:B:122:PRO:HA	4:B:2088:HOH:O	2.07	0.54
1:B:276:VAL:HB	1:B:319:VAL:CG1	2.35	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:A:231:ALA:HB2	1:B:778:ASN:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:HB3	1:A:275:LEU:HD12	1.90	0.54
1:B:535:MSE:O	1:B:538:MSE:HG2	2.06	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:A:221:GLU:HG2	1:B:187:ALA:HB1	1.88	0.54
1:B:416:VAL:HG23	1:B:417:GLY:N	2.22	0.54
1:B:775:ILE:HG13	4:B:2446:HOH:O	2.06	0.54
1:A:299:THR:O	1:A:299:THR:HG22	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: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:B:67:MSE:HG3	4:B:2052:HOH:O	2.08	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:387:THR:N	1:A:388:PRO:HD2	2.23	0.54
1:A:903:LYS:HE2	4:A:2271:HOH:O	2.07	0.54
1:A:486:GLN:HB3	1:A:490:ARG:HH11	1.73	0.53
1:A:671:MSE:HE2	1:A:672:GLU:O	2.07	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
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:A:263:ARG:O	1:A:267:VAL:HG23	2.09	0.53
1:B:234:PHE:HA	4:B:2151:HOH:O	2.07	0.53
1:A:616:LYS:HB2	4:A:2260:HOH:O	2.07	0.53
1:B:420:PHE:HZ	4:B:2263:HOH:O	1.81	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:A:257:ARG:HG3	1:A:258:GLU:HG3	1.89	0.53
1:A:816:LEU:HD13	4:A:2352:HOH:O	2.08	0.53
1:B:246:MSE:HE2	1:B:246:MSE:CA	2.33	0.53
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:642:ASN:ND2	1:B:645:LEU:HD12	2.24	0.52
1:B:871:ARG:HD2	4:B:2494:HOH:O	2.09	0.52
1:A:40:ILE:HG13	1:A:41:ILE:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HG3	4:A:2063:HOH:O	2.09	0.52
1:A:346:GLU:OE1	1:A:349:LYS:HD3	2.09	0.52
1:A:641:SER:HA	1:A:887:ILE:CD1	2.40	0.52
1:A:72:HIS:CE1	1:A:773:ARG:HD3	2.44	0.52
1:A:635:LYS:HA	1:A:642:ASN:OD1	2.09	0.52
1:B:45:VAL:HG11	1:B:86:TYR:CE2	2.45	0.52
1:B:817:LEU:HD13	4:B:2453:HOH:O	2.09	0.52
1:B:867:ARG:CZ	4:B:2488:HOH:O	2.57	0.52
1:B:206:GLU:HG2	4:B:2135:HOH:O	2.09	0.52
1:B:950:HIS:ND1	2:B:1977:ADP:O1B	2.43	0.52
1:B:789:ILE:HD12	1:B:815:PHE:CZ	2.45	0.52
1:A:324:GLU:CD	1:A:324:GLU:N	2.68	0.51
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:A:897:SER:C	4:A:2389:HOH:O	2.53	0.51
1:B:258:GLU:HG2	1:B:260:GLY:H	1.75	0.51
1:A:318:ARG:NH2	1:A:424:GLU:OE1	2.43	0.51
1:A:788:LYS:HD2	1:A:788:LYS:N	2.26	0.51
1:A:210:PRO:O	1:A:214:GLN:HG2	2.10	0.51
1:A:431:CYS:N	4:A:2191:HOH:O	2.44	0.51
1:B:246:MSE:HA	1:B:246:MSE:CE	2.33	0.51
1:B:543:LEU:HD12	4:B:2310:HOH:O	2.09	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:78:ASN:HD21	1:A:736:LYS:NZ	2.09	0.51
1:A:78:ASN:ND2	1:A:736:LYS:HZ3	2.08	0.51
1:A:212:LEU:HD13	1:A:245:ILE:HG22	1.92	0.51
1:A:302:ASP:OD2	1:A:304:GLU:HB3	2.10	0.51
1:B:877:HIS:HD2	4:B:2486:HOH:O	1.94	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:17:LEU:CA	1:A:28:ILE:HD13	2.41	0.51
1:A:246:MSE:HA	1:A:246:MSE:CE	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:LYS:HB3	1:B:306:ARG:HH12	1.75	0.51
1:B:445:LEU:HD22	4:B:2349:HOH:O	2.11	0.51
1:A:78:ASN:ND2	1:A:736:LYS:NZ	2.58	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:532:THR:CG2	1:B:535:MSE:H	2.24	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:256:GLU:O	1:B:262:LYS:HE3	2.11	0.50
1:B:396:GLU:HB2	2:B:1977:ADP:H5'2	1.91	0.50
1:B:568:GLU:OE1	1:B:597:HIS:ND1	2.41	0.50
1:A:385:HIS:HA	4:A:2183:HOH:O	2.11	0.50
1:A:386:ILE:HD13	4:A:2176:HOH:O	2.11	0.50
1:B:266:ALA:HB3	1:B:308:VAL:HG12	1.93	0.50
1:A:667:LYS:CG	1:A:725:TYR:HB3	2.42	0.50
1:B:779:ASP:OD2	1:B:782:ALA:HB3	2.11	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:B:634:ALA:HA	1:B:637:TYR:CD1	2.46	0.50
1:A:166:ARG:NH2	1:A:373:ASP:OD2	2.45	0.50
1:A:645:LEU:H	1:A:903:LYS:HZ3	1.58	0.50
1:A:167:MSE:HE1	1:A:171:ILE:HD11	1.93	0.50
1:B:420:PHE:HB3	1:B:619:LYS:O	2.11	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:775:ILE:HB	4:B:2445:HOH:O	2.12	0.49
1:B:914:PRO:HA	4:B:2517:HOH:O	2.13	0.49
1:A:640:LEU:HD11	1:A:884:ASP:OD2	2.13	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:798:GLY:HA2	1:A:851:MSE:HE1	1.94	0.49
1:B:58:LYS:HG2	1:B:58:LYS:O	2.12	0.49
1:B:699:ILE:CG2	1:B:700:GLY:N	2.76	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:123:VAL:HG13	1:A:370:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HG13	4:A:2128:HOH:O	2.13	0.48
1:A:306:ARG:N	4:A:2153:HOH:O	2.46	0.48
1:A:494:VAL:HG12	1:A:495:GLU:HG3	1.94	0.48
1:A:624:PHE:CE1	1:A:639:GLU:HG3	2.48	0.48
1:B:445:LEU:HD21	1:B:612:TYR:CE2	2.48	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:303:PRO:HG2	4:B:2189:HOH:O	2.13	0.48
1:B:372:ILE:HD11	1:B:410:ALA:CB	2.39	0.48
1:A:296:ASN:C	1:A:298:ALA:N	2.71	0.48
1:A:250:LEU:HD13	1:A:269:ILE:HG12	1.96	0.48
1:A:655:LEU:HB3	4:A:2290:HOH:O	2.13	0.48
1:B:775:ILE:HD11	4:B:2081:HOH:O	2.14	0.48
1:A:667:LYS:HE2	1:A:725:TYR:CG	2.49	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:877:HIS:HE1	1:A:907:ALA:O	1.96	0.47
1:B:204:ASP:HB3	4:B:2151:HOH:O	2.14	0.47
1:B:223:PRO:HB3	1:B:261:ILE:CD1	2.45	0.47
1:A:535:MSE:HE1	1:A:547:TRP:CG	2.50	0.47
1:A:736:LYS:NZ	1:A:770:ARG:HD2	2.28	0.47
1:B:78:ASN:HA	4:B:2064:HOH:O	2.14	0.47
1:B:240:PRO:HD2	4:B:2156:HOH:O	2.14	0.47
1:A:646:GLU:C	4:A:2271:HOH:O	2.58	0.47
1:B:773:ARG:HG2	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:432:ASN:HB2	4:B:2264:HOH:O	2.14	0.47
1:B:540:ILE:HB	4:B:2310:HOH:O	2.15	0.47
1:B:773:ARG:HA	4:B:2055:HOH:O	2.15	0.47
1:B:827:ARG:HG3	1:B:827:ARG:NH1	2.28	0.47
1:A:647:PHE:HB3	4:A:2271:HOH:O	2.15	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:816:LEU:HD23	1:B:830:PRO:HA	1.96	0.47
1:A:262:LYS:HB3	4:A:2141: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:765:ARG:NH2	4:B:2433:HOH:O	2.45	0.47
1:B:819:GLU:O	1:B:826:GLU:HA	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:CG	1:A:61:LYS:HG2	2.40	0.47
1:A:538:MSE:HB2	1:A:539:PRO:HD2	1.96	0.47
1:A:105:ILE:HG12	4:A:2040:HOH:O	2.14	0.47
1:A:160:LYS:HG3	1:A:199:THR:HG22	1.97	0.47
1:B:701:PRO:HG3	4:B:2007:HOH:O	2.14	0.47
1:A:921:GLU:CD	1:A:949:THR:HA	2.41	0.46
1:B:428:GLU:OE2	1:B:454:ARG:NE	2.46	0.46
1:B:16:LYS:HB3	1:B:28:ILE:HD12	1.96	0.46
1:B:820:ASN:HB2	1:B:826:GLU:HA	1.97	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:647:PHE:C	1:B:648:LYS:HD3	2.41	0.46
1:B:371:LEU:HD23	4:B:2240:HOH:O	2.16	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:B:67:MSE:HE1	1:B:109:ALA:CA	2.43	0.46
1:A:256:GLU:HG2	1:A:261:ILE:HD13	1.97	0.46
1:A:502:HIS:C	1:A:504:ASP:H	2.23	0.46
1:A:803:ARG:N	4:A:2338:HOH:O	2.49	0.46
1:A:473:ARG:NH2	4:A:2206:HOH:O	2.49	0.46
1:A:566:LEU:HD22	4:A:2253:HOH:O	2.14	0.46
1:A:654:TYR:CE2	1:B:521:ALA:HB2	2.51	0.46
1:A:916:LEU:CD2	1:A:944:GLY:HA3	2.46	0.46
1:A:77:SER:H	1:A:774:GLN:HE22	1.64	0.46
1:A:152:PHE:N	4:A:2074:HOH:O	2.49	0.46
1:A:253:GLY:O	1:A:256:GLU:HB2	2.16	0.46
1:A:970:MSE:HG2	1:A:971:THR:H	1.80	0.46
1:B:435:PHE:CD1	1:B:480:VAL:HG13	2.50	0.46
1:B:654:TYR:HE2	1:B:656:GLU:HG2	1.78	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:A:301:ALA:O	1:A:302:ASP:C	2.59	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:586:ASN:ND2	3:A:1976:SO4:O3	2.45	0.45
1:A:731:ARG:HH12	1:A:865:GLN:NE2	2.07	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:502:HIS:C	1:B:504:ASP:H	2.24	0.45
1:B:737:GLN:HG2	4:B:2105:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:HD21	1:A:736:LYS:HZ1	1.62	0.45
1:A:304:GLU:OE2	1:A:304:GLU:HA	2.16	0.45
1:B:0:HIS:HB3	4:B:2392:HOH:O	2.16	0.45
1:B:125:ILE:HG23	1:B:126:LYS:N	2.32	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:A:304:GLU:O	1:A:308:VAL:HG23	2.16	0.45
1:B:178:MSE:HE3	1:B:190:THR:OG1	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:609:ILE:HG13	1:B:627:PHE:HB2	1.98	0.45
1:A:342:GLN:HE21	1:A:342:GLN:HB3	1.66	0.45
1:A:716:GLU:HG3	1:A:771:ALA:HB2	1.97	0.45
1:B:76:GLN:HG3	1:B:775:ILE:HD11	1.99	0.45
1:B:652:PRO:HB3	1:B:914:PRO:O	2.17	0.45
1:B:814:SER:HA	1:B:836:ASN:OD1	2.17	0.45
1:B:824:LYS:HB3	1:B:824:LYS:HE2	1.65	0.45
1:B:820:ASN:O	1:B:826:GLU:HB2	2.16	0.45
1:B:831:MSE:C	1:B:832:MSE:HE2	2.42	0.45
1:A:69:ALA:O	1:A:73:ILE:HG13	2.16	0.45
1:A:212:LEU:CD1	1:A:246:MSE:HE3	2.46	0.45
1:A:773:ARG:NH1	1:A:846:GLU:OE1	2.46	0.45
1:A:948:ILE:HG21	4:A:2012:HOH:O	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:17:LEU:N	1:B:28:ILE:CD1	2.81	0.44
1:B:773:ARG:NH1	4:B:2445:HOH:O	2.49	0.44
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:A:949:THR:OG1	1:A:950:HIS:N	2.50	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: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:232:THR:C	4:A:2114:HOH:O	2.60	0.44
1:A:277:GLU:HG3	4:A:2135:HOH:O	2.17	0.44
1:A:737:GLN:HB3	1:A:925:TYR:CD2	2.52	0.44
1:B:494:VAL:HG12	1:B:495:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HB3	1:A:28:ILE:HD12	2.00	0.44
1:A:321:ASN:O	1:A:321:ASN:ND2	2.51	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:B:637:TYR:HB2	4:B:2360:HOH:O	2.17	0.44
1:A:749:LYS:HB3	1:A:753:GLU:HB2	1.99	0.44
1:A:765:ARG:HD3	4:A:2317:HOH:O	2.18	0.44
1:B:775:ILE:O	1:B:775:ILE:CG2	2.65	0.44
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.81	0.43
1:B:699:ILE:CG2	1:B:700:GLY:H	2.28	0.43
1:B:773:ARG:O	1:B:775:ILE:N	2.51	0.43
1:B:921:GLU:OE2	1:B:950:HIS:CD2	2.71	0.43
1:A:502:HIS:C	1:A:504:ASP:N	2.76	0.43
1:A:781:GLU:CD	4:A:2327:HOH:O	2.60	0.43
1:A:532:THR:HG22	1:A:535:MSE:HG3	2.01	0.43
1:B:306:ARG:CZ	4:B:2191:HOH:O	2.67	0.43
1:B:950:HIS:CB	2:B:1977:ADP:O1B	2.66	0.43
1:B:729:ASN:N	3:B:1979:SO4:O3	2.34	0.43
1:A:209:ILE:O	1:A:213:ILE:HG13	2.19	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:751:PRO:HB3	1:A:904:LEU:HD13	2.00	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:B:212:LEU:HD13	1:B:246:MSE:HE3	2.01	0.43
1:A:212:LEU:CD1	1:A:246:MSE:CE	2.97	0.43
1:A:248:PRO:HG2	4:A:2120:HOH:O	2.18	0.43
1:B:238:VAL:HG21	1:B:272:MSE:O	2.19	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:337:VAL:HG23	4:A:2163:HOH:O	2.19	0.42
1:A:182:LYS:HB3	1:A:185:VAL:HG23	2.01	0.42
1:A:447:LYS:C	4:A:2196:HOH:O	2.61	0.42
1:A:587:THR:OG1	1:B:870:THR:HG22	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: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:282:ILE:O	1:A:282:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD21	1:A:317:ARG:NH2	2.33	0.42
1:A:200:VAL:CG2	1:A:245:ILE:CD1	2.96	0.42
1:A:256:GLU:C	4:A:2126:HOH:O	2.62	0.42
1:B:41:ILE:HD12	1:B:46:PRO:HD3	2.00	0.42
1:A:81:PRO:HG2	4:A:2031:HOH:O	2.18	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:728:GLU:CD	1:A:728:GLU:H	2.27	0.42
1:A:776:ASN:HB3	1:A:779:ASP:CG	2.44	0.42
1:B:783:MSE:C	1:B:785:LYS:H	2.28	0.42
1:A:526:LEU:O	1:A:531:PHE:HB2	2.20	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:B:487:GLU:H	1:B:487:GLU:CD	2.28	0.42
1:A:239:THR:HB	1:A:240:PRO:CD	2.50	0.42
1:A:351:GLU:HG2	1:A:394:LEU:HD21	2.02	0.42
1:A:505:THR:O	1:A:539:PRO:HA	2.20	0.42
1:B:21:THR:HG23	1:B:23:ASP:HB2	2.01	0.42
1:B:76:GLN:CD	1:B:775:ILE:HG12	2.44	0.42
1:A:435:PHE:CD1	1:A:480:VAL:HG13	2.55	0.42
1:B:462:GLY:N	1:B:637:TYR:HE2	2.17	0.42
1:A:167:MSE:N	1:A:168:PRO:HD2	2.35	0.42
1:A:315:THR:O	1:A:319:VAL:HG23	2.20	0.42
1:B:123:VAL:HG12	1:B:367:ILE:HG23	2.02	0.42
1:B:597:HIS:H	1:B:597:HIS:HD1	1.68	0.42
1:A:39:ASN:ND2	4:A:2012:HOH:O	2.51	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:234:PHE:HB2	4:A:2131:HOH:O	2.20	0.41
1:A:658:VAL:HA	4:A:2276:HOH:O	2.19	0.41
1:A:804:LYS:HG2	3:A:1977:SO4:O3	2.20	0.41
1:A:68:GLN:O	1:A:72:HIS:HD2	2.03	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:671:MSE:HE3	1:A:719:PRO:CB	2.45	0.41
1:A:877:HIS:HD2	4:A:2374:HOH:O	2.02	0.41
1:B:668:VAL:CG1	1:B:671:MSE:HB2	2.50	0.41
1:A:215:CYS:C	4:A:2123:HOH:O	2.63	0.41
1:B:291:PRO:HG2	4:B:2185:HOH:O	2.20	0.41
1:A:142:TRP:HD1	4:A:2065:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:850:LYS:O	1:B:854:GLU:HG3	2.21	0.41
1:B:957:ASN:HD22	1:B:957:ASN:HA	1.68	0.41
1:A:390:MSE:C	1:A:392:ILE:H	2.28	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:A:781:GLU:C	1:A:783:MSE:H	2.27	0.41
1:B:300:ILE:HG21	1:B:305:ALA:HB3	2.03	0.41
1:B:425:ASP:CG	1:B:608:TYR:HH	2.29	0.41
1:B:131:HIS:HA	3:B:1983:SO4:O1	2.21	0.41
1:B:950:HIS:HB2	4:B:2533:HOH:O	2.21	0.41
1:A:239:THR:HB	1:A:240:PRO:HD2	2.03	0.41
1:B:867:ARG:NH2	4:B:2488:HOH:O	2.54	0.41
1:A:17:LEU:HA	1:A:28:ILE:HD13	2.02	0.40
1:A:67:MSE:HE2	1:A:109:ALA:HA	2.00	0.40
1:A:252:ARG:CZ	4:A:2109:HOH:O	2.68	0.40
1:A:430:LEU:O	1:A:484:PRO:HG2	2.21	0.40
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:B:451:ARG:HD3	1:B:453:LYS:HZ2	1.86	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:462:GLY:C	1:B:637:TYR:CE2	3.00	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:B:779:ASP:O	1:B:783:MSE:HG2	2.21	0.40
1:A:102:ASP:OD2	1:A:105:ILE:HG13	2.20	0.40
1:A:207:ARG:NH1	4:A:2104:HOH:O	2.55	0.40
1:A:264:LYS:HD2	1:A:264:LYS:HA	1.98	0.40
1:A:303:PRO:HG3	1:B:826:GLU:CD	2.47	0.40
1:A:884:ASP:HA	1:A:885:PRO:HD3	1.92	0.40
1:B:207:ARG:HA	4:B:2135:HOH:O	2.20	0.40
1:B:555:ARG:HH21	1:B:559:ARG:NH2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:824:LYS:HA	4:B:2470:HOH:O	2.22	0.40
1:B:958:LEU:HD23	1:B:958:LEU:HA	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%)	43	58
1	B	979/986 (99%)	945 (96%)	31 (3%)	3 (0%)	36	50
All	All	1950/1972 (99%)	1872 (96%)	73 (4%)	5 (0%)	36	50

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 [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	831/821 (101%)	809 (97%)	22 (3%)	40	63
1	B	838/821 (102%)	817 (98%)	21 (2%)	42	64
All	All	1669/1642 (102%)	1626 (97%)	43 (3%)	40	63

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	101	LYS
1	A	166	ARG
1	A	169	GLU
1	A	182	LYS
1	A	224	GLU
1	A	277	GLU
1	A	288	LYS
1	A	316	LEU
1	A	324	GLU
1	A	342	GLN
1	A	573	LEU
1	A	659	LYS
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
1	B	169	GLU
1	B	215	CYS
1	B	316	LEU
1	B	322	VAL
1	B	351	GLU
1	B	352	THR
1	B	516	VAL
1	B	534	GLU
1	B	573	LEU
1	B	737	GLN
1	B	748	ASP

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Mol	Chain	Res	Type
1	B	783	MSE
1	B	859	GLU
1	B	872	LYS
1	B	876	GLU
1	B	881	LEU
1	B	928	ARG
1	B	956	LYS
1	B	958	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	76	GLN
1	A	78	ASN
1	A	271	ASN
1	A	321	ASN
1	A	342	GLN
1	A	413	ASN
1	A	432	ASN
1	A	446	ASN
1	A	496	HIS
1	A	597	HIS
1	A	604	ASN
1	A	611	ASN
1	A	662	GLN
1	A	711	ASN
1	A	729	ASN
1	A	774	GLN
1	A	848	HIS
1	A	865	GLN
1	A	877	HIS
1	A	890	HIS
1	A	915	HIS
1	A	924	ASN
1	B	5	GLN
1	B	15	GLN
1	B	97	ASN
1	B	227	HIS
1	B	271	ASN
1	B	321	ASN
1	B	342	GLN

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Mol	Chain	Res	Type
1	B	413	ASN
1	B	419	ASN
1	B	560	ASN
1	B	604	ASN
1	B	611	ASN
1	B	642	ASN
1	B	711	ASN
1	B	729	ASN
1	B	737	GLN
1	B	756	GLN
1	B	784	ASN
1	B	848	HIS
1	B	865	GLN
1	B	877	HIS
1	B	890	HIS
1	B	915	HIS
1	B	924	ASN
1	B	957	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	SO4	B	1979	-	4,4,4	0.70	0	6,6,6	0.54	0
3	SO4	B	1981	-	4,4,4	0.69	0	6,6,6	0.08	0
3	SO4	A	1974	-	4,4,4	0.70	0	6,6,6	0.54	0
2	ADP	A	1973	-	28,29,29	1.31	3 (10%)	43,45,45	1.81	11 (25%)
3	SO4	B	1978	-	4,4,4	0.69	0	6,6,6	0.07	0
3	SO4	B	1984	-	4,4,4	0.70	0	6,6,6	0.55	0
3	SO4	B	1980	-	4,4,4	0.69	0	6,6,6	0.09	0
3	SO4	B	1983	-	4,4,4	0.69	0	6,6,6	0.07	0
3	SO4	B	1985	-	4,4,4	0.69	0	6,6,6	0.09	0
3	SO4	B	1982	-	4,4,4	0.68	0	6,6,6	0.08	0
3	SO4	A	1975	-	4,4,4	0.71	0	6,6,6	0.53	0
3	SO4	A	1978	-	4,4,4	0.69	0	6,6,6	0.53	0
3	SO4	A	1977	-	4,4,4	0.70	0	6,6,6	0.08	0
3	SO4	A	1976	-	4,4,4	0.70	0	6,6,6	0.54	0
2	ADP	B	1977	-	28,29,29	1.32	4 (14%)	43,45,45	1.82	10 (23%)

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	-	-	5/16/32/32	0/3/3/3
2	ADP	B	1977	-	-	2/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1973	ADP	PB-O1B	3.53	1.61	1.50
2	B	1977	ADP	PB-O1B	3.49	1.61	1.50
2	B	1977	ADP	C5-N7	-3.25	1.33	1.39
2	A	1973	ADP	C5-N7	-3.09	1.33	1.39
2	A	1973	ADP	C8-N9	-2.42	1.33	1.37
2	B	1977	ADP	C8-N9	-2.33	1.33	1.37
2	B	1977	ADP	C4-N9	-2.04	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1973	ADP	C5-C4-N3	-5.23	119.52	126.72
2	B	1977	ADP	C5-C4-N3	-5.01	119.82	126.72
2	B	1977	ADP	N3-C2-N1	-4.73	121.42	128.58
2	A	1973	ADP	N3-C2-N1	-4.70	121.47	128.58
2	A	1973	ADP	N3-C4-N9	3.68	133.43	127.17
2	B	1977	ADP	N3-C4-N9	3.62	133.32	127.17
2	A	1973	ADP	C2-N3-C4	3.56	120.53	111.83
2	B	1977	ADP	C2-N3-C4	3.52	120.43	111.83
2	B	1977	ADP	C4'-O4'-C1'	-3.29	102.21	109.47
2	B	1977	ADP	N9-C8-N7	-2.95	109.75	113.94
2	A	1973	ADP	N9-C8-N7	-2.87	109.87	113.94
2	A	1973	ADP	C4'-O4'-C1'	-2.73	103.45	109.47
2	A	1973	ADP	C4-C5-N7	-2.71	107.49	110.58
2	A	1973	ADP	C5-N7-C8	2.70	107.70	103.45
2	B	1977	ADP	C5-N7-C8	2.69	107.68	103.45
2	A	1973	ADP	O3B-PB-O3A	2.57	113.26	104.64
2	B	1977	ADP	C4-C5-N7	-2.55	107.67	110.58
2	B	1977	ADP	O3B-PB-O3A	2.54	113.16	104.64
2	B	1977	ADP	C4-N9-C8	2.19	108.04	105.74
2	A	1973	ADP	C4-N9-C8	2.08	107.92	105.74
2	A	1973	ADP	O4'-C1'-C2'	-2.01	102.31	106.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1973	ADP	C5'-O5'-PA-O2A
2	A	1973	ADP	C5'-O5'-PA-O3A
2	B	1977	ADP	C5'-O5'-PA-O2A
2	B	1977	ADP	C5'-O5'-PA-O3A
2	A	1973	ADP	PB-O3A-PA-O1A
2	A	1973	ADP	C5'-O5'-PA-O1A
2	A	1973	ADP	PB-O3A-PA-O2A

There are no ring outliers.

9 monomers are involved in 18 short contacts:

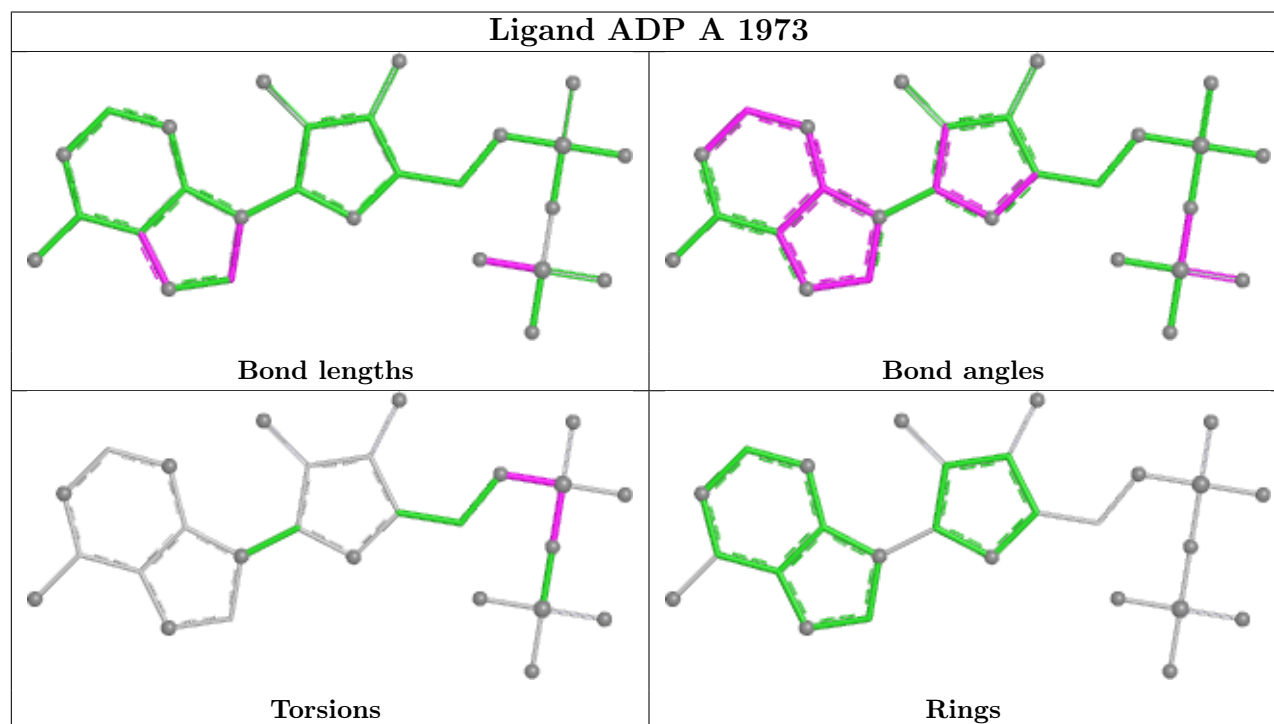
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1979	SO4	2	0
3	B	1981	SO4	1	0
3	A	1974	SO4	2	0
3	B	1983	SO4	1	0

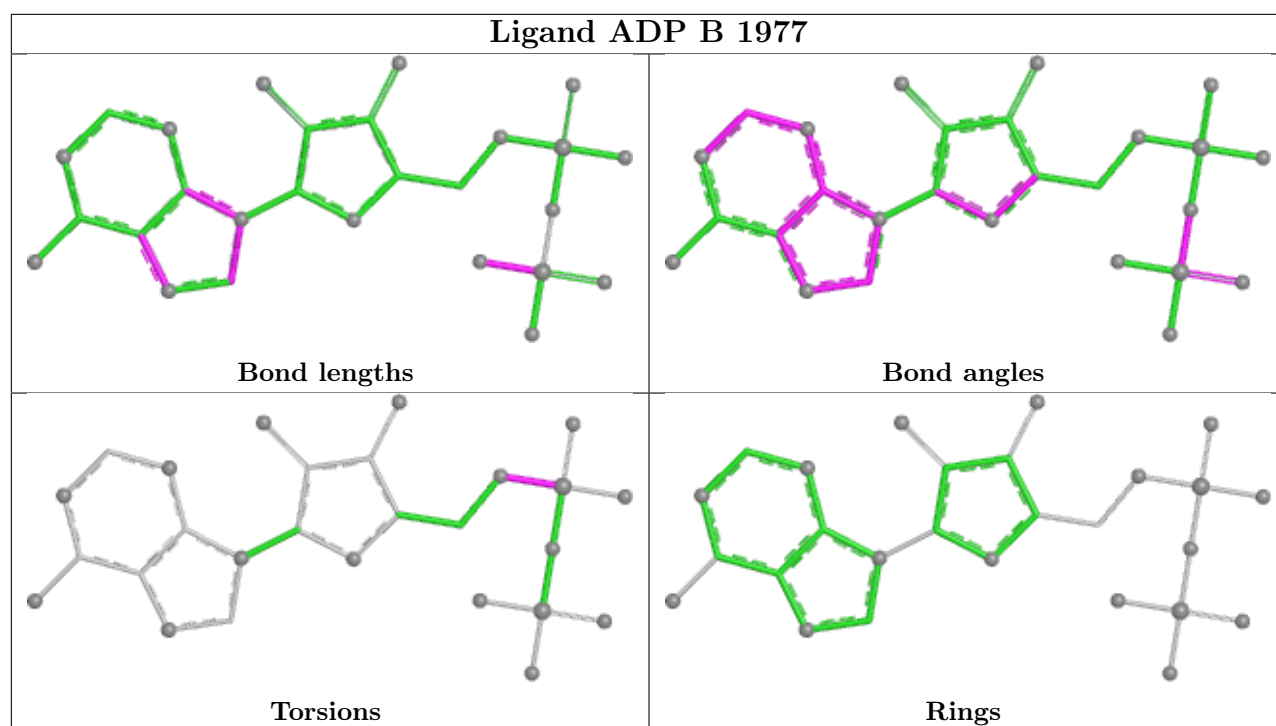
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1985	SO4	1	0
3	A	1975	SO4	1	0
3	A	1977	SO4	2	0
3	A	1976	SO4	2	0
2	B	1977	ADP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	0.07	48 (5%) 34 30	22, 44, 82, 108	0
1	B	959/986 (97%)	-0.31	26 (2%) 56 52	17, 33, 63, 106	0
All	All	1910/1972 (96%)	-0.12	74 (3%) 43 39	17, 39, 75, 108	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	PHE	5.3
1	A	641	SER	5.0
1	B	774	GLN	4.9
1	A	775	ILE	4.8
1	A	300	ILE	4.3
1	B	775	ILE	4.2
1	A	422	ASP	4.0
1	B	779	ASP	4.0
1	B	780	ALA	3.9
1	B	640	LEU	3.9
1	B	231	ALA	3.9
1	A	305	ALA	3.8
1	A	780	ALA	3.8
1	A	637	TYR	3.8
1	B	425	ASP	3.8
1	A	778	ASN	3.7
1	A	774	GLN	3.6
1	A	301	ALA	3.5
1	B	230	GLY	3.4
1	A	643	THR	3.3
1	A	297	PHE	3.3
1	A	306	ARG	3.3
1	A	779	ASP	3.2
1	A	424	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	645	LEU	3.2
1	A	304	GLU	3.1
1	A	640	LEU	3.0
1	A	423	GLU	3.0
1	A	299	THR	3.0
1	A	263	ARG	2.9
1	A	973	SER	2.9
1	B	977	TRP	2.9
1	A	971	THR	2.9
1	B	227	HIS	2.8
1	B	776	ASN	2.7
1	A	644	ASP	2.7
1	B	422	ASP	2.7
1	B	637	TYR	2.7
1	B	232	THR	2.7
1	A	303	PRO	2.7
1	A	957	ASN	2.7
1	B	504	ASP	2.6
1	A	427	GLY	2.6
1	A	307	GLU	2.6
1	A	420	PHE	2.6
1	A	952	ALA	2.6
1	A	309	THR	2.6
1	A	428	GLU	2.6
1	B	782	ALA	2.6
1	B	426	GLU	2.5
1	B	233	THR	2.5
1	B	639	GLU	2.5
1	B	636	ALA	2.5
1	B	421	ASP	2.4
1	A	421	ASP	2.4
1	A	642	ASN	2.4
1	A	352	THR	2.4
1	A	426	GLU	2.4
1	A	231	ALA	2.3
1	B	428	GLU	2.3
1	A	639	GLU	2.3
1	A	504	ASP	2.2
1	A	298	ALA	2.2
1	B	424	GLU	2.2
1	A	308	VAL	2.1
1	A	232	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	642	ASN	2.1
1	B	427	GLY	2.1
1	A	322	VAL	2.1
1	A	776	ASN	2.1
1	A	781	GLU	2.1
1	A	302	ASP	2.1
1	A	293	LEU	2.0
1	A	425	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

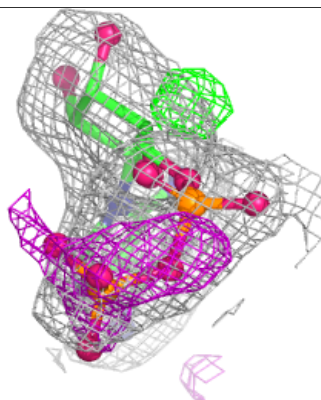
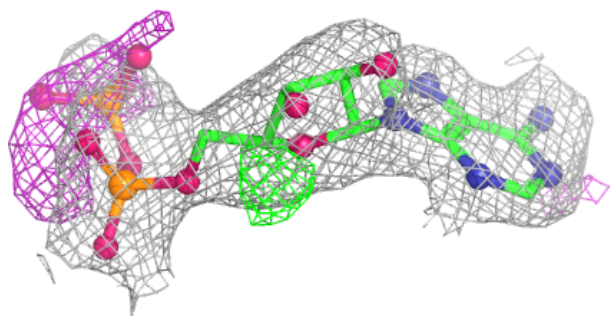
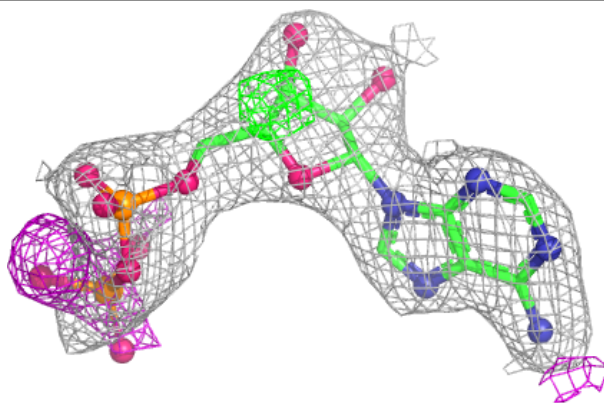
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

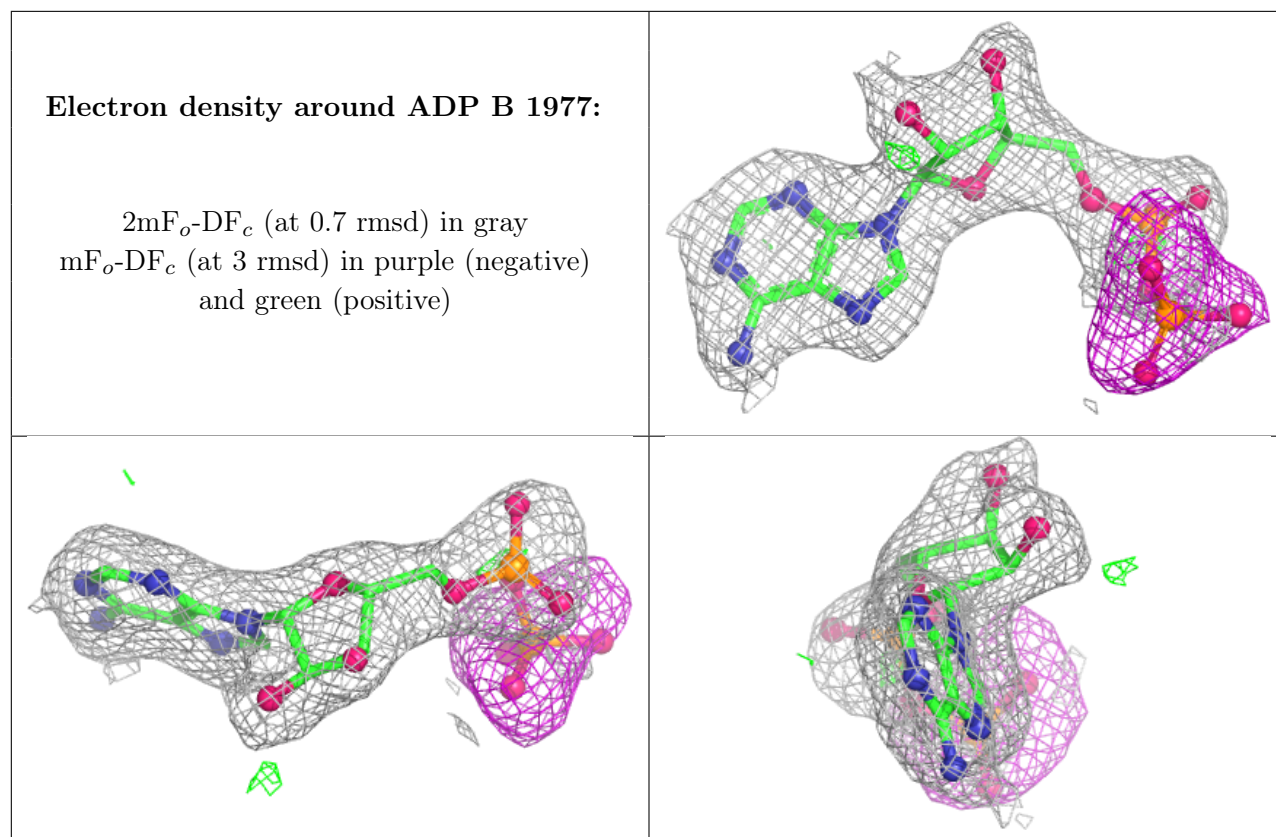
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	1981	5/5	0.69	0.17	85,85,86,86	0
3	SO4	B	1985	5/5	0.75	0.24	73,73,74,74	0
3	SO4	A	1975	5/5	0.80	0.12	83,84,84,85	0
3	SO4	A	1974	5/5	0.82	0.15	80,81,81,81	0
2	ADP	A	1973	27/27	0.82	0.12	33,53,80,81	0
3	SO4	A	1977	5/5	0.84	0.19	83,83,84,85	0
2	ADP	B	1977	27/27	0.87	0.14	24,37,70,72	0
3	SO4	B	1980	5/5	0.87	0.12	73,73,74,74	0
3	SO4	B	1979	5/5	0.88	0.17	59,61,62,63	0
3	SO4	A	1976	5/5	0.93	0.14	54,55,58,59	0
3	SO4	B	1983	5/5	0.94	0.14	63,65,65,66	0
3	SO4	B	1978	5/5	0.94	0.10	55,56,57,59	0
3	SO4	B	1982	5/5	0.95	0.10	63,63,63,65	0
3	SO4	A	1978	5/5	0.96	0.07	48,50,50,51	0
3	SO4	B	1984	5/5	0.99	0.04	37,38,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1973:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.