



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:11 PM UTC

PDB ID : 2IO7 / pdb_00002io7
Title : E. coli Bifunctional glutathionylspermidine synthetase/amidase Incomplex with Mg²⁺ and AMPPNP
Authors : Pai, C.H.; Chiang, B.Y.; Ko, T.P.; Chong, C.M.; Yen, F.J.; Coward, J.K.; Wang, A.H.-J.; Lin, C.H.
Deposited on : 2006-10-10
Resolution : 2.70 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

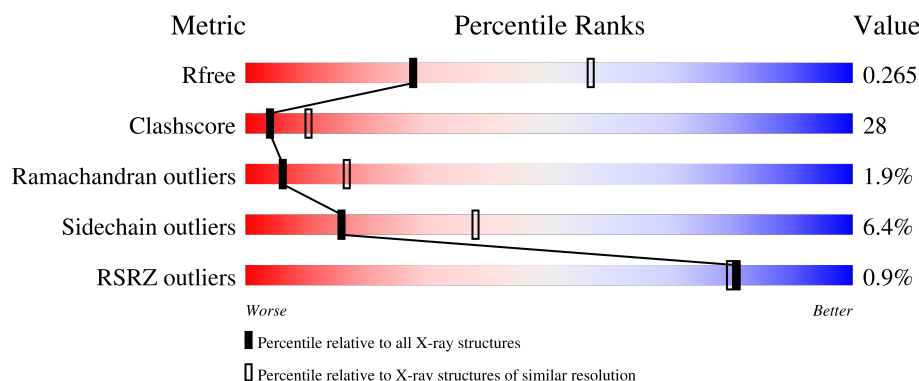
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

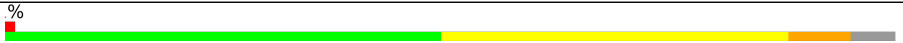
The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	619	
1	B	619	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9983 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.

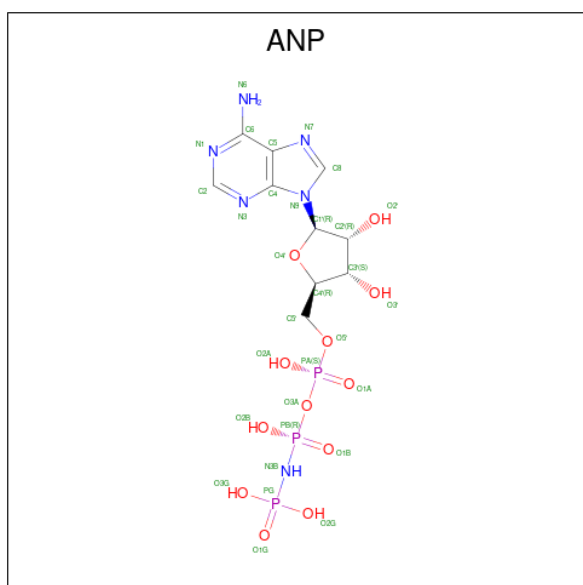
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4729	3028	810	872	19			
1	B	587	Total	C	N	O	S	0	0	0
			4726	3028	811	868	19			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

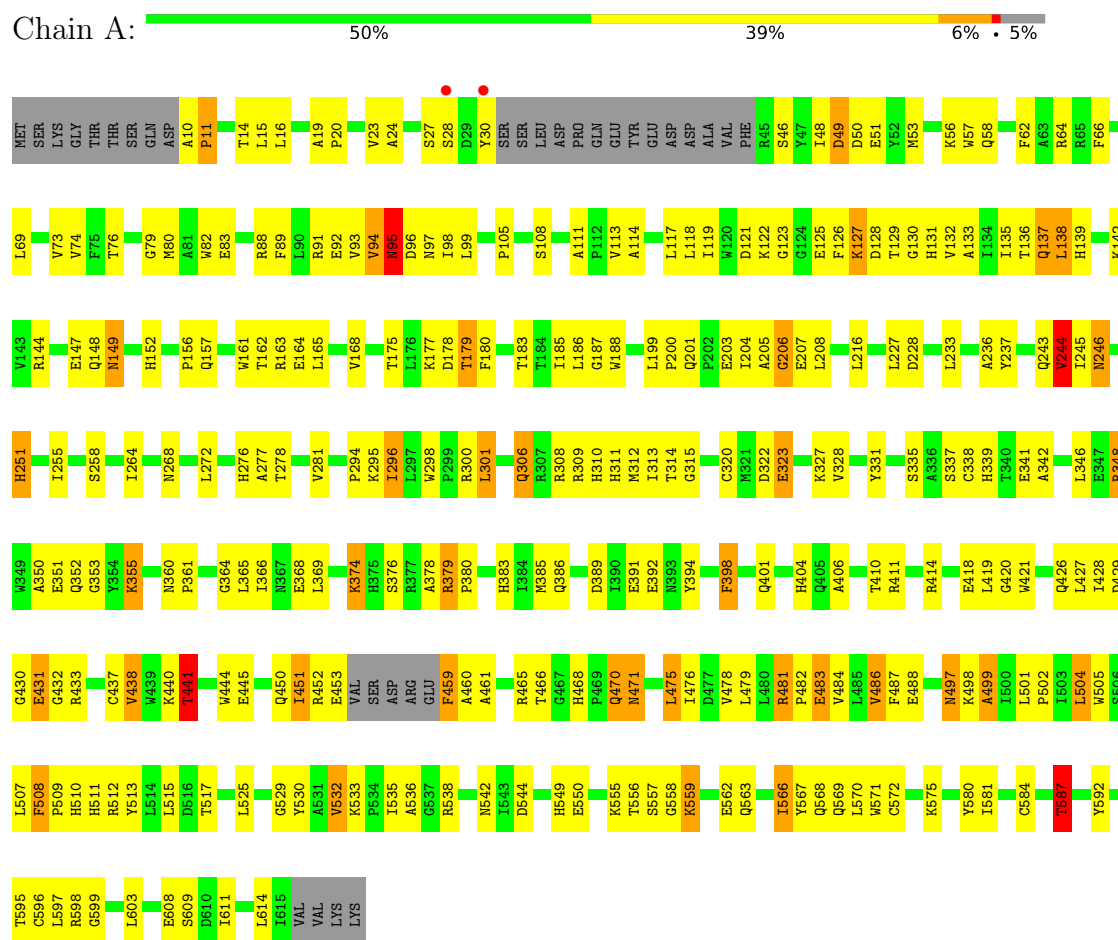
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	258	Total	O	0	0
			258	258		
4	B	204	Total	O	0	0
			204	204		

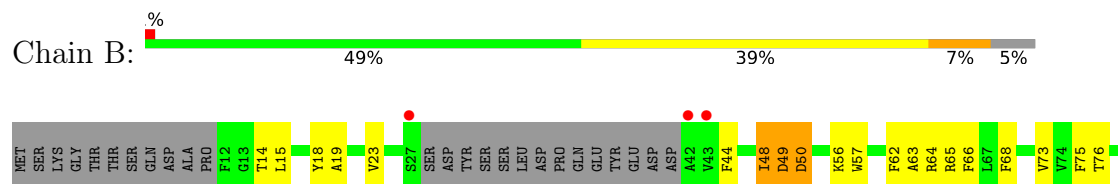
3 Residue-property plots

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: Bifunctional glutathionylspermidine synthetase/amidase



- Molecule 1: Bifunctional glutathionylspermidine synthetase/amidase



G578	G584	T585	F586	T587	N591	Y592	G593	G594	T595	C596	L597	R598	E601	S602	L603	V604	I605	K606	K607	E608	I611	E612	P613	L614	K618	LYS	P509	L427	L428	D429	G430	E431	G432	R433	C437	Y438	W439	K440	T441	W444	A447	F448	I451	R452	E453	VAL	ASP	ARG	GLU	PHE	A461	V462	H468	P469	Q470	N471	L475	I476	L479	L480	R481	P482	E483	V484	E488	T492	V493	N497	K498	A499	I500	L501	W571	C572	L573																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.01Å 75.54Å 84.06Å 70.67° 74.36° 78.22°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 90.4 (30.00-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.72Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.198 , 0.260 0.205 , 0.265	Depositor DCC
R_{free} test set	1720 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9983	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% 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: MG, ANP

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	0.73	0/4851	1.11	31/6587 (0.5%)
1	B	0.71	0/4846	1.10	24/6579 (0.4%)
All	All	0.72	0/9697	1.11	55/13166 (0.4%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	GLY	N-CA-C	-10.22	100.85	112.29
1	B	441	THR	N-CA-C	-9.64	101.63	113.97
1	B	93	VAL	N-CA-C	9.49	120.10	110.23
1	A	46	SER	N-CA-C	9.30	123.92	109.96
1	B	130	GLY	N-CA-C	-9.05	98.55	112.84
1	A	566	ILE	N-CA-C	-8.34	95.99	108.99
1	A	441	THR	N-CA-C	-8.32	103.26	113.41
1	A	438	VAL	N-CA-C	8.30	119.31	108.35
1	A	481	ARG	N-CA-C	-8.17	99.36	109.65
1	B	529	GLY	N-CA-C	-7.97	103.36	112.29
1	A	451	ILE	N-CA-C	-7.13	105.83	112.96
1	A	320	CYS	N-CA-C	-7.12	97.60	109.07
1	A	499	ALA	N-CA-C	-7.09	104.51	113.01
1	B	109	PRO	N-CA-C	-6.81	104.65	113.57
1	A	93	VAL	N-CA-C	6.78	117.53	110.62
1	B	438	VAL	N-CA-C	6.76	118.46	108.45
1	A	108	SER	N-CA-C	6.62	119.91	110.24
1	A	486	VAL	N-CA-C	6.58	118.89	108.89
1	A	453	GLU	CA-CB-CG	6.40	126.89	114.10
1	B	231	ASP	CA-C-N	6.34	126.08	119.05
1	B	231	ASP	C-N-CA	6.34	126.08	119.05
1	A	562	GLU	N-CA-C	6.20	120.56	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ILE	N-CA-C	-5.98	97.19	107.24
1	A	398	PHE	N-CA-C	-5.92	104.75	111.14
1	B	611	ILE	N-CA-C	-5.90	99.92	108.36
1	A	549	HIS	N-CA-C	-5.86	106.21	113.19
1	A	301	LEU	N-CA-C	-5.86	104.80	111.07
1	B	111	ALA	CA-C-N	5.85	127.16	119.84
1	B	111	ALA	C-N-CA	5.85	127.16	119.84
1	B	572	CYS	N-CA-C	5.84	118.47	110.24
1	A	111	ALA	CA-C-N	5.73	127.00	119.84
1	A	111	ALA	C-N-CA	5.73	127.00	119.84
1	A	587	THR	N-CA-C	-5.65	100.49	109.59
1	A	98	ILE	N-CA-C	5.65	115.99	107.80
1	B	585	THR	N-CA-C	-5.63	101.20	109.81
1	A	244	VAL	N-CA-C	5.60	115.22	108.06
1	A	406	ALA	N-CA-C	-5.44	106.61	113.20
1	B	121	ASP	N-CA-C	-5.38	103.59	110.53
1	B	530	TYR	N-CA-C	5.36	116.43	108.60
1	A	532	VAL	N-CA-C	-5.32	100.75	108.36
1	B	219	LYS	N-CA-C	-5.31	104.38	111.87
1	A	508	PHE	CA-C-N	5.29	126.46	119.84
1	A	508	PHE	C-N-CA	5.29	126.46	119.84
1	A	342	ALA	N-CA-C	5.26	116.82	111.14
1	B	328	VAL	CB-CA-C	-5.26	103.69	110.84
1	A	360	ASN	CA-C-O	5.25	122.70	119.29
1	A	306	GLN	N-CA-C	5.23	117.06	111.36
1	B	122	LYS	N-CA-C	-5.17	102.63	110.28
1	A	137	GLN	N-CA-C	5.07	116.22	108.52
1	A	466	THR	N-CA-C	-5.05	105.84	112.41
1	B	301	LEU	N-CA-C	-5.05	105.67	111.07
1	B	447	ALA	N-CA-C	-5.03	105.80	111.28
1	B	598	ARG	CA-C-N	-5.03	118.71	122.18
1	B	598	ARG	C-N-CA	-5.03	118.71	122.18
1	B	244	VAL	N-CA-C	5.02	115.89	108.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	4729	0	4601	258	0
1	B	4726	0	4616	266	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	4	0
4	A	258	0	0	8	0
4	B	204	0	0	7	0
All	All	9983	0	9243	521	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 28.

All (521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:HE3	1:A:355:LYS:H	1.14	1.10
1:B:84:ILE:HG22	1:B:189:MET:HE1	1.41	1.02
1:A:497:ASN:ND2	1:A:499:ALA:H	1.59	1.00
1:A:536:ALA:H	1:A:563:GLN:NE2	1.59	1.00
1:A:139:HIS:HB2	1:A:142:LYS:HG2	1.44	0.98
1:B:80:MET:HE3	1:B:129:THR:HA	1.44	0.98
1:A:392:GLU:OE1	1:A:441:THR:HG21	1.67	0.95
1:B:367:ASN:ND2	1:B:405:GLN:HE22	1.65	0.94
1:B:497:ASN:HD21	1:B:535:ILE:HB	1.33	0.90
1:A:389:ASP:HB3	1:A:391:GLU:HG2	1.53	0.90
1:B:497:ASN:HD22	1:B:498:LYS:N	1.69	0.89
1:A:421:TRP:H	1:A:471:ASN:HD21	1.21	0.87
1:A:497:ASN:C	1:A:497:ASN:HD22	1.82	0.87
1:A:483:GLU:CD	1:A:483:GLU:H	1.82	0.86
1:A:497:ASN:HD22	1:A:498:LYS:N	1.71	0.86
1:A:355:LYS:HE3	1:A:355:LYS:N	1.92	0.85
1:B:534:PRO:HB2	1:B:563:GLN:HE21	1.39	0.85
1:A:48:ILE:HD13	1:A:69:LEU:HD21	1.58	0.85
1:A:114:ALA:HA	1:A:135:ILE:HG22	1.59	0.85
1:B:524:GLU:OE1	1:B:524:GLU:N	2.10	0.85
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.42	0.84
1:B:268:ASN:HD21	1:B:592:TYR:H	1.24	0.83
1:B:96:ASP:CG	1:B:309:ARG:HH12	1.84	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LYS:HE3	1:B:323:GLU:H	1.44	0.82
1:A:64:ARG:HG3	1:A:74:VAL:HG23	1.61	0.82
1:A:598:ARG:HD3	1:A:611:ILE:HD13	1.61	0.82
1:B:523:ASP:O	1:B:526:VAL:HG12	1.80	0.81
1:A:10:ALA:HB1	1:A:14:THR:HG21	1.63	0.80
1:B:44:PHE:O	1:B:56:LYS:HG3	1.80	0.80
1:B:80:MET:HE3	1:B:129:THR:CA	2.14	0.78
1:A:268:ASN:HD21	1:A:592:TYR:H	1.31	0.77
1:A:341:GLU:HG2	1:A:611:ILE:HG13	1.65	0.77
1:A:355:LYS:H	1:A:355:LYS:CE	1.95	0.77
1:B:68:PHE:HE1	1:B:93:VAL:HG21	1.50	0.77
1:B:390:ILE:HD13	1:B:391:GLU:N	2.01	0.76
1:B:124:GLY:HA3	1:B:182:ASP:O	1.86	0.76
1:A:497:ASN:HD22	1:A:499:ALA:H	1.30	0.76
1:B:413:LEU:HD13	1:B:419:LEU:HD11	1.66	0.76
1:B:270:LEU:HD13	1:B:328:VAL:HG11	1.67	0.75
1:A:178:ASP:HB2	1:A:185:ILE:HD11	1.66	0.75
1:A:426:GLN:HA	1:A:481:ARG:HH22	1.51	0.75
1:A:497:ASN:HD21	1:A:535:ILE:HB	1.51	0.75
1:B:367:ASN:HD22	1:B:405:GLN:HE22	1.31	0.74
1:A:587:THR:HG23	4:A:5129:HOH:O	1.88	0.74
1:A:15:LEU:HD12	1:B:424:ALA:HB1	1.69	0.74
1:A:308:ARG:HA	1:A:311:HIS:CD2	2.24	0.73
1:A:331:TYR:OH	1:A:587:THR:HG21	1.88	0.73
1:A:300:ARG:HH22	1:A:482:PRO:HG3	1.53	0.73
1:B:544:ASP:OD1	1:B:555:LYS:HE2	1.89	0.73
1:B:511:HIS:HE1	1:B:513:TYR:CD2	2.07	0.72
1:B:383:HIS:HB2	1:B:438:VAL:HG12	1.71	0.72
1:A:48:ILE:O	1:A:49:ASP:HB2	1.89	0.72
1:B:341:GLU:HG2	1:B:611:ILE:HG13	1.72	0.71
1:A:62:PHE:HB2	1:A:148:GLN:NE2	2.05	0.71
1:A:300:ARG:NH2	1:A:482:PRO:HG3	2.04	0.71
1:B:520:THR:HG22	1:B:521:VAL:N	2.06	0.70
1:A:536:ALA:N	1:A:563:GLN:NE2	2.38	0.70
1:B:210:LYS:HE3	1:B:323:GLU:N	2.06	0.70
1:A:550:GLU:O	1:A:550:GLU:HG2	1.92	0.69
1:A:580:TYR:O	1:A:599:GLY:HA2	1.92	0.69
1:A:420:GLY:O	1:A:428:ILE:HG12	1.91	0.69
1:A:80:MET:HE3	1:A:128:ASP:O	1.92	0.69
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.57	0.69
1:B:309:ARG:HG3	1:B:309:ARG:HH11	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASN:ND2	1:B:613:PRO:HD3	2.08	0.68
1:A:277:ALA:HB2	1:A:504:LEU:HD13	1.75	0.68
1:A:481:ARG:HG3	1:A:483:GLU:OE1	1.94	0.68
1:B:337:SER:O	1:B:338:CYS:HB2	1.93	0.68
1:B:452:ARG:HG2	4:B:5320:HOH:O	1.93	0.68
1:A:308:ARG:HG3	1:A:308:ARG:NH1	2.09	0.67
1:B:517:THR:HB	1:B:568:GLN:HA	1.76	0.67
1:B:390:ILE:HD13	1:B:391:GLU:H	1.57	0.67
1:A:361:PRO:HG3	1:A:614:LEU:HD23	1.76	0.67
1:B:227:LEU:HB2	1:B:243:GLN:HE22	1.59	0.67
1:B:297:LEU:O	1:B:301:LEU:HD13	1.93	0.67
1:A:95:ASN:C	1:A:95:ASN:HD22	2.03	0.66
1:A:572:CYS:HB3	1:A:603:LEU:HD22	1.75	0.66
1:B:309:ARG:HD3	1:B:309:ARG:C	2.21	0.66
1:B:498:LYS:HB3	1:B:566:ILE:HG12	1.76	0.66
1:B:425:GLY:O	1:B:481:ARG:NH2	2.25	0.66
1:A:536:ALA:N	1:A:563:GLN:HE22	1.93	0.66
1:A:337:SER:O	1:A:338:CYS:HB2	1.95	0.65
1:A:536:ALA:H	1:A:563:GLN:HE22	1.36	0.65
1:B:226:TRP:HB2	1:B:352:GLN:HG2	1.79	0.65
1:A:48:ILE:CD1	1:A:69:LEU:HD21	2.26	0.65
1:A:483:GLU:CD	1:A:483:GLU:N	2.54	0.65
1:A:294:PRO:HD3	1:A:452:ARG:NH1	2.12	0.65
1:A:294:PRO:HD3	1:A:452:ARG:HH12	1.61	0.65
1:A:53:MET:O	1:A:64:ARG:HD2	1.97	0.65
1:A:351:GLU:O	1:A:351:GLU:HG2	1.97	0.65
1:B:80:MET:CE	1:B:129:THR:HA	2.25	0.65
1:A:497:ASN:ND2	1:A:499:ALA:N	2.39	0.64
1:A:536:ALA:H	1:A:563:GLN:HE21	1.39	0.64
1:B:314:THR:OG1	1:B:339:HIS:HE1	1.81	0.64
1:B:475:LEU:HD21	1:B:479:LEU:HD11	1.79	0.64
1:A:80:MET:CE	1:A:129:THR:HA	2.29	0.63
1:B:497:ASN:HD22	1:B:497:ASN:C	2.00	0.63
1:A:11:PRO:O	1:A:14:THR:HG22	1.97	0.63
1:B:76:THR:HG22	4:B:5184:HOH:O	1.98	0.63
1:B:532:VAL:HB	1:B:544:ASP:HB2	1.79	0.63
1:A:144:ARG:HG2	1:A:164:GLU:HG2	1.80	0.63
1:A:365:LEU:O	1:A:369:LEU:HB2	1.98	0.63
1:A:161:TRP:CZ3	1:A:164:GLU:HG3	2.34	0.62
1:A:315:GLY:H	1:A:587:THR:HG22	1.63	0.62
1:A:122:LYS:HB2	1:A:128:ASP:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ILE:HB	3:B:965:ANP:O3'	2.00	0.61
1:A:315:GLY:N	1:A:587:THR:HG22	2.16	0.61
1:B:520:THR:HG22	1:B:521:VAL:H	1.66	0.61
1:A:79:GLY:N	1:A:83:GLU:OE1	2.34	0.61
1:A:426:GLN:HA	1:A:481:ARG:NH2	2.16	0.61
1:A:121:ASP:HB2	1:A:186:LEU:HG	1.82	0.60
1:B:452:ARG:O	1:B:453:GLU:HG3	2.01	0.60
1:A:517:THR:HG23	1:A:568:GLN:HB2	1.82	0.60
1:B:151:ILE:HD12	1:B:151:ILE:N	2.16	0.60
1:B:241:ASN:O	1:B:244:VAL:HG22	2.01	0.60
1:B:48:ILE:O	1:B:49:ASP:HB2	2.00	0.60
1:B:348:ARG:NH1	1:B:352:GLN:NE2	2.50	0.60
1:B:379:ARG:HB2	1:B:437:CYS:HB2	1.84	0.60
1:B:497:ASN:ND2	1:B:499:ALA:H	2.00	0.60
1:B:204:ILE:HD13	1:B:205:ALA:N	2.17	0.59
1:A:445:GLU:HB3	4:A:5051:HOH:O	2.01	0.59
1:A:536:ALA:CA	1:A:563:GLN:HE22	2.14	0.59
1:A:597:LEU:O	1:A:598:ARG:HG2	2.02	0.59
1:B:245:ILE:HG13	1:B:246:ASN:N	2.15	0.59
1:B:354:TYR:CZ	1:B:356:GLY:HA3	2.37	0.59
1:A:216:LEU:HD13	1:A:353:GLY:O	2.02	0.59
1:B:227:LEU:HB2	1:B:243:GLN:NE2	2.16	0.59
1:A:497:ASN:ND2	1:A:498:LYS:N	2.47	0.59
1:B:294:PRO:HD2	1:B:297:LEU:HD12	1.84	0.59
1:A:597:LEU:HD11	1:A:614:LEU:HD13	1.85	0.59
1:B:104:PHE:CE2	1:B:110:ARG:HG2	2.38	0.59
1:A:364:GLY:N	4:A:5035:HOH:O	2.26	0.58
1:B:229:GLU:HB3	1:B:235:ASN:ND2	2.18	0.58
1:B:497:ASN:ND2	1:B:535:ILE:HB	2.10	0.58
1:B:97:ASN:HD22	1:B:98:ILE:H	1.49	0.58
1:A:497:ASN:HD22	1:A:499:ALA:N	2.01	0.58
1:A:243:GLN:C	1:A:244:VAL:HG12	2.27	0.58
1:A:30:TYR:HE2	1:A:58:GLN:HE22	1.51	0.58
1:A:308:ARG:NE	1:A:311:HIS:HD2	2.01	0.58
1:B:97:ASN:HD22	1:B:98:ILE:N	2.02	0.58
1:B:330:GLU:OE2	3:B:965:ANP:N3B	2.37	0.57
1:A:137:GLN:HG2	1:A:144:ARG:HB2	1.85	0.57
1:A:203:GLU:OE2	1:A:203:GLU:HA	2.05	0.57
1:B:401:GLN:OE1	1:B:401:GLN:HA	2.04	0.57
1:A:335:SER:OG	1:A:538:ARG:NH2	2.36	0.57
1:B:535:ILE:HG23	1:B:564:LYS:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD11	1:B:18:TYR:OH	2.05	0.56
1:B:246:ASN:HD21	1:B:613:PRO:HD3	1.70	0.56
1:A:20:PRO:HG2	1:A:136:THR:HB	1.87	0.56
1:A:355:LYS:N	1:A:355:LYS:CE	2.63	0.56
1:B:131:HIS:HE1	1:B:147:GLU:OE1	1.87	0.56
1:B:497:ASN:O	1:B:500:ILE:HG22	2.05	0.56
1:B:532:VAL:HG22	1:B:567:TYR:CE1	2.40	0.56
1:A:542:ASN:OD1	1:A:558:GLY:HA3	2.06	0.56
1:A:544:ASP:OD2	1:A:555:LYS:HE2	2.05	0.56
1:B:84:ILE:CG2	1:B:189:MET:HE1	2.24	0.56
1:B:303:LEU:HD13	1:B:307:ARG:NH2	2.20	0.56
1:B:308:ARG:HA	1:B:311:HIS:ND1	2.21	0.56
1:A:277:ALA:O	1:A:281:VAL:HG23	2.06	0.56
1:B:534:PRO:HB2	1:B:563:GLN:NE2	2.15	0.56
1:A:379:ARG:HG3	1:A:380:PRO:HD2	1.87	0.55
1:A:138:LEU:O	1:A:139:HIS:CD2	2.59	0.55
1:A:15:LEU:CD2	1:A:24:ALA:HB1	2.36	0.55
1:A:429:ASP:OD1	1:A:433:ARG:HG2	2.07	0.55
1:B:296:ILE:HD11	1:B:461:ALA:HA	1.88	0.55
1:B:337:SER:O	1:B:338:CYS:CB	2.53	0.55
1:A:80:MET:HG2	4:A:5188:HOH:O	2.05	0.55
1:B:94:VAL:HG13	4:B:5167:HOH:O	2.06	0.55
1:B:481:ARG:NH1	1:B:483:GLU:CD	2.64	0.55
1:B:570:LEU:O	1:B:571:TRP:HB2	2.05	0.55
1:A:335:SER:HG	1:A:538:ARG:HH22	1.54	0.55
1:B:125:GLU:HG2	1:B:180:PHE:CE2	2.42	0.55
1:B:422:ASP:OD2	1:B:426:GLN:HB2	2.07	0.55
1:B:497:ASN:HD22	1:B:498:LYS:H	1.53	0.55
1:A:497:ASN:ND2	1:A:535:ILE:HB	2.21	0.54
1:B:138:LEU:HD12	1:B:143:VAL:HG23	1.87	0.54
1:B:167:MET:HE3	1:B:169:VAL:CG2	2.36	0.54
1:A:512:ARG:HB2	4:A:5030:HOH:O	2.07	0.54
1:B:584:CYS:HB2	1:B:596:CYS:SG	2.47	0.54
1:A:296:ILE:HD11	1:A:461:ALA:HA	1.88	0.54
1:B:532:VAL:C	1:B:533:LYS:HG2	2.32	0.54
1:A:121:ASP:HB2	1:A:186:LEU:CG	2.37	0.54
1:B:498:LYS:HB2	1:B:535:ILE:HA	1.90	0.54
1:B:501:LEU:HB2	1:B:502:PRO:HD3	1.89	0.54
1:A:483:GLU:HG2	4:B:5349:HOH:O	2.07	0.54
1:B:127:LYS:H	1:B:127:LYS:HD2	1.72	0.54
1:A:64:ARG:CG	1:A:74:VAL:HG23	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HG22	1:A:114:ALA:N	2.21	0.53
1:B:215:ARG:HG3	1:B:215:ARG:NH1	2.22	0.53
1:B:355:LYS:HD2	1:B:355:LYS:N	2.23	0.53
1:B:538:ARG:O	1:B:539:CYS:HB2	2.08	0.53
1:A:501:LEU:HB2	1:A:502:PRO:HD3	1.91	0.53
1:B:451:ILE:O	1:B:453:GLU:N	2.33	0.53
1:B:476:ILE:HG12	1:B:476:ILE:O	2.07	0.53
1:B:497:ASN:C	1:B:497:ASN:ND2	2.63	0.53
1:A:314:THR:OG1	1:A:339:HIS:HE1	1.91	0.53
1:B:82:TRP:HD1	1:B:129:THR:O	1.90	0.53
1:A:118:LEU:C	1:A:119:ILE:HD13	2.34	0.53
1:B:80:MET:HE3	1:B:129:THR:N	2.23	0.53
1:B:376:SER:O	1:B:378:ALA:N	2.37	0.53
1:B:601:GLU:CD	1:B:601:GLU:H	2.17	0.53
1:B:319:PHE:CE2	1:B:328:VAL:HG13	2.44	0.53
1:B:342:ALA:HA	1:B:346:LEU:HD12	1.91	0.53
1:A:542:ASN:HA	1:A:556:THR:O	2.08	0.52
1:B:306:GLN:O	1:B:306:GLN:HG2	2.09	0.52
1:A:16:LEU:HD21	1:A:27:SER:HB2	1.91	0.52
1:A:51:GLU:OE1	1:A:91:ARG:NH2	2.39	0.52
1:A:313:ILE:HD11	1:A:487:PHE:CE2	2.44	0.52
1:A:507:LEU:C	1:A:509:PRO:HD3	2.34	0.52
1:A:15:LEU:HD23	1:A:24:ALA:HB1	1.91	0.52
1:B:216:LEU:HD13	1:B:353:GLY:O	2.10	0.52
1:B:268:ASN:ND2	1:B:592:TYR:H	2.02	0.52
1:B:413:LEU:CD1	1:B:419:LEU:HD11	2.37	0.52
1:A:313:ILE:HB	1:A:488:GLU:OE1	2.10	0.52
1:B:381:PHE:CD1	1:B:409:GLU:HB2	2.45	0.52
1:A:80:MET:HE3	1:A:128:ASP:C	2.35	0.52
1:B:104:PHE:O	1:B:187:GLY:HA3	2.10	0.51
1:B:314:THR:HA	1:B:587:THR:O	2.09	0.51
1:B:119:ILE:CG1	1:B:189:MET:HE2	2.40	0.51
1:B:518:ASP:OD2	1:B:519:PHE:N	2.38	0.51
1:B:542:ASN:ND2	1:B:561:ALA:HB2	2.25	0.51
1:A:312:MET:HA	1:A:488:GLU:OE2	2.11	0.51
1:A:512:ARG:CB	1:A:512:ARG:HH11	2.23	0.51
1:B:96:ASP:OD1	1:B:309:ARG:NH1	2.42	0.51
1:A:245:ILE:HG13	1:A:246:ASN:ND2	2.26	0.51
1:A:255:ILE:HG23	1:A:614:LEU:HD11	1.93	0.51
1:B:387:ASP:OD1	1:B:388:LYS:N	2.43	0.51
1:B:411:ARG:HG2	1:B:411:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ARG:C	1:B:453:GLU:HG3	2.36	0.51
1:A:95:ASN:ND2	1:A:97:ASN:HB3	2.26	0.51
1:B:532:VAL:O	1:B:533:LYS:HG2	2.11	0.51
1:A:125:GLU:HB3	1:A:183:THR:HG21	1.93	0.51
1:A:392:GLU:OE1	1:A:441:THR:CG2	2.50	0.51
1:A:536:ALA:HB3	1:A:563:GLN:HE22	1.75	0.51
1:B:388:LYS:HG3	1:B:414:ARG:NH2	2.26	0.51
1:A:451:ILE:HG13	1:A:476:ILE:HD12	1.92	0.51
1:A:56:LYS:HB3	1:A:57:TRP:CD1	2.46	0.50
1:B:348:ARG:NH1	1:B:352:GLN:HE22	2.09	0.50
1:B:137:GLN:CG	1:B:144:ARG:HB2	2.42	0.50
1:A:131:HIS:HE1	1:A:147:GLU:OE2	1.95	0.50
1:A:96:ASP:CG	1:A:309:ARG:HH21	2.19	0.50
1:A:389:ASP:C	1:A:391:GLU:N	2.67	0.50
1:A:559:LYS:H	1:A:559:LYS:HD2	1.77	0.50
1:A:113:VAL:CG2	1:A:114:ALA:N	2.73	0.50
1:A:139:HIS:HB2	1:A:142:LYS:CG	2.28	0.50
1:A:427:LEU:HD11	1:A:478:VAL:HG22	1.94	0.50
1:B:112:PRO:HB3	1:B:188:TRP:CD2	2.47	0.50
1:B:431:GLU:OE2	1:B:431:GLU:HA	2.12	0.50
1:A:168:VAL:HG22	1:A:175:THR:HB	1.94	0.50
1:A:595:THR:HG22	1:A:596:CYS:N	2.27	0.50
1:B:481:ARG:HB3	1:B:484:VAL:HG23	1.94	0.50
1:B:138:LEU:HD11	1:B:167:MET:HE1	1.94	0.50
1:B:253:TYR:CZ	1:B:581:ILE:HD11	2.47	0.50
1:A:121:ASP:OD2	1:A:122:LYS:N	2.45	0.49
1:A:350:ALA:C	1:A:352:GLN:N	2.68	0.49
1:A:532:VAL:HB	1:A:544:ASP:HB2	1.94	0.49
1:A:246:ASN:N	1:A:246:ASN:HD22	2.10	0.49
1:A:584:CYS:HB2	1:A:596:CYS:SG	2.53	0.49
1:B:580:TYR:CE2	1:B:603:LEU:HD12	2.48	0.49
1:B:96:ASP:OD2	1:B:309:ARG:NH1	2.46	0.49
1:B:303:LEU:HD13	1:B:307:ARG:HH21	1.78	0.49
1:B:522:ASN:HD22	1:B:524:GLU:CD	2.20	0.49
1:A:389:ASP:C	1:A:391:GLU:H	2.20	0.49
1:B:488:GLU:HB3	1:B:492:THR:HG21	1.93	0.49
1:A:437:CYS:O	1:A:438:VAL:HG23	2.13	0.49
1:A:245:ILE:HG13	1:A:246:ASN:N	2.28	0.49
1:A:139:HIS:CB	1:A:142:LYS:HG2	2.30	0.49
1:B:314:THR:HG21	1:B:339:HIS:CE1	2.48	0.49
1:A:82:TRP:HB3	1:A:130:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:HB2	1:B:200:PRO:HD2	1.95	0.48
1:A:121:ASP:HB2	1:A:186:LEU:CD2	2.43	0.48
1:A:227:LEU:HB2	1:A:243:GLN:OE1	2.13	0.48
1:B:65:ARG:O	1:B:66:PHE:C	2.55	0.48
1:A:23:VAL:HG21	1:A:66:PHE:CD1	2.49	0.48
1:B:155:LEU:HB3	1:B:156:PRO:HD2	1.95	0.48
1:B:523:ASP:O	1:B:526:VAL:CG1	2.57	0.48
1:A:156:PRO:O	1:A:157:GLN:C	2.56	0.48
1:A:404:HIS:NE2	1:A:410:THR:OG1	2.45	0.48
1:A:88:ARG:O	1:A:89:PHE:HB3	2.13	0.48
1:A:163:ARG:NH1	1:A:179:THR:OG1	2.47	0.48
1:A:264:ILE:HG12	1:A:592:TYR:CD2	2.49	0.48
1:B:204:ILE:HD13	1:B:205:ALA:H	1.77	0.48
1:B:527:LYS:O	1:B:548:HIS:HB2	2.13	0.48
1:B:532:VAL:HG22	1:B:567:TYR:CD1	2.49	0.48
1:A:125:GLU:HB3	1:A:183:THR:CG2	2.43	0.48
1:A:535:ILE:HG22	1:A:566:ILE:HG23	1.94	0.48
1:B:270:LEU:HD13	1:B:328:VAL:CG1	2.40	0.48
1:A:168:VAL:CG2	1:A:175:THR:HB	2.43	0.48
1:B:418:GLU:HG2	1:B:430:GLY:CA	2.43	0.48
1:B:595:THR:HG22	1:B:596:CYS:N	2.28	0.48
1:A:27:SER:OG	1:A:152:HIS:HB3	2.14	0.48
1:A:164:GLU:C	1:A:165:LEU:HD23	2.38	0.48
1:A:460:ALA:HB2	1:B:114:ALA:CB	2.44	0.48
1:B:210:LYS:CE	1:B:323:GLU:H	2.21	0.48
1:B:352:GLN:OE1	1:B:352:GLN:HA	2.13	0.48
1:B:523:ASP:C	1:B:526:VAL:HG12	2.38	0.48
1:B:196:GLU:C	1:B:198:SER:H	2.22	0.47
1:B:382:VAL:O	1:B:410:THR:HA	2.13	0.47
1:B:440:LYS:HE2	1:B:444:TRP:NE1	2.29	0.47
1:B:444:TRP:HB2	1:B:493:VAL:CG1	2.44	0.47
1:B:520:THR:CG2	1:B:521:VAL:N	2.74	0.47
1:B:444:TRP:HB2	1:B:493:VAL:HG11	1.94	0.47
1:B:475:LEU:HD22	1:B:479:LEU:HG	1.96	0.47
1:A:137:GLN:OE1	1:A:144:ARG:HD2	2.14	0.47
1:A:308:ARG:NH1	1:A:308:ARG:CG	2.75	0.47
1:A:308:ARG:HE	1:A:311:HIS:CD2	2.31	0.47
1:A:532:VAL:O	1:A:533:LYS:HG2	2.15	0.47
1:B:517:THR:CG2	1:B:568:GLN:HG3	2.45	0.47
1:A:80:MET:HE3	1:A:129:THR:HA	1.96	0.47
1:B:56:LYS:HA	1:B:57:TRP:HA	1.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:OH	1:A:58:GLN:OE1	2.33	0.47
1:A:92:GLU:HB3	1:A:95:ASN:HD21	1.78	0.47
1:A:598:ARG:HD3	1:A:611:ILE:CD1	2.40	0.47
1:B:15:LEU:HD11	1:B:18:TYR:CZ	2.50	0.47
1:B:273:MET:HG2	1:B:508:PHE:CE2	2.50	0.47
1:B:309:ARG:HD3	1:B:309:ARG:O	2.14	0.47
1:B:468:HIS:CE1	1:B:470:GLN:HE21	2.32	0.47
1:A:80:MET:SD	1:A:129:THR:HA	2.54	0.47
1:A:138:LEU:O	1:A:139:HIS:HD2	1.97	0.47
1:A:308:ARG:CD	1:A:311:HIS:HD2	2.28	0.47
1:A:15:LEU:CD1	1:B:424:ALA:HB1	2.40	0.47
1:B:475:LEU:CD2	1:B:479:LEU:HD11	2.44	0.47
1:A:306:GLN:OE1	1:B:94:VAL:HA	2.16	0.46
1:A:430:GLY:C	1:A:432:GLY:H	2.23	0.46
1:B:63:ALA:HA	1:B:134:ILE:HD11	1.98	0.46
1:B:176:LEU:HD12	1:B:188:TRP:CZ3	2.49	0.46
1:B:447:ALA:HB2	1:B:475:LEU:HD13	1.97	0.46
3:B:965:ANP:O5'	3:B:965:ANP:H8	2.14	0.46
1:A:80:MET:N	1:A:83:GLU:OE1	2.38	0.46
1:A:121:ASP:HB2	1:A:186:LEU:HD21	1.98	0.46
1:B:461:ALA:O	1:B:462:VAL:C	2.58	0.46
3:A:964:ANP:O5'	3:A:964:ANP:H8	2.14	0.46
1:B:309:ARG:HH11	1:B:309:ARG:CG	2.27	0.46
1:B:573:LEU:HD22	1:B:581:ILE:O	2.16	0.46
1:A:508:PHE:N	1:A:509:PRO:HD3	2.31	0.46
1:B:178:ASP:OD1	1:B:179:THR:N	2.48	0.46
1:A:308:ARG:HE	1:A:311:HIS:HD2	1.61	0.46
1:A:350:ALA:C	1:A:352:GLN:H	2.23	0.46
1:B:290:LEU:HD13	1:B:519:PHE:CZ	2.50	0.46
1:A:475:LEU:HD22	1:A:479:LEU:HG	1.97	0.46
1:A:481:ARG:HB3	1:A:484:VAL:CG2	2.46	0.46
1:B:547:SER:C	1:B:549:HIS:H	2.22	0.46
1:B:560:PHE:CD1	1:B:560:PHE:N	2.83	0.46
1:A:19:ALA:HB1	1:A:20:PRO:CD	2.46	0.46
1:A:459:PHE:HB3	4:A:5213:HOH:O	2.15	0.46
1:B:102:GLN:HA	1:B:102:GLN:NE2	2.30	0.46
1:B:137:GLN:HG2	1:B:144:ARG:HB2	1.96	0.46
1:B:367:ASN:HD22	1:B:405:GLN:NE2	2.08	0.46
1:B:549:HIS:C	1:B:550:GLU:HG3	2.41	0.46
1:B:97:ASN:ND2	1:B:98:ILE:N	2.64	0.46
1:B:297:LEU:HD13	1:B:448:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:C	1:B:95:ASN:HD22	2.23	0.45
1:B:427:LEU:HD12	1:B:481:ARG:HD2	1.98	0.45
1:A:268:ASN:ND2	1:A:592:TYR:H	2.07	0.45
1:A:581:ILE:CG2	1:A:597:LEU:HD22	2.46	0.45
1:B:291:PHE:CD1	1:B:291:PHE:N	2.83	0.45
1:B:580:TYR:CZ	1:B:603:LEU:HD12	2.51	0.45
1:A:10:ALA:N	4:A:5066:HOH:O	2.49	0.45
1:B:348:ARG:CZ	1:B:352:GLN:HE22	2.28	0.45
1:B:497:ASN:ND2	1:B:498:LYS:N	2.51	0.45
1:A:119:ILE:CD1	1:A:132:VAL:HG23	2.46	0.45
1:A:246:ASN:HD22	1:A:246:ASN:H	1.64	0.45
1:B:226:TRP:H	1:B:226:TRP:CD1	2.34	0.45
1:A:251:HIS:ND1	1:A:251:HIS:C	2.73	0.45
1:B:348:ARG:O	1:B:352:GLN:HB2	2.17	0.45
1:B:517:THR:HG22	1:B:568:GLN:HG3	1.98	0.45
1:A:56:LYS:HA	1:A:57:TRP:HA	1.65	0.45
1:A:206:GLY:O	1:A:323:GLU:HA	2.16	0.45
1:A:296:ILE:HD11	1:A:461:ALA:CA	2.46	0.45
1:A:525:LEU:HD21	1:A:567:TYR:O	2.17	0.45
1:B:127:LYS:HD2	1:B:127:LYS:N	2.32	0.45
1:A:341:GLU:CG	1:A:611:ILE:HG13	2.42	0.45
1:B:73:VAL:HG21	1:B:90:LEU:HD13	1.99	0.45
1:B:233:LEU:HD12	1:B:344:LEU:CD2	2.46	0.45
1:B:386:GLN:HG3	1:B:387:ASP:O	2.16	0.45
1:A:511:HIS:HE1	1:A:513:TYR:CD2	2.35	0.45
1:A:517:THR:HG21	1:A:566:ILE:HD13	1.98	0.45
1:A:228:ASP:OD2	1:A:228:ASP:C	2.59	0.45
1:A:10:ALA:HB1	1:A:14:THR:CG2	2.41	0.45
1:A:530:TYR:HA	1:A:570:LEU:N	2.32	0.45
1:B:536:ALA:H	1:B:563:GLN:NE2	2.14	0.45
1:A:350:ALA:O	1:A:352:GLN:N	2.50	0.44
1:B:481:ARG:HG2	1:B:481:ARG:HH11	1.81	0.44
1:A:122:LYS:HB2	1:A:127:LYS:O	2.18	0.44
1:A:364:GLY:O	1:A:365:LEU:C	2.60	0.44
1:A:536:ALA:CB	1:A:563:GLN:HE22	2.30	0.44
1:B:164:GLU:O	1:B:165:LEU:HD23	2.17	0.44
1:B:568:GLN:O	1:B:569:GLN:C	2.59	0.44
1:A:575:LYS:HE2	1:A:580:TYR:OH	2.16	0.44
1:B:346:LEU:HA	1:B:346:LEU:HD23	1.76	0.44
1:B:246:ASN:HD21	1:B:613:PRO:CD	2.31	0.44
1:A:64:ARG:HG3	1:A:74:VAL:CG2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLU:HB3	1:B:235:ASN:HD21	1.81	0.44
1:B:307:ARG:HG3	1:B:308:ARG:HG2	1.99	0.44
1:B:381:PHE:CZ	1:B:411:ARG:HB2	2.53	0.44
1:B:196:GLU:O	1:B:197:TYR:HB2	2.18	0.44
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.73	0.44
1:B:56:LYS:HB3	1:B:57:TRP:CD1	2.53	0.44
1:B:112:PRO:HB3	1:B:188:TRP:CE2	2.52	0.44
1:B:379:ARG:HB2	1:B:437:CYS:CB	2.47	0.44
1:B:547:SER:C	1:B:549:HIS:N	2.76	0.44
1:A:126:PHE:O	1:A:127:LYS:C	2.60	0.44
1:B:376:SER:C	1:B:378:ALA:H	2.24	0.44
1:A:132:VAL:HG22	1:A:133:ALA:N	2.32	0.44
1:A:328:VAL:O	1:A:328:VAL:HG13	2.18	0.44
1:A:508:PHE:O	1:A:511:HIS:HB2	2.18	0.44
1:B:19:ALA:HB2	1:B:62:PHE:HZ	1.83	0.44
1:A:73:VAL:HG11	1:A:99:LEU:HD12	2.00	0.43
1:A:117:LEU:O	1:A:188:TRP:HA	2.17	0.43
1:A:205:ALA:O	1:A:207:GLU:N	2.51	0.43
1:B:121:ASP:HB2	1:B:186:LEU:HG	2.00	0.43
1:B:532:VAL:C	1:B:533:LYS:CG	2.91	0.43
1:A:450:GLN:OE1	1:A:476:ILE:HG22	2.19	0.43
1:B:399:MET:HE3	1:B:439:TRP:CZ2	2.52	0.43
1:B:347:GLU:OE1	1:B:360:ASN:HB3	2.19	0.43
1:B:480:LEU:O	1:B:482:PRO:HD3	2.18	0.43
1:B:542:ASN:OD1	1:B:558:GLY:HA3	2.18	0.43
1:A:149:ASN:HD22	1:A:149:ASN:HA	1.57	0.43
1:A:418:GLU:HG3	1:A:430:GLY:CA	2.48	0.43
1:B:430:GLY:C	1:B:432:GLY:N	2.75	0.43
1:B:348:ARG:CZ	1:B:352:GLN:NE2	2.81	0.43
1:B:554:ASP:OD2	1:B:555:LYS:N	2.52	0.43
1:A:94:VAL:O	1:A:94:VAL:HG13	2.19	0.43
1:A:376:SER:C	1:A:378:ALA:H	2.26	0.43
1:A:468:HIS:HE1	1:A:470:GLN:HB2	1.84	0.43
1:B:348:ARG:NH1	1:B:352:GLN:CD	2.77	0.43
1:B:384:ILE:HD11	1:B:410:THR:HG21	1.99	0.43
1:B:399:MET:HG2	1:B:439:TRP:CE2	2.54	0.43
1:A:499:ALA:O	1:A:502:PRO:HD2	2.19	0.43
1:A:227:LEU:HD23	1:A:348:ARG:HG3	2.01	0.43
1:A:298:TRP:CD1	1:A:298:TRP:N	2.85	0.43
1:B:444:TRP:CB	1:B:493:VAL:HG11	2.47	0.43
1:B:498:LYS:HD2	4:B:5081:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLY:N	1:A:127:LYS:O	2.52	0.43
1:B:151:ILE:N	1:B:151:ILE:CD1	2.80	0.43
1:B:597:LEU:HD11	1:B:614:LEU:HD13	2.01	0.43
1:A:418:GLU:CG	1:A:430:GLY:H	2.32	0.43
1:A:470:GLN:O	1:A:471:ASN:C	2.62	0.43
1:A:95:ASN:HD22	1:A:97:ASN:H	1.65	0.42
1:A:595:THR:CG2	1:A:596:CYS:N	2.81	0.42
1:B:88:ARG:HH11	1:B:88:ARG:HG2	1.84	0.42
1:B:498:LYS:C	1:B:500:ILE:N	2.74	0.42
1:A:30:TYR:HE2	1:A:58:GLN:NE2	2.17	0.42
1:A:204:ILE:HD11	1:A:208:LEU:HD13	2.01	0.42
1:B:234:GLN:O	1:B:237:TYR:HB3	2.19	0.42
1:B:429:ASP:CG	1:B:433:ARG:HG2	2.45	0.42
1:A:88:ARG:HG3	1:A:201:GLN:HB2	2.01	0.42
1:A:385:MET:HE2	1:A:385:MET:HB3	1.88	0.42
1:A:118:LEU:HD12	1:A:187:GLY:O	2.19	0.42
1:A:199:LEU:HA	1:A:200:PRO:HD3	1.83	0.42
1:B:147:GLU:CD	1:B:150:VAL:HG21	2.45	0.42
1:B:308:ARG:NE	1:B:311:HIS:ND1	2.68	0.42
1:A:428:ILE:HA	1:A:433:ARG:O	2.20	0.42
1:A:440:LYS:HE2	1:A:444:TRP:CD1	2.55	0.42
1:B:84:ILE:C	1:B:86:SER:H	2.27	0.42
1:B:229:GLU:CB	1:B:235:ASN:ND2	2.83	0.42
1:B:591:ASN:O	1:B:592:TYR:C	2.62	0.42
1:B:80:MET:HE3	1:B:128:ASP:C	2.45	0.42
1:A:48:ILE:O	1:A:49:ASP:CB	2.65	0.42
1:A:460:ALA:HB2	1:B:114:ALA:HB3	2.01	0.42
1:A:598:ARG:NH1	1:A:609:SER:O	2.53	0.42
1:B:93:VAL:HG23	1:B:94:VAL:N	2.35	0.42
1:B:138:LEU:HD11	1:B:167:MET:CE	2.49	0.42
1:B:316:ARG:NH1	3:B:965:ANP:O2G	2.52	0.42
1:B:430:GLY:C	1:B:432:GLY:H	2.27	0.42
1:A:50:ASP:HB3	1:A:310:HIS:CD2	2.54	0.42
1:A:233:LEU:O	1:A:236:ALA:HB3	2.20	0.42
1:A:80:MET:CG	4:A:5188:HOH:O	2.67	0.41
1:A:178:ASP:O	1:A:180:PHE:N	2.53	0.41
1:B:372:ALA:HA	4:B:5311:HOH:O	2.20	0.41
1:B:521:VAL:HG11	1:B:530:TYR:CE2	2.55	0.41
1:B:585:THR:HA	1:B:594:GLY:O	2.20	0.41
1:A:178:ASP:C	1:A:180:PHE:N	2.79	0.41
1:B:598:ARG:HD3	1:B:611:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:O	1:A:168:VAL:HG23	2.19	0.41
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.88	0.41
1:A:374:LYS:HE3	1:A:374:LYS:HA	2.02	0.41
1:B:73:VAL:CG2	1:B:90:LEU:HD13	2.50	0.41
1:B:120:TRP:HB2	1:B:131:HIS:HB3	2.03	0.41
1:B:509:PRO:O	1:B:510:HIS:HB2	2.20	0.41
1:A:118:LEU:HD12	1:A:118:LEU:HA	1.90	0.41
1:B:64:ARG:NH1	1:B:75:PHE:O	2.53	0.41
1:B:512:ARG:HG2	1:B:512:ARG:HH11	1.86	0.41
1:A:530:TYR:CD1	1:A:530:TYR:C	2.98	0.41
1:A:28:SER:HB2	1:A:57:TRP:HB2	2.03	0.41
1:B:138:LEU:HD11	1:B:167:MET:SD	2.60	0.41
1:B:139:HIS:HB2	1:B:142:LYS:HG3	2.03	0.41
1:B:386:GLN:HA	1:B:441:THR:OG1	2.21	0.41
1:A:322:ASP:OD2	1:A:322:ASP:C	2.64	0.41
1:A:366:ILE:HG12	1:A:398:PHE:CZ	2.56	0.41
1:B:194:ASP:C	1:B:194:ASP:OD1	2.64	0.41
1:A:96:ASP:O	1:A:276:HIS:HD2	2.03	0.41
1:A:228:ASP:HB2	1:A:348:ARG:NH2	2.36	0.41
1:B:68:PHE:CE1	1:B:93:VAL:HG21	2.42	0.41
1:B:84:ILE:C	1:B:86:SER:N	2.79	0.41
1:B:429:ASP:OD1	1:B:429:ASP:C	2.63	0.41
1:A:105:PRO:HD3	1:A:199:LEU:HG	2.01	0.40
1:A:162:THR:O	1:A:163:ARG:CG	2.69	0.40
1:A:295:LYS:O	1:A:296:ILE:C	2.64	0.40
1:A:401:GLN:NE2	1:A:401:GLN:HA	2.37	0.40
1:A:581:ILE:HD12	1:A:581:ILE:N	2.36	0.40
1:B:19:ALA:HB3	1:B:23:VAL:HB	2.03	0.40
1:B:578:GLY:O	1:B:579:LYS:HG2	2.21	0.40
1:A:568:GLN:O	1:A:569:GLN:C	2.64	0.40
1:B:150:VAL:C	1:B:151:ILE:HD12	2.45	0.40
1:A:386:GLN:NE2	1:A:414:ARG:HD2	2.35	0.40
1:A:411:ARG:HH21	1:A:431:GLU:HG3	1.86	0.40
1:B:118:LEU:C	1:B:119:ILE:HD13	2.46	0.40
1:B:339:HIS:HB3	1:B:398:PHE:CE2	2.56	0.40
1:A:327:LYS:HG3	1:A:515:LEU:HD21	2.04	0.40
1:A:512:ARG:NH1	1:A:512:ARG:HB3	2.36	0.40
1:B:119:ILE:HG13	1:B:189:MET:HE2	2.03	0.40
1:B:228:ASP:HB3	1:B:234:GLN:NE2	2.36	0.40
1:B:468:HIS:HE1	1:B:470:GLN:HE21	1.68	0.40
1:B:517:THR:HB	1:B:568:GLN:CA	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:HA	1:A:394:TYR:CD2	2.56	0.40
1:A:383:HIS:CE1	1:A:433:ARG:HD2	2.56	0.40
1:A:505:TRP:CH2	1:A:510:HIS:HA	2.57	0.40
1:A:580:TYR:C	1:A:581:ILE:HD12	2.46	0.40
1:B:50:ASP:OD2	1:B:50:ASP:N	2.54	0.40
1:B:417:ASP:HB2	4:B:5324:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/619 (94%)	513 (88%)	58 (10%)	10 (2%)	7	19
1	B	581/619 (94%)	521 (90%)	48 (8%)	12 (2%)	5	15
All	All	1162/1238 (94%)	1034 (89%)	106 (9%)	22 (2%)	6	17

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	B	461	ALA
1	B	571	TRP
1	A	11	PRO
1	A	206	GLY
1	B	96	ASP
1	B	452	ARG
1	A	49	ASP
1	A	76	THR
1	A	95	ASN
1	B	49	ASP
1	B	338	CYS

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Mol	Chain	Res	Type
1	A	431	GLU
1	B	127	LYS
1	B	295	LYS
1	B	377	ARG
1	B	551	GLU
1	A	179	THR
1	A	571	TRP
1	B	550	GLU
1	A	296	ILE
1	B	482	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	500/530 (94%)	467 (93%)	33 (7%)	15	36
1	B	500/530 (94%)	469 (94%)	31 (6%)	16	39
All	All	1000/1060 (94%)	936 (94%)	64 (6%)	16	38

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	95	ASN
1	A	138	LEU
1	A	149	ASN
1	A	177	LYS
1	A	244	VAL
1	A	246	ASN
1	A	251	HIS
1	A	258	SER
1	A	272	LEU
1	A	278	THR
1	A	301	LEU
1	A	323	GLU

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Mol	Chain	Res	Type
1	A	348	ARG
1	A	355	LYS
1	A	368	GLU
1	A	374	LYS
1	A	379	ARG
1	A	419	LEU
1	A	441	THR
1	A	459	PHE
1	A	465	ARG
1	A	470	GLN
1	A	471	ASN
1	A	475	LEU
1	A	483	GLU
1	A	486	VAL
1	A	497	ASN
1	A	504	LEU
1	A	557	SER
1	A	559	LYS
1	A	587	THR
1	A	608	GLU
1	B	14	THR
1	B	50	ASP
1	B	95	ASN
1	B	143	VAL
1	B	153	SER
1	B	173	CYS
1	B	204	ILE
1	B	219	LYS
1	B	233	LEU
1	B	258	SER
1	B	265	LYS
1	B	309	ARG
1	B	328	VAL
1	B	348	ARG
1	B	352	GLN
1	B	369	LEU
1	B	379	ARG
1	B	382	VAL
1	B	390	ILE
1	B	417	ASP
1	B	470	GLN
1	B	471	ASN

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Mol	Chain	Res	Type
1	B	475	LEU
1	B	476	ILE
1	B	497	ASN
1	B	517	THR
1	B	560	PHE
1	B	566	ILE
1	B	606	LYS
1	B	608	GLU
1	B	618	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	70	ASN
1	A	95	ASN
1	A	131	HIS
1	A	141	ASN
1	A	149	ASN
1	A	159	GLN
1	A	201	GLN
1	A	235	ASN
1	A	241	ASN
1	A	246	ASN
1	A	261	GLN
1	A	268	ASN
1	A	276	HIS
1	A	310	HIS
1	A	311	HIS
1	A	339	HIS
1	A	352	GLN
1	A	397	GLN
1	A	405	GLN
1	A	471	ASN
1	A	497	ASN
1	A	563	GLN
1	A	565	ASN
1	A	582	GLN
1	B	55	HIS
1	B	58	GLN
1	B	70	ASN
1	B	95	ASN

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Mol	Chain	Res	Type
1	B	97	ASN
1	B	102	GLN
1	B	131	HIS
1	B	141	ASN
1	B	157	GLN
1	B	159	GLN
1	B	171	ASN
1	B	235	ASN
1	B	246	ASN
1	B	261	GLN
1	B	268	ASN
1	B	286	ASN
1	B	339	HIS
1	B	367	ASN
1	B	397	GLN
1	B	470	GLN
1	B	497	ASN
1	B	563	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ANP	B	965	2	33,33,33	3.73	6 (18%)	45,52,52	1.63	10 (22%)
3	ANP	A	964	2	33,33,33	3.80	8 (24%)	45,52,52	1.56	7 (15%)

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
3	ANP	B	965	2	-	7/18/38/38	0/3/3/3
3	ANP	A	964	2	-	6/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	965	ANP	PB-O3A	19.11	1.82	1.59
3	A	964	ANP	PB-O3A	19.00	1.82	1.59
3	A	964	ANP	C2-N1	5.44	1.43	1.33
3	B	965	ANP	C2-N1	5.27	1.43	1.33
3	A	964	ANP	PA-O3A	-4.95	1.54	1.59
3	B	965	ANP	PA-O3A	-4.33	1.54	1.59
3	A	964	ANP	C5-C6	3.59	1.51	1.41
3	A	964	ANP	PG-N3B	-3.01	1.55	1.63
3	B	965	ANP	C5-C6	2.93	1.49	1.41
3	A	964	ANP	C2-N3	2.75	1.38	1.33
3	A	964	ANP	C4-N3	2.68	1.39	1.34
3	B	965	ANP	PB-O1B	2.32	1.49	1.46
3	B	965	ANP	C2-N3	2.24	1.37	1.33
3	A	964	ANP	C6-N1	2.09	1.41	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	965	ANP	O2G-PG-O1G	-6.21	97.88	113.45
3	A	964	ANP	O2G-PG-O1G	-5.69	99.19	113.45
3	B	965	ANP	N3-C2-N1	-3.69	122.99	128.58
3	A	964	ANP	N3-C2-N1	-3.58	123.17	128.58
3	B	965	ANP	O2G-PG-O3G	3.07	115.83	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	964	ANP	C2-N1-C6	2.74	123.22	118.73
3	B	965	ANP	C2-N1-C6	2.54	122.89	118.73
3	A	964	ANP	O2B-PB-O1B	2.46	115.14	109.87
3	A	964	ANP	O2G-PG-O3G	2.34	113.86	107.59
3	B	965	ANP	O2B-PB-O1B	2.33	114.86	109.87
3	B	965	ANP	O1G-PG-N3B	2.12	114.89	111.77
3	B	965	ANP	O1B-PB-N3B	2.11	114.88	111.77
3	B	965	ANP	O3'-C3'-C2'	2.10	118.54	111.82
3	B	965	ANP	C3'-C2'-C1'	2.07	105.38	101.46
3	A	964	ANP	O3'-C3'-C2'	2.06	118.42	111.82
3	A	964	ANP	O2A-PA-O3A	2.05	112.82	107.27
3	B	965	ANP	C4'-O4'-C1'	2.05	113.99	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	964	ANP	PB-N3B-PG-O1G
3	A	964	ANP	PG-N3B-PB-O1B
3	A	964	ANP	PG-N3B-PB-O3A
3	A	964	ANP	PA-O3A-PB-O2B
3	B	965	ANP	PB-N3B-PG-O1G
3	B	965	ANP	PG-N3B-PB-O1B
3	B	965	ANP	PG-N3B-PB-O3A
3	B	965	ANP	PA-O3A-PB-O2B
3	A	964	ANP	PB-O3A-PA-O2A
3	B	965	ANP	PB-O3A-PA-O2A
3	B	965	ANP	PA-O3A-PB-O1B
3	A	964	ANP	PB-O3A-PA-O1A
3	B	965	ANP	PB-O3A-PA-O1A

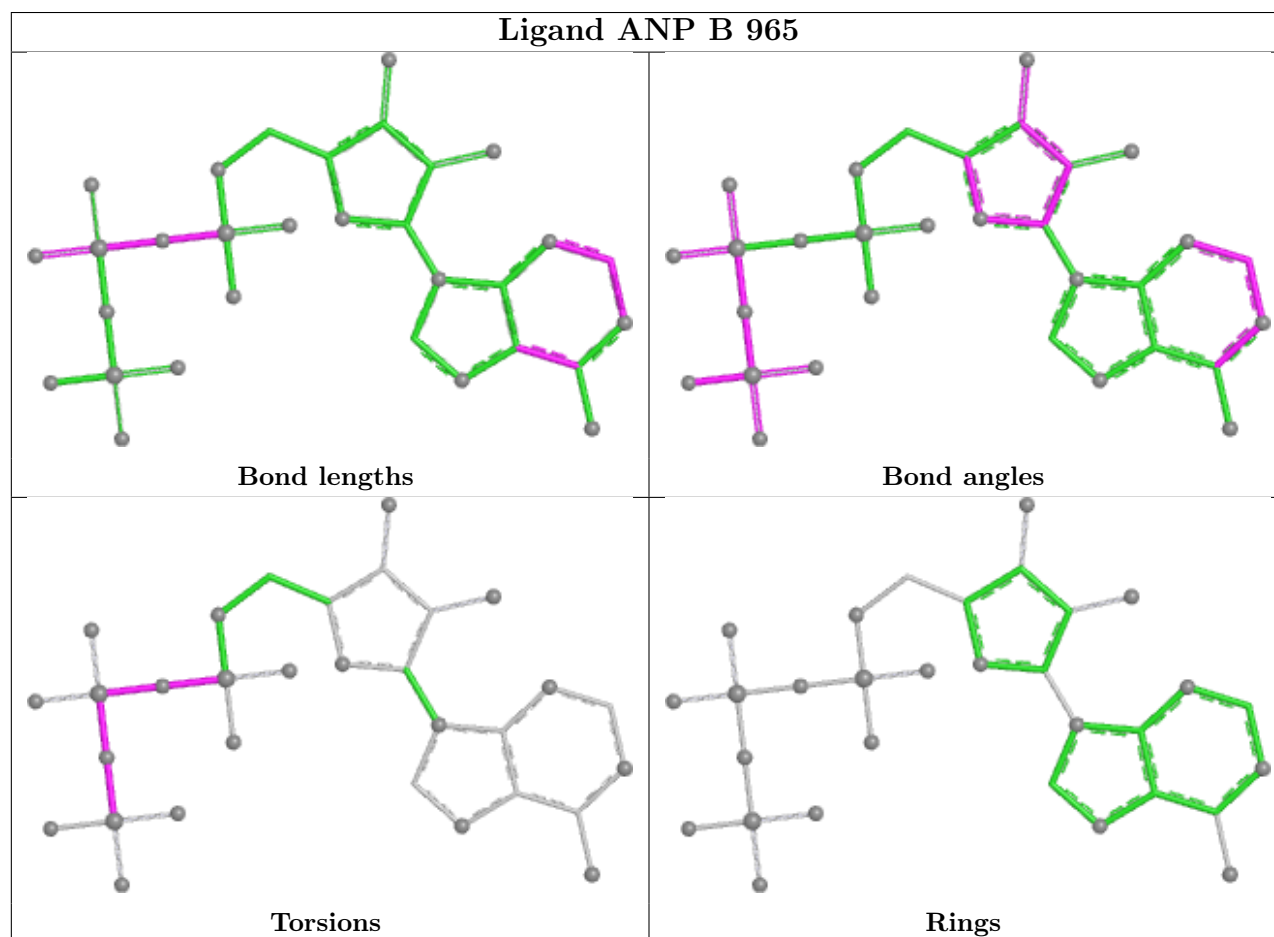
There are no ring outliers.

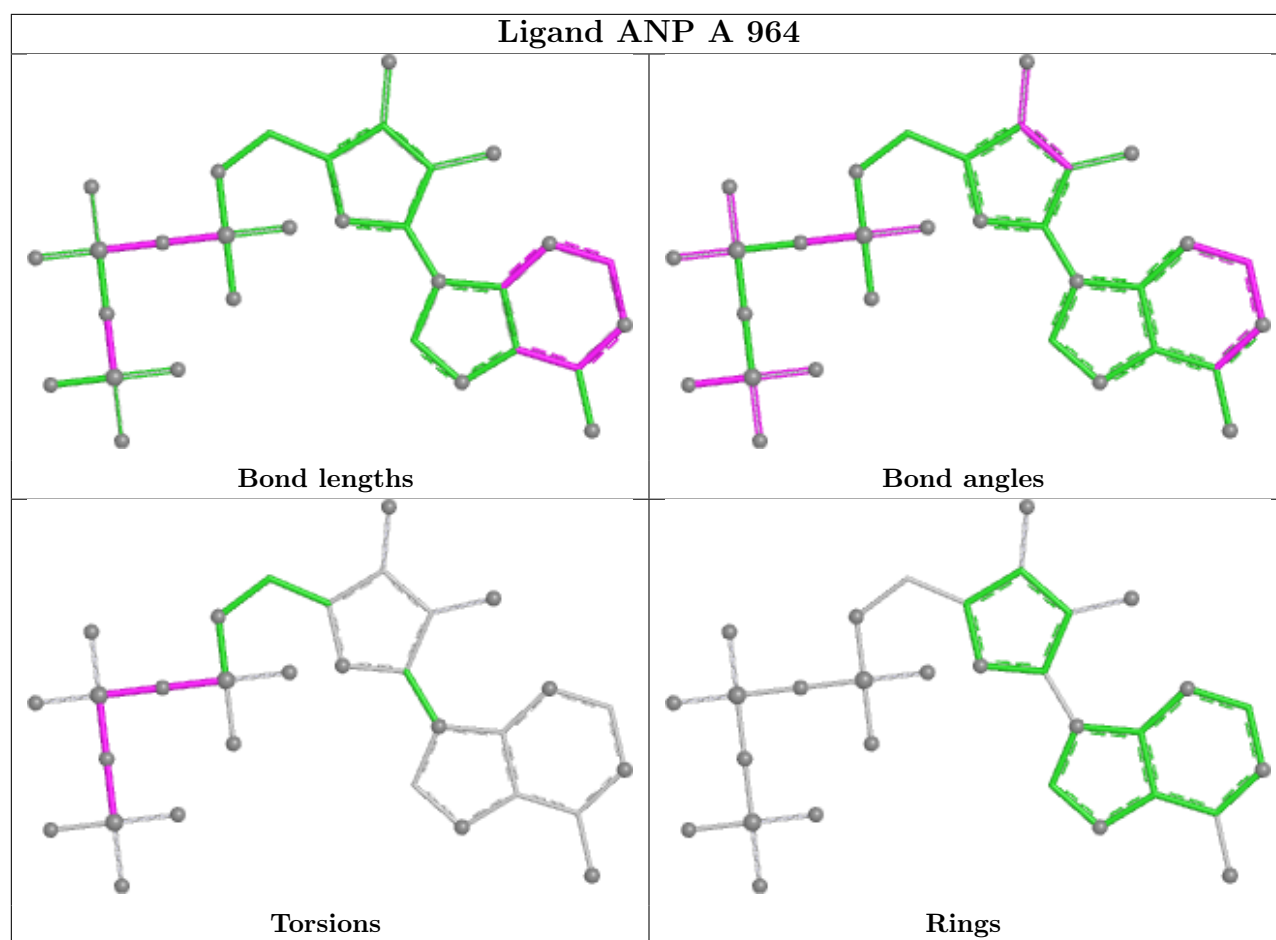
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	965	ANP	4	0
3	A	964	ANP	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	587/619 (94%)	-0.15	2 (0%) 90 89	1, 16, 38, 63	0
1	B	587/619 (94%)	-0.09	8 (1%) 73 72	1, 17, 39, 59	0
All	All	1174/1238 (94%)	-0.12	10 (0%) 81 80	1, 17, 38, 63	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ALA	4.0
1	B	43	VAL	3.1
1	B	460	ALA	2.8
1	B	461	ALA	2.7
1	B	223	ASP	2.7
1	A	30	TYR	2.6
1	B	424	ALA	2.5
1	A	28	SER	2.3
1	B	141	ASN	2.3
1	B	27	SER	2.2

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](#)

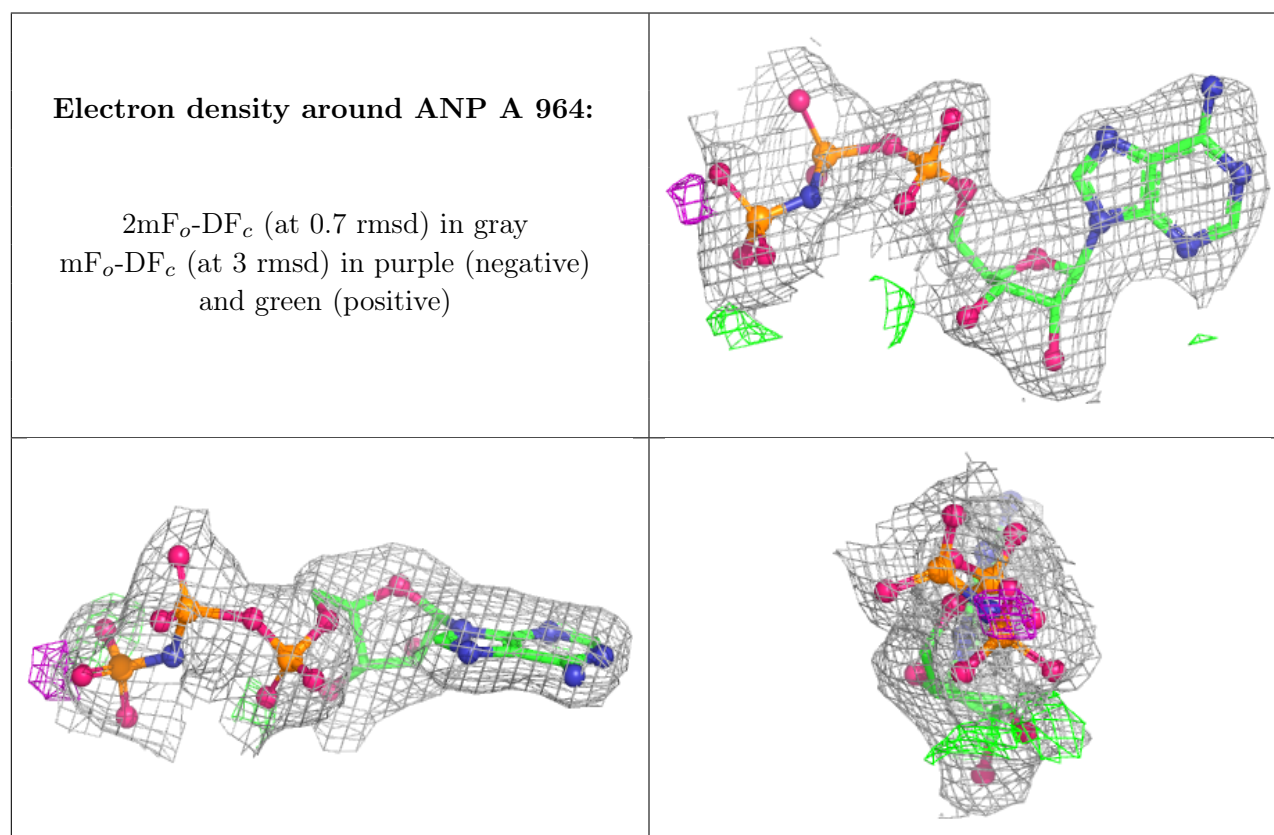
There are no oligosaccharides in this entry.

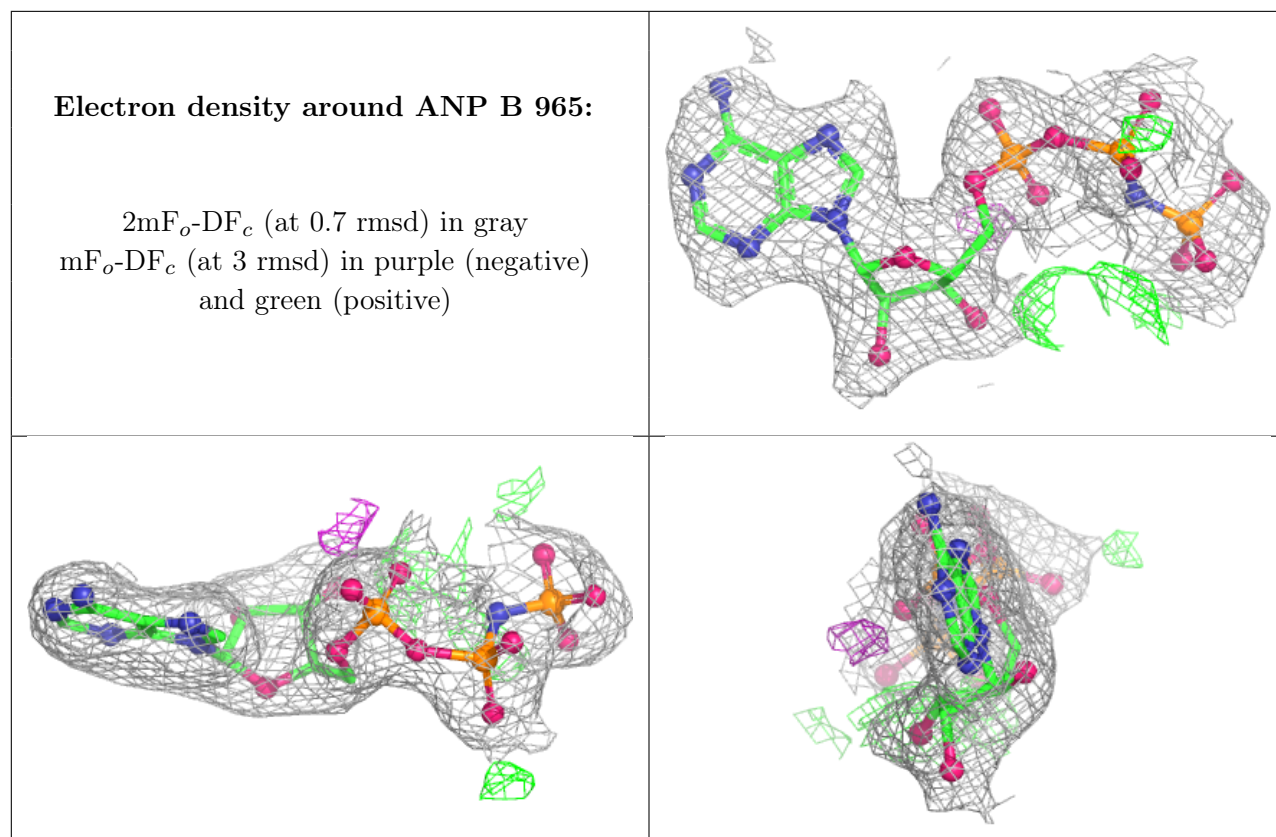
6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
2	MG	A	5002	1/1	0.95	0.06	1,1,1,1	0
2	MG	B	5004	1/1	0.95	0.05	1,1,1,1	0
2	MG	A	5001	1/1	0.97	0.04	1,1,1,1	0
3	ANP	A	964	31/31	0.97	0.07	3,8,14,15	0
3	ANP	B	965	31/31	0.97	0.06	7,13,15,16	0
2	MG	B	5003	1/1	0.98	0.05	1,1,1,1	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.