



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 07:50 PM EDT

PDB ID : 1WAJ / pdb_00001waj
Title : DNA POLYMERASE FROM BACTERIOPHAGE RB69
Authors : Wang, J.; Satter, A.K.M.A.; Wang, C.C.; Karam, J.D.; Konigsberg, W.H.;
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Deposited on : 1997-04-13
Resolution : 2.80 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

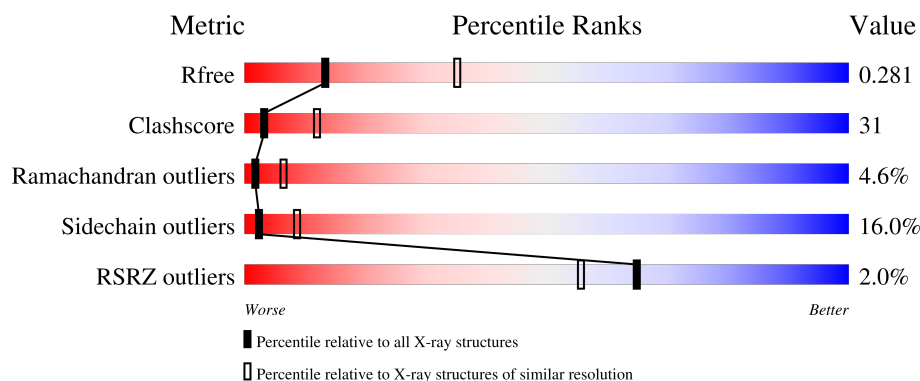
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	903	

2 Entry composition [i](#)

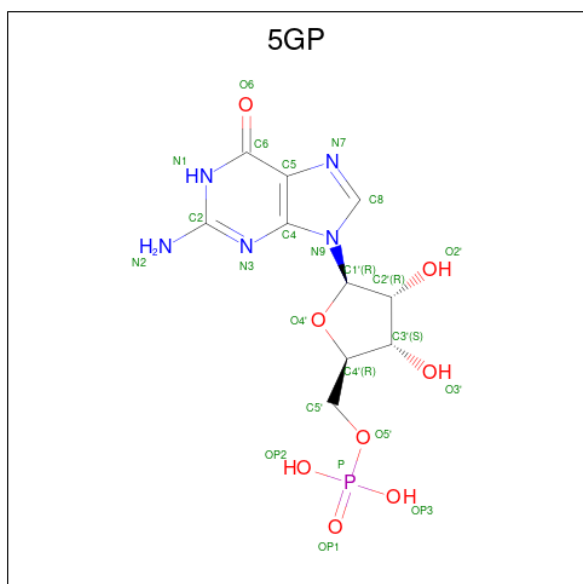
There are 3 unique types of molecules in this entry. The entry contains 7465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	903	7380	4739	1226	1382	33	0	0	0

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	24	10	5	8	1	4	0

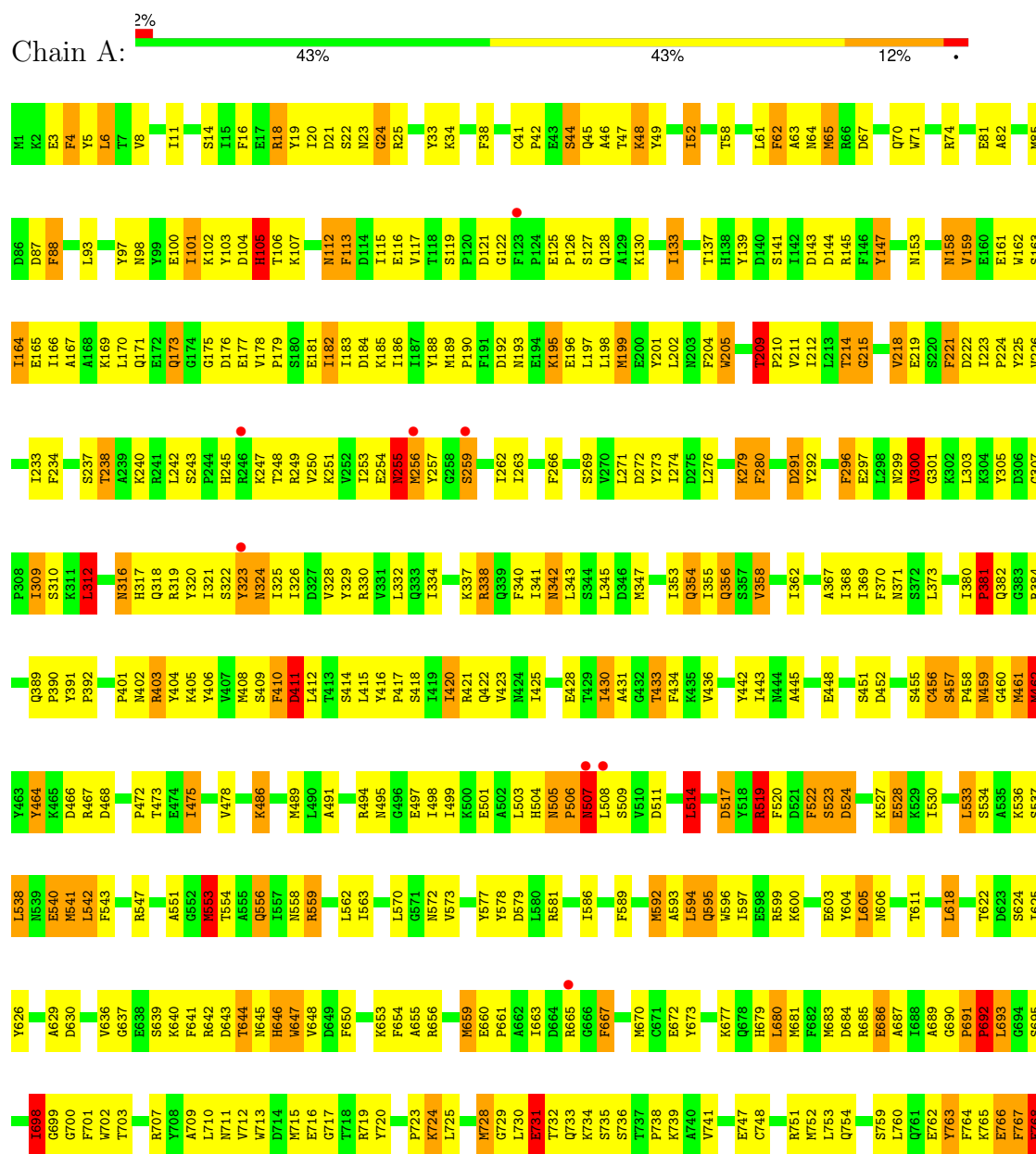
- Molecule 3 is water.

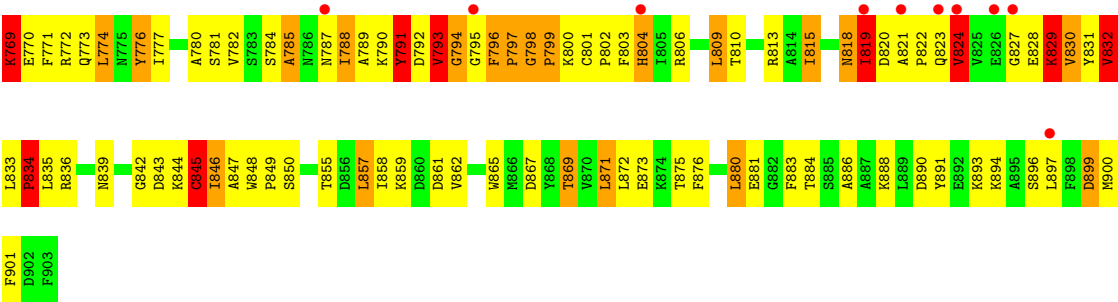
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		

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: DNA POLYMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.41Å 117.60Å 199.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.80) 85.9 (40.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.80Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , 0.280 0.223 , 0.281	Depositor DCC
R_{free} test set	2092 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7465	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: 5GP

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	0.84	6/7561 (0.1%)	1.30	91/10217 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	553	MET	SD-CE	7.57	1.98	1.79
1	A	212	ILE	CA-CB	-6.15	1.46	1.54
1	A	256	MET	SD-CE	6.08	1.94	1.79
1	A	819	ILE	CA-CB	6.07	1.62	1.54
1	A	824	VAL	CA-CB	6.00	1.60	1.54
1	A	691	PRO	CA-C	5.08	1.55	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ILE	N-CA-C	21.25	130.08	110.74
1	A	522	PHE	N-CA-C	19.17	131.58	111.07
1	A	62	PHE	N-CA-C	10.92	126.93	113.50
1	A	318	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	A	48	LYS	N-CA-C	-9.43	90.71	110.80
1	A	514	LEU	N-CA-C	9.33	124.59	110.14
1	A	209	THR	CA-C-N	9.03	128.97	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	THR	C-N-CA	9.03	128.97	120.03
1	A	380	ILE	CA-C-N	8.84	130.88	119.84
1	A	380	ILE	C-N-CA	8.84	130.88	119.84
1	A	100	GLU	N-CA-C	-8.58	99.21	110.53
1	A	731	GLU	N-CA-C	8.52	123.04	112.47
1	A	732	THR	N-CA-C	-8.38	103.04	113.18
1	A	798	GLY	CA-C-N	8.12	129.99	119.84
1	A	798	GLY	C-N-CA	8.12	129.99	119.84
1	A	833	LEU	CA-C-N	7.97	129.80	119.84
1	A	833	LEU	C-N-CA	7.97	129.80	119.84
1	A	65	MET	N-CA-C	7.82	120.79	111.33
1	A	830	VAL	N-CA-C	7.73	118.26	108.82
1	A	680	LEU	N-CA-C	7.64	127.08	110.80
1	A	256	MET	N-CA-C	-7.45	103.18	111.82
1	A	122	GLY	N-CA-C	7.26	122.93	113.27
1	A	899	ASP	N-CA-C	-7.21	100.40	110.35
1	A	389	GLN	CA-C-N	7.18	128.82	119.84
1	A	389	GLN	C-N-CA	7.18	128.82	119.84
1	A	486	LYS	N-CA-C	-7.16	103.48	111.71
1	A	828	GLU	N-CA-C	7.14	119.25	108.46
1	A	896	SER	N-CA-C	-7.14	97.96	109.96
1	A	839	ASN	CA-C-N	7.12	128.02	120.12
1	A	839	ASN	C-N-CA	7.12	128.02	120.12
1	A	767	PHE	N-CA-C	-7.00	97.43	108.63
1	A	712	VAL	N-CA-C	6.96	118.31	108.36
1	A	457	SER	CA-C-N	6.92	128.49	119.84
1	A	457	SER	C-N-CA	6.92	128.49	119.84
1	A	538	LEU	N-CA-C	-6.86	99.09	109.79
1	A	318	GLN	CG-CD-NE2	6.65	126.38	116.40
1	A	307	GLY	CA-C-N	6.62	126.58	120.03
1	A	307	GLY	C-N-CA	6.62	126.58	120.03
1	A	794	GLY	N-CA-C	-6.59	97.57	113.18
1	A	113	PHE	N-CA-C	6.57	118.93	109.14
1	A	540	GLU	N-CA-C	-6.55	104.22	111.36
1	A	106	THR	N-CA-C	-6.54	105.16	113.01
1	A	677	LYS	N-CA-C	6.47	118.41	111.36
1	A	475	ILE	CB-CA-C	-6.42	103.75	111.97
1	A	692	PRO	N-CA-C	6.39	125.63	112.47
1	A	769	LYS	N-CA-C	-6.28	103.14	111.24
1	A	785	ALA	N-CA-C	-6.28	98.93	108.67
1	A	768	GLU	N-CA-C	-6.28	97.43	110.80
1	A	456	CYS	N-CA-C	6.27	119.23	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	PHE	N-CA-C	6.22	119.04	111.82
1	A	262	ILE	N-CA-C	-6.22	99.75	108.27
1	A	698	ILE	N-CA-C	6.03	120.00	113.43
1	A	46	ALA	N-CA-C	-5.98	98.78	108.41
1	A	18	ARG	N-CA-C	-5.97	99.55	109.46
1	A	517	ASP	N-CA-C	-5.96	100.78	110.20
1	A	507	ASN	N-CA-C	5.96	123.49	110.80
1	A	573	VAL	N-CA-C	5.90	119.31	111.17
1	A	121	ASP	N-CA-C	-5.86	100.44	109.76
1	A	495	ASN	N-CA-C	-5.84	104.87	112.23
1	A	211	VAL	N-CA-C	-5.83	106.00	111.48
1	A	519	ARG	N-CA-C	5.79	117.59	111.28
1	A	215	GLY	N-CA-C	-5.78	102.17	110.38
1	A	725	LEU	N-CA-C	5.75	118.16	107.99
1	A	182	ILE	CB-CA-C	-5.73	104.56	112.24
1	A	624	SER	N-CA-C	5.67	118.46	109.50
1	A	305	TYR	N-CA-C	5.64	117.42	108.79
1	A	279	LYS	N-CA-C	5.58	118.56	111.69
1	A	269	SER	N-CA-C	5.55	118.35	107.57
1	A	159	VAL	N-CA-C	5.55	115.30	108.53
1	A	158	ASN	N-CA-C	-5.49	102.39	110.52
1	A	133	ILE	N-CA-C	-5.48	102.45	109.30
1	A	533	LEU	N-CA-C	5.39	118.49	110.52
1	A	461	MET	N-CA-C	5.37	122.23	110.80
1	A	505	ASN	N-CA-C	-5.34	98.01	109.81
1	A	411	ASP	N-CA-C	5.30	118.04	109.40
1	A	846	ILE	CB-CA-C	-5.27	102.53	110.55
1	A	776	TYR	N-CA-C	5.24	117.40	111.11
1	A	832	VAL	CB-CA-C	-5.23	102.71	111.29
1	A	221	PHE	N-CA-C	5.22	119.12	111.34
1	A	829	LYS	N-CA-C	5.21	121.90	110.80
1	A	355	ILE	N-CA-C	5.18	115.61	110.23
1	A	354	GLN	N-CA-C	-5.13	102.69	110.28
1	A	425	ILE	N-CA-C	5.13	115.61	108.84
1	A	14	SER	N-CA-C	5.12	117.16	109.23
1	A	605	LEU	N-CA-C	5.08	117.22	111.02
1	A	691	PRO	CA-C-N	5.07	126.18	119.84
1	A	691	PRO	C-N-CA	5.07	126.18	119.84
1	A	570	LEU	N-CA-C	-5.07	105.84	111.36
1	A	179	PRO	N-CA-C	5.06	118.82	111.03
1	A	259	SER	N-CA-C	5.06	121.57	110.80
1	A	508	LEU	N-CA-C	-5.05	99.70	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	TYR	Sidechain

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	7380	0	7265	450	0
2	A	24	0	12	0	0
3	A	61	0	0	12	0
All	All	7465	0	7277	450	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 31.

All (450) 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:593:ALA:HA	1:A:670:MET:HE1	1.35	1.09
1:A:253:ILE:HG22	1:A:254:GLU:H	1.05	1.07
1:A:752:MET:HG2	1:A:760:LEU:HD12	1.45	0.98
1:A:253:ILE:CG2	1:A:254:GLU:H	1.80	0.94
1:A:52:ILE:HD13	1:A:52:ILE:H	1.32	0.93
1:A:643:ASP:HB3	1:A:646:HIS:HB3	1.52	0.91
1:A:253:ILE:HG22	1:A:254:GLU:N	1.74	0.89
1:A:431:ALA:HA	1:A:464:TYR:HE1	1.39	0.88
1:A:188:TYR:HE1	1:A:190:PRO:HG3	1.37	0.88
1:A:116:GLU:HG3	1:A:324:ASN:HD21	1.39	0.87
1:A:597:ILE:HB	1:A:667:PHE:HE1	1.40	0.85
1:A:11:ILE:HD13	1:A:16:PHE:HD2	1.41	0.85
1:A:791:TYR:OH	1:A:801:CYS:HA	1.77	0.84
1:A:254:GLU:O	1:A:255:ASN:HB2	1.78	0.81
1:A:214:THR:HG22	1:A:215:GLY:H	1.44	0.80
1:A:356:GLN:NE2	1:A:356:GLN:H	1.79	0.80
1:A:356:GLN:H	1:A:356:GLN:HE21	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:H	1:A:541:MET:HE1	1.45	0.80
1:A:214:THR:HG21	1:A:273:TYR:HD2	1.48	0.79
1:A:830:VAL:HG12	1:A:831:TYR:N	1.97	0.79
1:A:832:VAL:HA	1:A:846:ILE:O	1.81	0.79
1:A:233:ILE:HG13	1:A:234:PHE:CD1	2.17	0.79
1:A:643:ASP:HB3	1:A:646:HIS:CB	2.14	0.78
1:A:511:ASP:HB2	3:A:905:HOH:O	1.82	0.77
1:A:162:TRP:HB3	1:A:188:TYR:CE2	2.20	0.77
1:A:667:PHE:CE2	1:A:681:MET:HB3	2.19	0.76
1:A:330:ARG:O	1:A:334:ILE:HG13	1.85	0.76
1:A:34:LYS:HD2	1:A:63:ALA:HA	1.66	0.76
1:A:647:TRP:CD1	1:A:648:VAL:N	2.54	0.76
1:A:700:GLY:HA3	1:A:710:LEU:HD23	1.67	0.76
1:A:663:ILE:HG21	1:A:683:MET:HE2	1.71	0.73
1:A:405:LYS:HA	1:A:698:ILE:O	1.88	0.72
1:A:834:PRO:O	1:A:835:LEU:HB2	1.87	0.72
1:A:522:PHE:O	1:A:523:SER:HB3	1.88	0.71
1:A:809:LEU:O	1:A:813:ARG:HG3	1.90	0.71
1:A:739:LYS:HG2	3:A:951:HOH:O	1.90	0.71
1:A:272:ASP:OD1	1:A:274:ILE:HG22	1.90	0.71
1:A:356:GLN:HE21	1:A:356:GLN:N	1.87	0.71
1:A:713:TRP:CZ3	1:A:723:PRO:HG3	2.25	0.71
1:A:193:ASN:HD21	1:A:195:LYS:HB2	1.57	0.70
1:A:489:MET:SD	1:A:553:MET:CB	2.79	0.70
1:A:52:ILE:H	1:A:52:ILE:CD1	2.03	0.70
1:A:218:VAL:HG13	1:A:223:ILE:HD11	1.73	0.70
1:A:830:VAL:HG11	1:A:847:ALA:HB1	1.73	0.70
1:A:52:ILE:HD13	1:A:52:ILE:N	2.07	0.70
1:A:796:PHE:CD2	1:A:797:PRO:HD2	2.27	0.70
1:A:41:CYS:SG	1:A:45:GLN:HG3	2.32	0.69
1:A:296:PHE:C	1:A:296:PHE:CD1	2.68	0.69
1:A:796:PHE:HD2	1:A:797:PRO:HD2	1.56	0.69
1:A:830:VAL:HG12	1:A:831:TYR:H	1.58	0.69
1:A:830:VAL:CG1	1:A:847:ALA:HB1	2.22	0.69
1:A:489:MET:SD	1:A:553:MET:HB3	2.33	0.69
1:A:597:ILE:HD13	1:A:667:PHE:HD1	1.58	0.68
1:A:404:TYR:CZ	1:A:618:LEU:HD21	2.28	0.68
1:A:787:ASN:C	1:A:789:ALA:H	1.99	0.68
1:A:173:GLN:HE21	1:A:173:GLN:N	1.91	0.68
1:A:112:ASN:C	1:A:112:ASN:HD22	2.01	0.68
1:A:597:ILE:HD13	1:A:667:PHE:CD1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:HE21	1:A:130:LYS:HD2	1.58	0.67
1:A:653:LYS:HD2	1:A:656:ARG:NH1	2.10	0.67
1:A:504:HIS:O	1:A:506:PRO:HD3	1.94	0.67
1:A:205:TRP:HZ3	1:A:242:LEU:O	1.77	0.66
1:A:499:ILE:HG21	1:A:542:LEU:HB2	1.77	0.66
1:A:188:TYR:CE1	1:A:190:PRO:HG3	2.26	0.66
1:A:788:ILE:HG22	1:A:791:TYR:HB3	1.77	0.66
1:A:794:GLY:C	1:A:796:PHE:H	2.01	0.66
1:A:596:TRP:CG	1:A:670:MET:HE3	2.31	0.66
1:A:403:ARG:NH1	1:A:888:LYS:HB2	2.10	0.66
1:A:145:ARG:HD3	1:A:185:LYS:O	1.96	0.66
1:A:341:ILE:O	1:A:345:LEU:HD23	1.96	0.66
1:A:663:ILE:HD13	1:A:683:MET:CE	2.26	0.66
1:A:846:ILE:HG22	1:A:847:ALA:N	2.11	0.66
1:A:21:ASP:OD1	1:A:25:ARG:HB2	1.96	0.65
1:A:507:ASN:HA	1:A:534:SER:HA	1.79	0.65
1:A:785:ALA:C	1:A:787:ASN:H	2.04	0.65
1:A:431:ALA:HA	1:A:464:TYR:CE1	2.26	0.65
1:A:788:ILE:O	1:A:791:TYR:HD2	1.79	0.65
1:A:834:PRO:HB3	1:A:867:ASP:HB3	1.79	0.65
1:A:734:LYS:HG3	3:A:943:HOH:O	1.96	0.65
1:A:280:PHE:CD1	1:A:280:PHE:N	2.64	0.64
1:A:422:GLN:HE22	1:A:681:MET:HG2	1.62	0.64
1:A:530:ILE:HA	1:A:533:LEU:HD23	1.80	0.64
1:A:738:PRO:HB2	1:A:741:VAL:HG23	1.79	0.64
1:A:147:TYR:CD1	1:A:147:TYR:N	2.65	0.63
1:A:316:ASN:C	1:A:316:ASN:HD22	2.05	0.63
1:A:459:ASN:HD22	1:A:459:ASN:H	1.46	0.63
1:A:748:CYS:O	1:A:752:MET:HG3	1.98	0.63
1:A:81:GLU:HB2	3:A:924:HOH:O	1.98	0.63
1:A:414:SER:O	1:A:417:PRO:HD2	1.99	0.62
1:A:280:PHE:N	1:A:280:PHE:HD1	1.97	0.62
1:A:8:VAL:HG11	1:A:93:LEU:HD21	1.80	0.62
1:A:219:GLU:HA	1:A:223:ILE:HD12	1.81	0.62
1:A:491:ALA:HB3	1:A:519:ARG:O	2.00	0.62
1:A:489:MET:SD	1:A:553:MET:HB2	2.39	0.62
1:A:279:LYS:C	1:A:280:PHE:HD1	2.07	0.61
1:A:434:PHE:CE2	1:A:460:GLY:HA2	2.35	0.61
1:A:644:THR:HB	1:A:692:PRO:O	2.00	0.61
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.83	0.61
1:A:752:MET:CG	1:A:760:LEU:HD12	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:TRP:O	1:A:650:PHE:HB3	1.99	0.61
1:A:830:VAL:CG1	1:A:831:TYR:N	2.64	0.61
1:A:4:PHE:HD1	1:A:4:PHE:N	1.99	0.61
1:A:787:ASN:C	1:A:789:ALA:N	2.57	0.61
1:A:846:ILE:HG22	1:A:847:ALA:H	1.66	0.60
1:A:581:ARG:HG3	1:A:581:ARG:HH11	1.66	0.60
1:A:667:PHE:HE2	1:A:681:MET:HB3	1.64	0.60
1:A:647:TRP:HH2	1:A:691:PRO:O	1.84	0.60
1:A:3:GLU:HB2	1:A:20:ILE:O	2.02	0.60
1:A:391:TYR:HB2	1:A:392:PRO:HD2	1.84	0.60
1:A:685:ARG:HG2	1:A:686:GLU:N	2.16	0.60
1:A:824:VAL:HA	3:A:920:HOH:O	2.02	0.60
1:A:11:ILE:HD13	1:A:16:PHE:CD2	2.31	0.60
1:A:188:TYR:O	1:A:189:MET:HG3	2.02	0.59
1:A:362:ILE:HD11	1:A:572:ASN:HB3	1.84	0.59
1:A:328:VAL:O	1:A:332:LEU:HD23	2.03	0.59
1:A:831:TYR:CE2	1:A:850:SER:HA	2.36	0.59
1:A:342:ASN:O	1:A:345:LEU:HB2	2.03	0.59
1:A:445:ALA:HA	1:A:673:TYR:CE2	2.38	0.58
1:A:4:PHE:N	1:A:4:PHE:CD1	2.71	0.58
1:A:835:LEU:HD21	1:A:846:ILE:HG13	1.84	0.58
1:A:162:TRP:HB3	1:A:188:TYR:HE2	1.67	0.58
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.85	0.58
1:A:685:ARG:NH2	1:A:717:GLY:H	2.00	0.57
1:A:667:PHE:CD2	1:A:681:MET:HB3	2.39	0.57
1:A:803:PHE:O	1:A:806:ARG:HB3	2.03	0.57
1:A:443:ILE:HG22	1:A:592:MET:HG3	1.86	0.57
1:A:647:TRP:CD1	1:A:647:TRP:C	2.82	0.57
1:A:799:PRO:O	1:A:800:LYS:HB2	2.05	0.57
1:A:536:LYS:O	1:A:536:LYS:HD3	2.05	0.56
1:A:821:ALA:N	1:A:822:PRO:HD2	2.20	0.56
1:A:788:ILE:O	1:A:791:TYR:CD2	2.56	0.56
1:A:170:LEU:HB2	1:A:173:GLN:NE2	2.21	0.56
1:A:325:ILE:HD12	1:A:325:ILE:H	1.70	0.56
1:A:347:MET:HA	1:A:558:ASN:HD21	1.71	0.56
1:A:835:LEU:HA	1:A:865:TRP:O	2.06	0.56
1:A:234:PHE:HB3	1:A:238:THR:HG21	1.87	0.56
1:A:713:TRP:CH2	1:A:723:PRO:HG3	2.40	0.56
1:A:147:TYR:N	1:A:147:TYR:HD1	2.04	0.55
1:A:410:PHE:CD1	1:A:410:PHE:N	2.74	0.55
1:A:781:SER:O	1:A:831:TYR:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ASN:O	1:A:822:PRO:HD3	2.06	0.55
1:A:818:ASN:HA	1:A:822:PRO:HG3	1.88	0.55
1:A:728:MET:HE2	1:A:729:GLY:H	1.71	0.55
1:A:434:PHE:CZ	1:A:460:GLY:HA2	2.40	0.55
1:A:832:VAL:HG22	1:A:847:ALA:HB2	1.87	0.55
1:A:163:SER:OG	1:A:166:ILE:HG13	2.07	0.55
1:A:408:MET:HE1	1:A:655:ALA:HB2	1.88	0.55
1:A:830:VAL:CG1	1:A:831:TYR:H	2.17	0.55
1:A:857:LEU:HD23	1:A:857:LEU:H	1.72	0.55
1:A:198:LEU:HD12	1:A:233:ILE:HD11	1.88	0.55
1:A:701:PHE:CE1	1:A:709:ALA:HB3	2.42	0.55
1:A:303:LEU:HD23	1:A:323:TYR:HB2	1.87	0.54
1:A:128:GLN:HG2	1:A:130:LYS:HG3	1.88	0.54
1:A:249:ARG:HD2	1:A:251:LYS:HE3	1.89	0.54
1:A:472:PRO:HA	1:A:475:ILE:HD12	1.90	0.54
1:A:403:ARG:O	1:A:403:ARG:HG2	2.05	0.54
1:A:459:ASN:HD22	1:A:459:ASN:N	2.02	0.54
1:A:347:MET:HE2	1:A:358:VAL:HG13	1.88	0.54
1:A:195:LYS:O	1:A:199:MET:HB2	2.07	0.54
1:A:719:ARG:HG3	1:A:720:TYR:N	2.22	0.54
1:A:338:ARG:HG3	1:A:340:PHE:CE1	2.43	0.53
1:A:793:VAL:C	1:A:795:GLY:H	2.13	0.53
1:A:653:LYS:HD2	1:A:656:ARG:HH12	1.73	0.53
1:A:685:ARG:HG2	1:A:686:GLU:H	1.72	0.53
1:A:832:VAL:H	1:A:847:ALA:HA	1.73	0.53
1:A:442:TYR:HB3	1:A:592:MET:HE3	1.91	0.53
1:A:514:LEU:N	1:A:541:MET:HE1	2.18	0.53
1:A:524:ASP:HA	1:A:527:LYS:HB2	1.90	0.53
1:A:767:PHE:HA	1:A:770:GLU:HG2	1.90	0.53
1:A:193:ASN:ND2	1:A:195:LYS:HB2	2.22	0.53
1:A:810:THR:HG21	1:A:845:CYS:O	2.09	0.53
1:A:820:ASP:C	1:A:822:PRO:HD2	2.33	0.53
1:A:171:GLN:HG2	1:A:177:GLU:OE2	2.08	0.53
1:A:4:PHE:CE2	1:A:103:TYR:HA	2.44	0.53
1:A:790:LYS:O	1:A:792:ASP:N	2.42	0.53
1:A:594:LEU:O	1:A:597:ILE:HG22	2.09	0.53
1:A:164:ILE:HG13	3:A:963:HOH:O	2.07	0.52
1:A:897:LEU:H	1:A:897:LEU:HD12	1.73	0.52
1:A:504:HIS:C	1:A:506:PRO:HD3	2.34	0.52
1:A:312:LEU:HD12	1:A:320:TYR:HA	1.90	0.52
1:A:685:ARG:HH22	1:A:717:GLY:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:O	1:A:45:GLN:HG2	2.09	0.52
1:A:759:SER:O	1:A:762:GLU:HG2	2.09	0.52
1:A:836:ARG:HG3	1:A:867:ASP:HA	1.92	0.52
1:A:186:ILE:HD12	1:A:186:ILE:N	2.25	0.52
1:A:214:THR:HG21	1:A:273:TYR:CD2	2.37	0.52
1:A:263:ILE:HD12	1:A:263:ILE:N	2.25	0.52
1:A:416:TYR:O	1:A:420:ILE:HD12	2.10	0.52
1:A:772:ARG:HG3	1:A:772:ARG:HH11	1.74	0.52
1:A:834:PRO:CB	1:A:867:ASP:HB3	2.40	0.52
1:A:577:TYR:N	1:A:577:TYR:CD1	2.78	0.52
1:A:115:ILE:HD11	1:A:221:PHE:HE1	1.75	0.52
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.45	0.52
1:A:443:ILE:HD12	1:A:595:GLN:HB2	1.92	0.52
1:A:104:ASP:OD2	1:A:107:LYS:HG3	2.10	0.51
1:A:410:PHE:HB3	1:A:683:MET:HG2	1.91	0.51
1:A:82:ALA:HB3	3:A:935:HOH:O	2.08	0.51
1:A:33:TYR:HB3	1:A:65:MET:HE3	1.92	0.51
1:A:64:ASN:O	1:A:67:ASP:HB2	2.10	0.51
1:A:178:VAL:O	1:A:183:ILE:HD11	2.11	0.51
1:A:218:VAL:O	1:A:223:ILE:HG13	2.09	0.51
1:A:233:ILE:C	1:A:234:PHE:HD1	2.17	0.51
1:A:303:LEU:HD23	1:A:323:TYR:CA	2.40	0.51
1:A:536:LYS:HD3	1:A:536:LYS:C	2.35	0.51
1:A:604:TYR:HD1	1:A:605:LEU:HD23	1.75	0.51
1:A:296:PHE:C	1:A:296:PHE:HD1	2.18	0.51
1:A:618:LEU:HB3	1:A:626:TYR:O	2.11	0.51
1:A:763:TYR:CD1	1:A:763:TYR:C	2.89	0.51
1:A:796:PHE:HB3	1:A:797:PRO:HD2	1.93	0.50
1:A:869:THR:O	1:A:873:GLU:HG3	2.10	0.50
1:A:6:LEU:HB2	1:A:18:ARG:O	2.11	0.50
1:A:169:LYS:HB2	1:A:175:GLY:HA3	1.92	0.50
1:A:309:ILE:HD13	1:A:309:ILE:O	2.11	0.50
1:A:604:TYR:CD1	1:A:605:LEU:HD23	2.46	0.50
1:A:173:GLN:HE21	1:A:173:GLN:H	1.60	0.50
1:A:273:TYR:OH	1:A:340:PHE:HB2	2.11	0.50
1:A:784:SER:HA	1:A:829:LYS:HA	1.94	0.50
1:A:899:ASP:C	1:A:901:PHE:H	2.20	0.50
1:A:193:ASN:OD1	1:A:196:GLU:HG3	2.12	0.50
1:A:402:ASN:HA	1:A:886:ALA:O	2.12	0.50
1:A:434:PHE:HE1	1:A:442:TYR:OH	1.94	0.50
1:A:699:GLY:O	1:A:753:LEU:HD22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ILE:HG22	1:A:819:ILE:O	2.12	0.50
1:A:736:SER:HA	1:A:782:VAL:O	2.12	0.49
1:A:119:SER:O	1:A:310:SER:HB2	2.12	0.49
1:A:686:GLU:HG3	1:A:687:ALA:H	1.78	0.49
1:A:368:ILE:HG22	1:A:369:ILE:N	2.27	0.49
1:A:415:LEU:O	1:A:416:TYR:C	2.55	0.49
1:A:112:ASN:HD22	1:A:113:PHE:N	2.10	0.49
1:A:353:ILE:HG13	1:A:354:GLN:O	2.13	0.49
1:A:411:ASP:O	1:A:683:MET:HA	2.12	0.49
1:A:5:TYR:HA	1:A:19:TYR:HB2	1.94	0.49
1:A:464:TYR:HD1	1:A:464:TYR:H	1.60	0.49
1:A:763:TYR:C	1:A:763:TYR:HD1	2.21	0.49
1:A:205:TRP:CZ3	1:A:242:LEU:O	2.63	0.49
1:A:62:PHE:O	1:A:63:ALA:HB3	2.12	0.49
1:A:199:MET:HE2	1:A:234:PHE:CE2	2.48	0.49
1:A:459:ASN:H	1:A:459:ASN:ND2	2.10	0.49
1:A:606:ASN:HB2	1:A:611:THR:OG1	2.13	0.49
1:A:245:HIS:HE1	3:A:915:HOH:O	1.96	0.49
1:A:551:ALA:O	1:A:554:THR:HG22	2.13	0.49
1:A:165:GLU:CD	1:A:165:GLU:H	2.20	0.48
1:A:85:MET:HG3	1:A:87:ASP:O	2.12	0.48
1:A:186:ILE:H	1:A:186:ILE:CD1	2.26	0.48
1:A:461:MET:HE1	1:A:581:ARG:HD2	1.94	0.48
1:A:703:THR:HG22	1:A:707:ARG:HH11	1.79	0.48
1:A:819:ILE:O	1:A:820:ASP:HB2	2.12	0.48
1:A:186:ILE:HD12	1:A:186:ILE:H	1.77	0.48
1:A:728:MET:HE2	1:A:729:GLY:N	2.27	0.48
1:A:771:PHE:HZ	1:A:871:LEU:HD13	1.77	0.48
1:A:402:ASN:OD1	1:A:888:LYS:HE2	2.14	0.48
1:A:403:ARG:HH11	1:A:888:LYS:HB2	1.78	0.48
1:A:533:LEU:HB3	1:A:538:LEU:HG	1.96	0.48
1:A:199:MET:HE2	1:A:234:PHE:HE2	1.78	0.48
1:A:370:PHE:CD1	1:A:370:PHE:C	2.92	0.48
1:A:354:GLN:HG3	3:A:936:HOH:O	2.13	0.48
1:A:300:VAL:HG23	1:A:301:GLY:H	1.78	0.47
1:A:689:ALA:HB1	1:A:711:ASN:O	2.14	0.47
1:A:6:LEU:HD21	1:A:20:ILE:HG12	1.96	0.47
1:A:116:GLU:HG3	1:A:324:ASN:ND2	2.20	0.47
1:A:329:TYR:O	1:A:332:LEU:HB2	2.14	0.47
1:A:402:ASN:CG	1:A:403:ARG:H	2.22	0.47
1:A:553:MET:HG3	1:A:554:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:GLN:HA	3:A:962:HOH:O	2.13	0.47
1:A:642:ARG:O	1:A:643:ASP:HB2	2.14	0.47
1:A:843:ASP:O	1:A:844:LYS:HG3	2.14	0.47
1:A:883:PHE:N	1:A:883:PHE:CD1	2.79	0.47
1:A:104:ASP:CG	1:A:107:LYS:HG3	2.40	0.47
1:A:796:PHE:CB	1:A:797:PRO:HD2	2.44	0.47
1:A:221:PHE:CD1	1:A:221:PHE:C	2.92	0.47
1:A:663:ILE:HD13	1:A:683:MET:HE3	1.95	0.47
1:A:8:VAL:HG23	1:A:354:GLN:HE21	1.80	0.47
1:A:71:TRP:O	1:A:74:ARG:HB3	2.15	0.47
1:A:489:MET:CG	1:A:553:MET:HB3	2.44	0.47
1:A:20:ILE:CG2	1:A:24:GLY:HA2	2.44	0.47
1:A:24:GLY:HA3	1:A:107:LYS:HE3	1.97	0.47
1:A:117:VAL:HG22	1:A:133:ILE:HA	1.96	0.47
1:A:181:GLU:OE1	1:A:181:GLU:N	2.48	0.47
1:A:597:ILE:CB	1:A:667:PHE:HE1	2.20	0.47
1:A:466:ASP:CG	1:A:467:ARG:H	2.23	0.46
1:A:188:TYR:HE1	1:A:190:PRO:CG	2.18	0.46
1:A:214:THR:HG23	1:A:271:LEU:O	2.15	0.46
1:A:198:LEU:O	1:A:199:MET:C	2.59	0.46
1:A:489:MET:HG3	1:A:553:MET:HB3	1.96	0.46
1:A:836:ARG:NH1	1:A:865:TRP:HA	2.30	0.46
1:A:597:ILE:HB	1:A:667:PHE:CE1	2.32	0.46
1:A:667:PHE:CD2	1:A:681:MET:CB	2.99	0.46
1:A:679:HIS:O	1:A:681:MET:N	2.47	0.46
1:A:876:PHE:O	1:A:880:LEU:HB2	2.14	0.46
1:A:125:GLU:HB2	1:A:128:GLN:CD	2.40	0.46
1:A:791:TYR:OH	1:A:802:PRO:HD3	2.15	0.46
1:A:815:ILE:HA	1:A:815:ILE:HD12	1.72	0.46
1:A:836:ARG:HH11	1:A:865:TRP:HA	1.80	0.46
1:A:167:ALA:HA	1:A:176:ASP:HB2	1.97	0.46
1:A:643:ASP:O	1:A:646:HIS:HB3	2.16	0.46
1:A:321:ILE:O	1:A:325:ILE:HD12	2.15	0.45
1:A:464:TYR:CD1	1:A:464:TYR:N	2.85	0.45
1:A:528:GLU:C	1:A:530:ILE:N	2.71	0.45
1:A:249:ARG:CD	1:A:251:LYS:HE3	2.45	0.45
1:A:254:GLU:O	1:A:257:TYR:HD2	1.99	0.45
1:A:457:SER:HB3	1:A:459:ASN:ND2	2.31	0.45
1:A:821:ALA:N	1:A:822:PRO:CD	2.80	0.45
1:A:125:GLU:HB2	1:A:128:GLN:NE2	2.30	0.45
1:A:332:LEU:HD13	1:A:332:LEU:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:GLU:HB3	1:A:763:TYR:CE2	2.51	0.45
1:A:291:ASP:HB2	1:A:292:TYR:H	1.49	0.45
1:A:65:MET:HE2	1:A:88:PHE:HB3	1.99	0.45
1:A:405:LYS:O	1:A:690:GLY:HA2	2.16	0.45
1:A:629:ALA:O	1:A:630:ASP:C	2.60	0.45
1:A:751:ARG:NE	1:A:763:TYR:HD2	2.15	0.45
1:A:316:ASN:C	1:A:316:ASN:ND2	2.73	0.45
1:A:431:ALA:HB2	1:A:464:TYR:CD1	2.51	0.45
1:A:733:GLN:O	1:A:734:LYS:C	2.60	0.45
1:A:455:SER:O	1:A:462:MET:HA	2.15	0.45
1:A:402:ASN:ND2	1:A:403:ARG:H	2.14	0.45
1:A:597:ILE:HD12	1:A:600:LYS:HB2	1.99	0.45
1:A:767:PHE:CD1	1:A:767:PHE:C	2.95	0.45
1:A:253:ILE:O	1:A:254:GLU:HG3	2.16	0.45
1:A:589:PHE:CD1	1:A:589:PHE:C	2.95	0.45
1:A:844:LYS:O	1:A:845:CYS:HB3	2.16	0.45
1:A:163:SER:HB3	1:A:166:ILE:HD12	1.99	0.44
1:A:169:LYS:HB2	1:A:175:GLY:CA	2.48	0.44
1:A:5:TYR:HA	1:A:19:TYR:CB	2.48	0.44
1:A:533:LEU:HD12	1:A:537:SER:HB2	1.99	0.44
1:A:785:ALA:C	1:A:787:ASN:N	2.73	0.44
1:A:792:ASP:O	1:A:793:VAL:C	2.60	0.44
1:A:115:ILE:HD12	1:A:115:ILE:C	2.43	0.44
1:A:143:ASP:O	1:A:144:ASP:HB3	2.17	0.44
1:A:169:LYS:C	1:A:175:GLY:HA3	2.43	0.44
1:A:491:ALA:HA	1:A:494:ARG:HH21	1.82	0.44
1:A:686:GLU:O	1:A:715:MET:HA	2.17	0.44
1:A:699:GLY:C	1:A:753:LEU:HD22	2.43	0.44
1:A:771:PHE:O	1:A:774:LEU:HG	2.16	0.44
1:A:322:SER:O	1:A:326:ILE:HG12	2.17	0.44
1:A:578:TYR:CG	1:A:579:ASP:N	2.85	0.44
1:A:641:PHE:HA	1:A:646:HIS:CE1	2.52	0.44
1:A:644:THR:HG23	1:A:645:ASN:H	1.82	0.44
1:A:18:ARG:NH2	1:A:210:PRO:O	2.51	0.44
1:A:153:ASN:HB2	1:A:192:ASP:O	2.18	0.44
1:A:369:ILE:O	1:A:370:PHE:C	2.59	0.44
1:A:422:GLN:HE21	1:A:422:GLN:HB2	1.60	0.44
1:A:497:GLU:OE1	1:A:497:GLU:HA	2.18	0.44
1:A:604:TYR:CD1	1:A:604:TYR:C	2.96	0.44
1:A:692:PRO:O	1:A:693:LEU:CB	2.65	0.44
1:A:695:SER:HB2	1:A:754:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:N	1:A:158:ASN:HD22	2.15	0.44
1:A:247:LYS:HB3	1:A:266:PHE:CD2	2.52	0.43
1:A:430:ILE:HG23	1:A:430:ILE:O	2.17	0.43
1:A:538:LEU:O	1:A:540:GLU:N	2.45	0.43
1:A:760:LEU:HD23	1:A:760:LEU:C	2.43	0.43
1:A:433:THR:CG2	1:A:434:PHE:N	2.80	0.43
1:A:686:GLU:HG3	1:A:687:ALA:N	2.33	0.43
1:A:137:THR:OG1	1:A:324:ASN:HB3	2.18	0.43
1:A:247:LYS:O	1:A:266:PHE:HB2	2.19	0.43
1:A:457:SER:HA	1:A:458:PRO:HD3	1.79	0.43
1:A:20:ILE:HG23	1:A:24:GLY:HA2	1.99	0.43
1:A:406:TYR:HB3	1:A:629:ALA:HB3	1.99	0.43
1:A:724:LYS:NZ	1:A:724:LYS:HB3	2.34	0.43
1:A:692:PRO:HG3	1:A:713:TRP:CZ2	2.54	0.43
1:A:256:MET:HE2	1:A:788:ILE:HG12	2.00	0.43
1:A:636:VAL:HG12	1:A:636:VAL:O	2.17	0.43
1:A:647:TRP:O	1:A:650:PHE:N	2.52	0.43
1:A:741:VAL:HG13	1:A:876:PHE:HD1	1.83	0.43
1:A:303:LEU:HD21	1:A:319:ARG:HG3	2.01	0.43
1:A:254:GLU:HB3	1:A:255:ASN:H	1.49	0.43
1:A:253:ILE:CG2	1:A:254:GLU:N	2.46	0.42
1:A:367:ALA:O	1:A:371:ASN:ND2	2.52	0.42
1:A:457:SER:HB3	1:A:459:ASN:HD21	1.84	0.42
1:A:738:PRO:HG3	1:A:780:ALA:O	2.18	0.42
1:A:798:GLY:HA2	1:A:799:PRO:HD2	1.66	0.42
1:A:503:LEU:O	1:A:506:PRO:HG3	2.19	0.42
1:A:663:ILE:HD13	1:A:683:MET:HE2	2.01	0.42
1:A:702:TRP:CD1	1:A:702:TRP:N	2.87	0.42
1:A:417:PRO:O	1:A:421:ARG:HG3	2.18	0.42
1:A:464:TYR:HD1	1:A:464:TYR:N	2.16	0.42
1:A:751:ARG:HE	1:A:763:TYR:HD2	1.68	0.42
1:A:776:TYR:CE1	1:A:777:ILE:HG13	2.54	0.42
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.87	0.42
1:A:460:GLY:O	1:A:461:MET:HE2	2.19	0.42
1:A:225:TYR:O	1:A:226:VAL:C	2.62	0.42
1:A:240:LYS:NZ	1:A:248:THR:HG22	2.34	0.42
1:A:74:ARG:HA	3:A:926:HOH:O	2.18	0.42
1:A:420:ILE:HD11	1:A:586:ILE:HD13	2.01	0.42
1:A:653:LYS:HD2	1:A:653:LYS:HA	1.87	0.42
1:A:731:GLU:HB3	1:A:734:LYS:HD2	2.01	0.42
1:A:861:ASP:O	1:A:862:VAL:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.49	0.42
1:A:818:ASN:CA	1:A:822:PRO:HG3	2.50	0.42
1:A:139:TYR:CE1	1:A:141:SER:HA	2.54	0.42
1:A:475:ILE:H	1:A:475:ILE:HG13	1.70	0.42
1:A:731:GLU:CB	1:A:734:LYS:HD2	2.50	0.42
1:A:145:ARG:HE	1:A:185:LYS:HD2	1.85	0.42
1:A:201:TYR:O	1:A:204:PHE:HB3	2.19	0.42
1:A:296:PHE:HD1	1:A:296:PHE:O	2.03	0.42
1:A:846:ILE:CG2	1:A:847:ALA:N	2.80	0.42
1:A:486:LYS:HB2	1:A:556:GLN:HG3	2.02	0.42
1:A:514:LEU:N	1:A:514:LEU:HD12	2.35	0.42
1:A:774:LEU:N	1:A:774:LEU:HD23	2.35	0.42
1:A:818:ASN:O	1:A:819:ILE:HB	2.20	0.42
1:A:831:TYR:CD2	1:A:850:SER:HA	2.54	0.42
1:A:4:PHE:HA	1:A:97:TYR:CE2	2.54	0.41
1:A:47:THR:HB	1:A:48:LYS:O	2.20	0.41
1:A:105:HIS:C	1:A:107:LYS:N	2.78	0.41
1:A:654:PHE:CD1	1:A:654:PHE:C	2.98	0.41
1:A:797:PRO:HB2	1:A:798:GLY:H	1.76	0.41
1:A:881:GLU:OE1	1:A:891:TYR:HE2	2.03	0.41
1:A:893:LYS:HG2	1:A:894:LYS:O	2.19	0.41
1:A:218:VAL:CG1	1:A:219:GLU:N	2.82	0.41
1:A:243:SER:C	1:A:245:HIS:N	2.77	0.41
1:A:423:VAL:HA	1:A:455:SER:OG	2.19	0.41
1:A:38:PHE:CE1	1:A:49:TYR:CD2	3.09	0.41
1:A:167:ALA:HA	1:A:176:ASP:OD2	2.20	0.41
1:A:182:ILE:O	1:A:185:LYS:HB2	2.20	0.41
1:A:517:ASP:OD1	1:A:519:ARG:NE	2.53	0.41
1:A:542:LEU:O	1:A:543:PHE:C	2.63	0.41
1:A:420:ILE:HG21	1:A:475:ILE:HD11	2.02	0.41
1:A:765:LYS:O	1:A:768:GLU:HB3	2.20	0.41
1:A:224:PRO:HA	1:A:263:ILE:HD13	2.02	0.41
1:A:793:VAL:C	1:A:795:GLY:N	2.78	0.41
1:A:858:ILE:O	1:A:859:LYS:C	2.63	0.41
1:A:125:GLU:HA	1:A:126:PRO:HD3	1.94	0.41
1:A:461:MET:CE	1:A:581:ARG:HD2	2.51	0.41
1:A:205:TRP:O	1:A:209:THR:N	2.54	0.41
1:A:221:PHE:CD1	1:A:222:ASP:N	2.89	0.41
1:A:647:TRP:CG	1:A:648:VAL:N	2.88	0.41
1:A:747:GLU:O	1:A:748:CYS:C	2.62	0.41
1:A:766:GLU:O	1:A:769:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HG22	1:A:791:TYR:CB	2.47	0.41
1:A:819:ILE:C	1:A:821:ALA:H	2.28	0.41
1:A:830:VAL:HG12	1:A:847:ALA:HB1	2.02	0.41
1:A:842:GLY:O	1:A:843:ASP:HB2	2.21	0.41
1:A:170:LEU:HD22	1:A:170:LEU:N	2.36	0.41
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.95	0.41
1:A:303:LEU:HD23	1:A:323:TYR:HA	2.02	0.41
1:A:52:ILE:HD12	1:A:381:PRO:HD3	2.03	0.40
1:A:112:ASN:C	1:A:112:ASN:ND2	2.71	0.40
1:A:343:LEU:HD23	1:A:343:LEU:C	2.47	0.40
1:A:538:LEU:HA	1:A:541:MET:HB3	2.02	0.40
1:A:559:ARG:HA	1:A:559:ARG:HD3	1.90	0.40
1:A:719:ARG:CG	1:A:720:TYR:N	2.84	0.40
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.86	0.40
1:A:848:TRP:HB2	1:A:849:PRO:CD	2.51	0.40
1:A:250:VAL:O	1:A:251:LYS:HG3	2.21	0.40
1:A:297:GLU:OE1	1:A:338:ARG:NH1	2.54	0.40
1:A:422:GLN:NE2	1:A:679:HIS:O	2.54	0.40
1:A:534:SER:N	3:A:905:HOH:O	2.53	0.40
1:A:599:ARG:O	1:A:603:GLU:HB2	2.21	0.40
1:A:409:SER:C	1:A:410:PHE:CD1	2.99	0.40
1:A:763:TYR:O	1:A:764:PHE:C	2.65	0.40
1:A:347:MET:CE	1:A:358:VAL:HG13	2.52	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	901/903 (100%)	732 (81%)	128 (14%)	41 (5%)	2 6

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	255	ASN
1	A	259	SER
1	A	300	VAL
1	A	381	PRO
1	A	451	SER
1	A	507	ASN
1	A	680	LEU
1	A	768	GLU
1	A	791	TYR
1	A	793	VAL
1	A	799	PRO
1	A	819	ILE
1	A	829	LYS
1	A	98	ASN
1	A	312	LEU
1	A	390	PRO
1	A	509	SER
1	A	622	THR
1	A	637	GLY
1	A	692	PRO
1	A	797	PRO
1	A	818	ASN
1	A	827	GLY
1	A	44	SER
1	A	291	ASP
1	A	832	VAL
1	A	102	LYS
1	A	161	GLU
1	A	316	ASN
1	A	462	MET
1	A	804	HIS
1	A	834	PRO
1	A	845	CYS
1	A	24	GLY
1	A	523	SER
1	A	659	MET
1	A	735	SER
1	A	766	GLU
1	A	401	PRO
1	A	506	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	802/802 (100%)	674 (84%)	128 (16%)	2 9

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	6	LEU
1	A	22	SER
1	A	23	ASN
1	A	44	SER
1	A	52	ILE
1	A	58	THR
1	A	61	LEU
1	A	70	GLN
1	A	101	ILE
1	A	105	HIS
1	A	112	ASN
1	A	127	SER
1	A	147	TYR
1	A	164	ILE
1	A	173	GLN
1	A	184	ASP
1	A	195	LYS
1	A	197	LEU
1	A	199	MET
1	A	205	TRP
1	A	209	THR
1	A	214	THR
1	A	218	VAL
1	A	237	SER
1	A	238	THR
1	A	255	ASN
1	A	280	PHE
1	A	296	PHE
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	300	VAL
1	A	309	ILE
1	A	312	LEU
1	A	324	ASN
1	A	337	LYS
1	A	338	ARG
1	A	342	ASN
1	A	356	GLN
1	A	358	VAL
1	A	373	LEU
1	A	381	PRO
1	A	382	GLN
1	A	384	ARG
1	A	403	ARG
1	A	410	PHE
1	A	411	ASP
1	A	412	LEU
1	A	418	SER
1	A	420	ILE
1	A	428	GLU
1	A	430	ILE
1	A	433	THR
1	A	436	VAL
1	A	448	GLU
1	A	452	ASP
1	A	456	CYS
1	A	459	ASN
1	A	462	MET
1	A	464	TYR
1	A	468	ASP
1	A	473	THR
1	A	478	VAL
1	A	498	ILE
1	A	501	GLU
1	A	505	ASN
1	A	507	ASN
1	A	514	LEU
1	A	519	ARG
1	A	520	PHE
1	A	524	ASP
1	A	528	GLU
1	A	541	MET

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Mol	Chain	Res	Type
1	A	542	LEU
1	A	547	ARG
1	A	553	MET
1	A	556	GLN
1	A	559	ARG
1	A	562	LEU
1	A	563	ILE
1	A	592	MET
1	A	594	LEU
1	A	595	GLN
1	A	618	LEU
1	A	625	ILE
1	A	639	SER
1	A	640	LYS
1	A	644	THR
1	A	646	HIS
1	A	647	TRP
1	A	659	MET
1	A	665	ARG
1	A	667	PHE
1	A	672	GLU
1	A	684	ASP
1	A	686	GLU
1	A	692	PRO
1	A	693	LEU
1	A	698	ILE
1	A	716	GLU
1	A	724	LYS
1	A	728	MET
1	A	731	GLU
1	A	763	TYR
1	A	768	GLU
1	A	769	LYS
1	A	773	GLN
1	A	774	LEU
1	A	788	ILE
1	A	791	TYR
1	A	793	VAL
1	A	796	PHE
1	A	804	HIS
1	A	809	LEU
1	A	815	ILE

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Mol	Chain	Res	Type
1	A	823	GLN
1	A	824	VAL
1	A	834	PRO
1	A	845	CYS
1	A	855	THR
1	A	857	LEU
1	A	869	THR
1	A	871	LEU
1	A	872	LEU
1	A	875	THR
1	A	880	LEU
1	A	884	THR
1	A	890	ASP
1	A	900	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	128	GLN
1	A	131	HIS
1	A	158	ASN
1	A	173	GLN
1	A	232	ASN
1	A	316	ASN
1	A	324	ASN
1	A	354	GLN
1	A	356	GLN
1	A	422	GLN
1	A	459	ASN
1	A	504	HIS
1	A	676	ASN
1	A	773	GLN
1	A	787	ASN
1	A	812	ASN

5.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	5GP	A	904	-	26,26,26	1.83	8 (30%)	39,40,40	1.78	10 (25%)

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	5GP	A	904	-	-	5/10/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	904	5GP	C5'-C4'	3.93	1.63	1.51
2	A	904	5GP	C3'-C4'	3.30	1.61	1.53
2	A	904	5GP	O4'-C1'	2.95	1.48	1.42
2	A	904	5GP	C2'-C3'	2.91	1.61	1.53
2	A	904	5GP	O6-C6	2.87	1.29	1.23
2	A	904	5GP	O3'-C3'	2.84	1.50	1.43
2	A	904	5GP	O4'-C4'	2.67	1.50	1.45
2	A	904	5GP	C5-C6	2.00	1.51	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	904	5GP	O5'-C5'-C4'	5.00	126.03	108.99
2	A	904	5GP	O6-C6-C5	3.67	136.22	126.53
2	A	904	5GP	C5'-C4'-C3'	-3.27	103.42	115.21
2	A	904	5GP	O4'-C4'-C5'	3.00	118.94	109.33
2	A	904	5GP	O4'-C1'-C2'	-2.84	100.53	106.62
2	A	904	5GP	C5-C6-N1	-2.61	106.62	113.25
2	A	904	5GP	N9-C4-N3	-2.53	120.90	125.95
2	A	904	5GP	C5-C4-N9	2.31	109.80	105.66
2	A	904	5GP	C4-C5-N7	-2.13	107.29	110.67
2	A	904	5GP	O4'-C1'-N9	2.07	113.05	108.36

There are no chirality outliers.

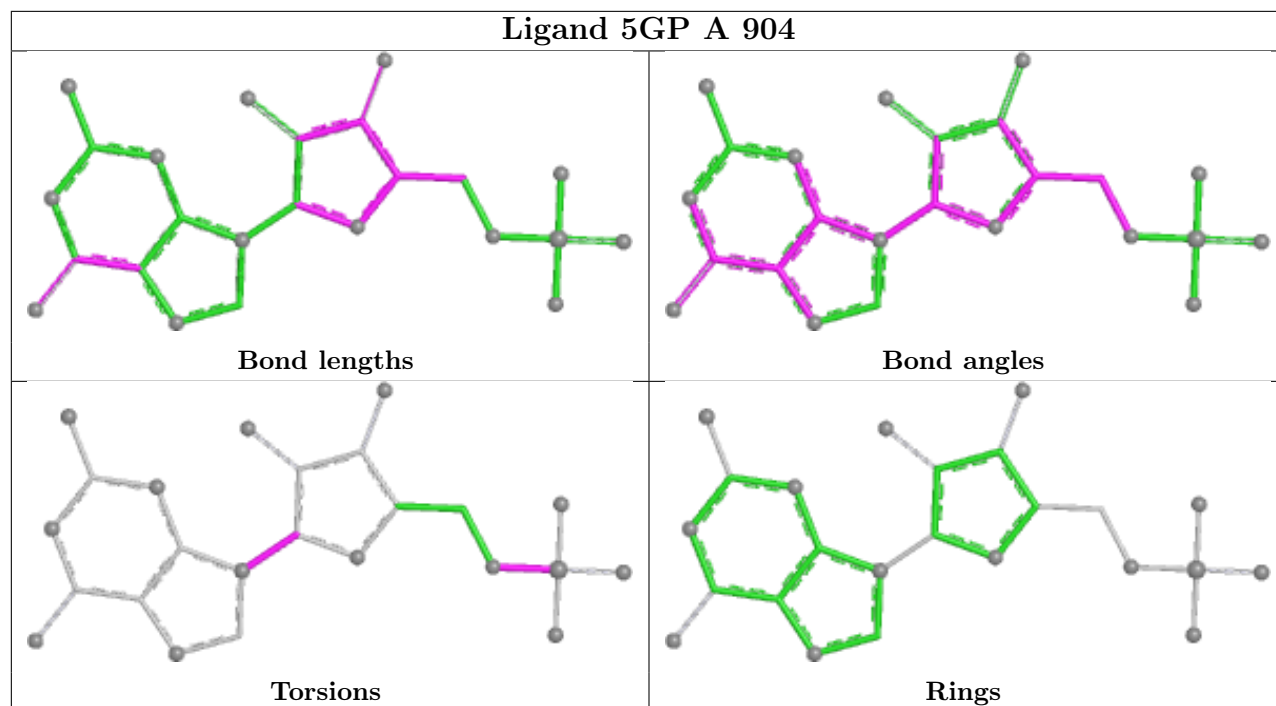
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	904	5GP	O4'-C1'-N9-C4
2	A	904	5GP	C5'-O5'-P-OP3
2	A	904	5GP	O4'-C1'-N9-C8
2	A	904	5GP	C5'-O5'-P-OP1
2	A	904	5GP	C5'-O5'-P-OP2

There are no ring outliers.

No monomer is involved in short contacts.

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	903/903 (100%)	-0.07	18 (1%) 65 56	45, 73, 100, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	ASN	4.2
1	A	821	ALA	4.0
1	A	665	ARG	3.9
1	A	826	GLU	3.7
1	A	323	TYR	3.1
1	A	827	GLY	3.0
1	A	123	PHE	2.7
1	A	819	ILE	2.6
1	A	823	GLN	2.6
1	A	256	MET	2.6
1	A	259	SER	2.5
1	A	787	ASN	2.5
1	A	246	ARG	2.4
1	A	824	VAL	2.4
1	A	804	HIS	2.4
1	A	897	LEU	2.3
1	A	795	GLY	2.1
1	A	508	LEU	2.1

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 [i](#)

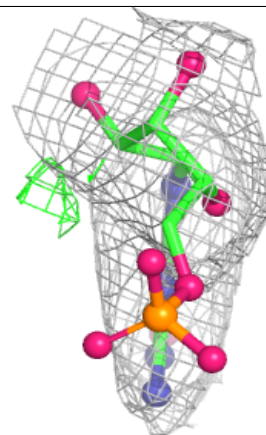
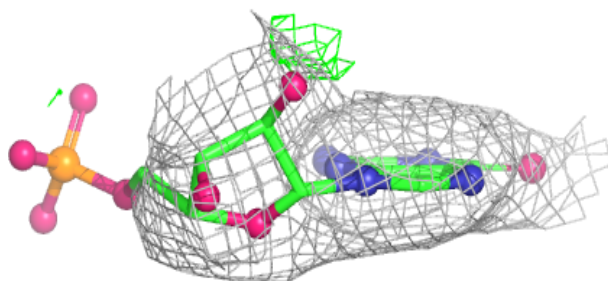
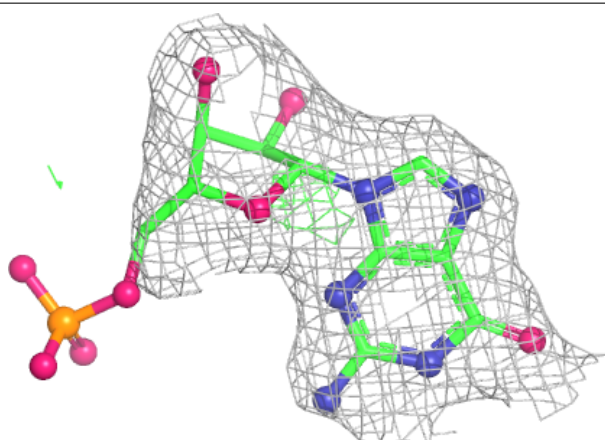
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5GP	A	904	24/24	0.93	0.10	70,72,74,74	4

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 5GP A 904:

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 ⓘ

There are no such residues in this entry.