



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:03 PM UTC

PDB ID : 5H7L / pdb_00005h7l
Title : Complex of Elongation factor 2-50S ribosomal protein L12
Authors : Tanzawa, T.; Kato, K.; Uchiumi, T.; Yao, M.
Deposited on : 2016-11-18
Resolution : 3.10 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

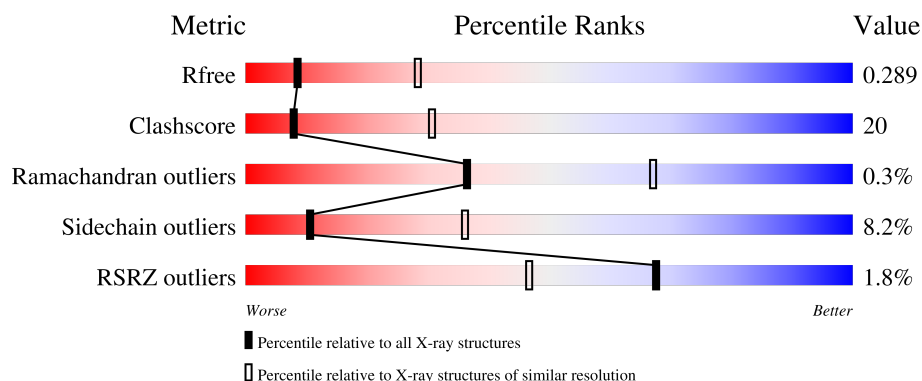
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	743	3% 52% 36% 5% 7%
1	B	743	% 56% 32% • • 7%
2	E	11	73% 9% 18%
2	G	11	64% 27% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11115 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	694	Total	C	N	O	S	0	0	0
			5476	3477	959	1006	34			
1	B	691	Total	C	N	O	S	0	0	0
			5452	3463	955	1000	34			

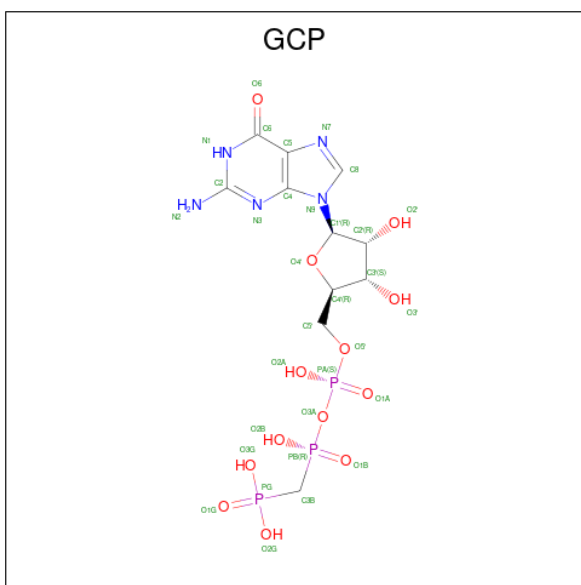
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O59521
A	2	VAL	-	expression tag	UNP O59521
A	3	GLU	-	expression tag	UNP O59521
A	736	LEU	-	expression tag	UNP O59521
A	737	GLU	-	expression tag	UNP O59521
A	738	HIS	-	expression tag	UNP O59521
A	739	HIS	-	expression tag	UNP O59521
A	740	HIS	-	expression tag	UNP O59521
A	741	HIS	-	expression tag	UNP O59521
A	742	HIS	-	expression tag	UNP O59521
A	743	HIS	-	expression tag	UNP O59521
B	1	MET	-	expression tag	UNP O59521
B	2	VAL	-	expression tag	UNP O59521
B	3	GLU	-	expression tag	UNP O59521
B	736	LEU	-	expression tag	UNP O59521
B	737	GLU	-	expression tag	UNP O59521
B	738	HIS	-	expression tag	UNP O59521
B	739	HIS	-	expression tag	UNP O59521
B	740	HIS	-	expression tag	UNP O59521
B	741	HIS	-	expression tag	UNP O59521
B	742	HIS	-	expression tag	UNP O59521
B	743	HIS	-	expression tag	UNP O59521

- Molecule 2 is a protein called 50S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	10	Total 64	C 43	N 10	O 11	0	0	0
2	E	9	Total 59	C 40	N 9	O 10	0	0	0

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{13}\text{P}_3$).

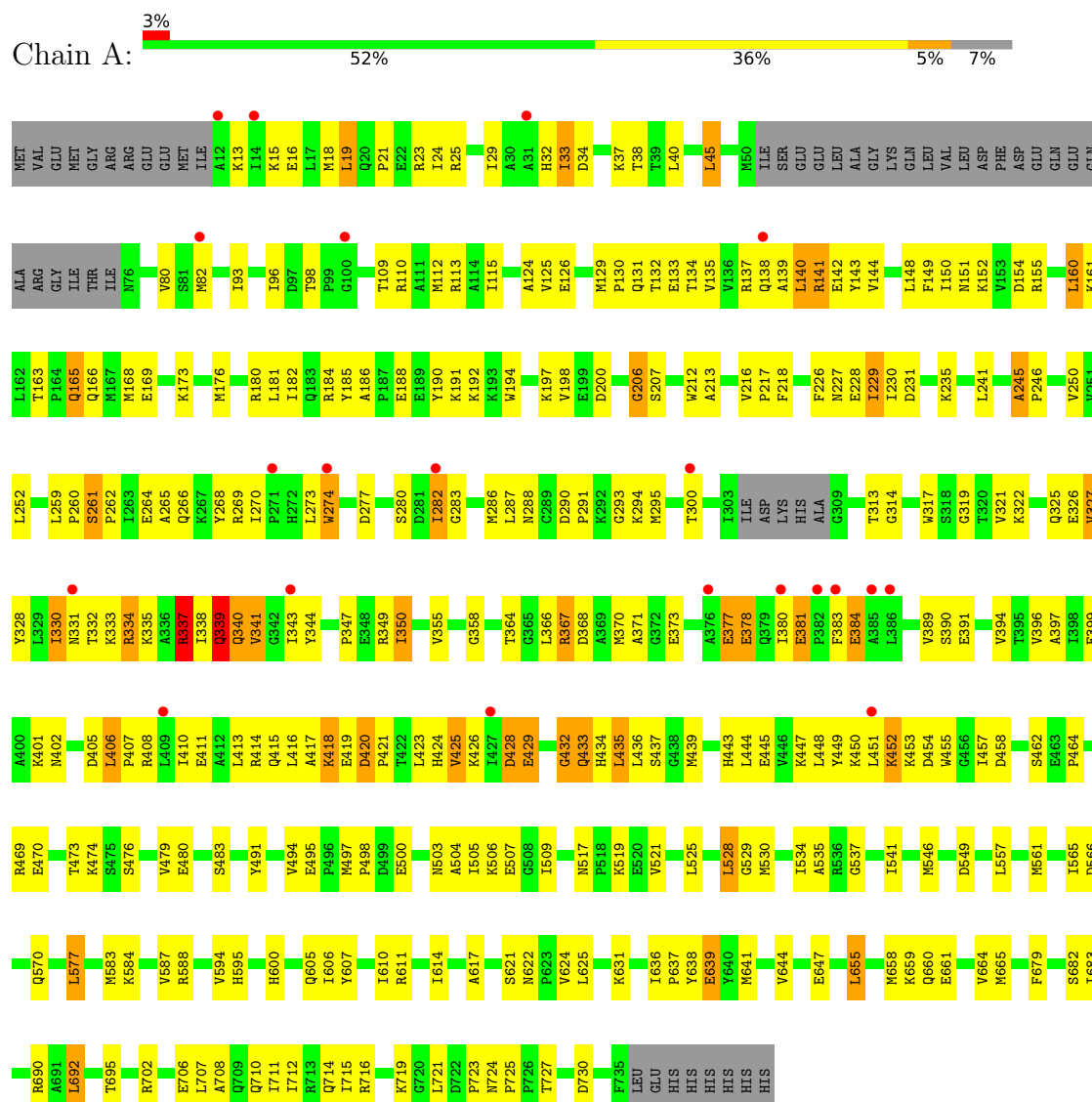


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	B	1	Total 32	C 11	N 5	O 13	P 3	0	0

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 2



• Molecule 1: Elongation factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.77Å 121.90Å 199.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 3.10 48.43 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.43-3.10) 99.3 (48.43-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.285 0.238 , 0.289	Depositor DCC
R_{free} test set	1796 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.1	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	0.93	EDS
Total number of atoms	11115	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: GCP

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	0.70	0/5577	1.14	14/7541 (0.2%)
1	B	0.69	0/5552	1.13	24/7508 (0.3%)
2	E	0.45	0/59	0.90	0/78
2	G	0.41	0/64	0.90	0/85
All	All	0.69	0/11252	1.14	38/15212 (0.2%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ILE	N-CA-C	-10.01	102.92	112.83
1	B	20	GLN	CA-C-N	8.16	128.35	119.87
1	B	20	GLN	C-N-CA	8.16	128.35	119.87
1	B	457	ILE	N-CA-C	7.91	119.60	108.93
1	B	636	ILE	N-CA-C	7.57	117.57	109.01
1	B	206	GLY	N-CA-C	7.53	120.75	110.58
1	A	378	GLU	N-CA-C	-7.49	96.69	108.90
1	A	534	ILE	N-CA-C	-7.47	105.85	111.90
1	A	206	GLY	N-CA-C	7.37	120.04	110.45
1	A	420	ASP	CA-C-N	7.37	127.07	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ASP	C-N-CA	7.37	127.07	119.56
1	B	295	MET	N-CA-C	7.20	119.59	110.24
1	B	455	TRP	N-CA-C	6.59	121.61	113.50
1	A	453	LYS	N-CA-C	-6.57	105.39	113.41
1	B	448	LEU	CA-C-N	-6.28	112.59	122.65
1	B	448	LEU	C-N-CA	-6.28	112.59	122.65
1	B	725	PRO	O-C-N	6.21	124.17	121.31
1	B	104	PHE	N-CA-C	-5.97	101.62	110.46
1	A	339	GLN	CB-CG-CD	5.87	122.58	112.60
1	B	244	LYS	N-CA-C	-5.72	106.65	113.97
1	B	441	GLU	N-CA-C	5.61	117.08	111.07
1	A	449	TYR	N-CA-C	-5.54	106.38	113.02
1	B	141	ARG	N-CA-C	-5.48	104.53	111.11
1	A	432	GLY	N-CA-C	5.47	126.15	113.18
1	B	108	VAL	N-CA-C	5.45	116.18	110.62
1	A	330	ILE	N-CA-C	5.41	116.79	110.62
1	A	381	GLU	N-CA-C	-5.37	103.41	110.39
1	B	430	GLU	N-CA-C	-5.25	107.54	114.31
1	A	337	ARG	N-CA-C	5.22	116.78	108.79
1	B	375	VAL	N-CA-C	5.18	115.32	107.80
1	B	517	ASN	CA-C-N	5.18	124.80	119.05
1	B	517	ASN	C-N-CA	5.18	124.80	119.05
1	B	641	MET	CB-CG-SD	-5.17	97.19	112.70
1	B	482	LYS	CB-CA-C	5.16	118.27	109.80
1	A	245	ALA	CA-C-N	5.13	125.37	119.83
1	A	245	ALA	C-N-CA	5.13	125.37	119.83
1	B	95	LEU	CA-CB-CG	5.08	134.07	116.30
1	B	379	GLN	N-CA-C	5.03	116.92	108.73

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	GLU	Peptide
1	A	452	LYS	Peptide
1	B	272	HIS	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	5476	0	5594	246	0
1	B	5452	0	5581	196	0
2	E	59	0	62	2	0
2	G	64	0	67	3	0
3	A	32	0	14	3	0
3	B	32	0	14	2	0
All	All	11115	0	11332	441	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 (441) 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:104:PHE:HB3	1:B:106:GLY:H	1.25	0.98
1:A:184:ARG:NH1	1:A:639:GLU:OE2	2.01	0.94
1:B:216:VAL:HG22	2:G:106:LEU:HD11	1.46	0.94
1:A:401:LYS:HE2	1:A:402:ASN:ND2	1.84	0.93
1:B:143:TYR:HE2	1:B:272:HIS:CD2	1.87	0.92
1:B:641:MET:HE3	1:B:667:ILE:HD11	1.55	0.89
1:A:282:ILE:HD13	1:A:294:LYS:HZ3	1.38	0.88
1:B:160:LEU:HD23	1:B:162:LEU:HD13	1.58	0.85
1:B:349:ARG:NH2	1:B:352:MET:SD	2.53	0.81
1:B:272:HIS:O	1:B:272:HIS:ND1	2.13	0.81
1:A:710:GLN:O	1:A:714:GLN:HG3	1.80	0.81
1:B:525:LEU:HB3	1:B:530:MET:HE3	1.62	0.80
1:A:326:GLU:HA	1:A:337:ARG:HG2	1.62	0.80
1:B:184:ARG:NH1	1:B:639:GLU:OE2	2.15	0.79
1:B:138:GLN:HG2	1:B:692:LEU:HD21	1.65	0.79
1:A:38:THR:OG1	3:A:801:GCP:O2B	2.00	0.78
1:A:138:GLN:O	1:A:141:ARG:NH2	2.17	0.77
1:A:266:GLN:NE2	1:A:317:TRP:HE3	1.82	0.77
1:A:137:ARG:NH2	1:A:690:ARG:O	2.16	0.77
1:B:134:THR:HG23	1:B:692:LEU:HD11	1.65	0.77
1:B:646:ARG:O	1:B:650:GLN:HG3	1.85	0.76
1:A:141:ARG:HG2	1:A:142:GLU:N	1.99	0.76
1:A:80:VAL:HG22	1:A:347:PRO:HA	1.67	0.76
1:A:45:LEU:HD23	1:A:80:VAL:HG12	1.68	0.75
1:A:473:THR:HG22	1:A:622:ASN:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:NZ	1:A:98:THR:O	2.20	0.73
1:A:416:LEU:HA	1:A:419:GLU:HB3	1.70	0.72
1:A:339:GLN:HE21	1:A:339:GLN:N	1.88	0.72
1:A:337:ARG:HD2	1:A:338:ILE:H	1.55	0.71
1:A:503:ASN:O	1:A:507:GLU:HG2	1.90	0.71
1:B:104:PHE:HB3	1:B:106:GLY:N	2.04	0.70
1:B:482:LYS:HD2	1:B:483:SER:O	1.91	0.70
1:B:380:ILE:HG22	1:B:381:GLU:H	1.55	0.70
1:A:384:GLU:N	1:A:384:GLU:OE1	2.25	0.70
1:A:450:LYS:HE2	1:A:455:TRP:NE1	2.07	0.70
1:B:113:ARG:HH21	1:B:383:PHE:HB3	1.56	0.70
1:A:231:ASP:OD2	1:A:235:LYS:NZ	2.25	0.69
1:B:137:ARG:NH1	1:B:690:ARG:O	2.21	0.69
1:B:327:VAL:HG11	1:B:375:VAL:HG13	1.75	0.69
1:B:21:PRO:HA	1:B:24:ILE:HD12	1.75	0.68
1:A:410:ILE:HD12	1:A:411:GLU:HG2	1.73	0.68
1:A:658:MET:HE1	1:B:658:MET:HE1	1.74	0.68
1:B:345:MET:H	1:B:349:ARG:HB2	1.58	0.68
1:B:619:MET:HG3	1:B:731:VAL:HG21	1.75	0.68
1:B:350:ILE:HG22	1:B:351:ASN:H	1.59	0.68
1:A:659:LYS:NZ	1:A:661:GLU:OE2	2.20	0.68
1:A:110:ARG:NH2	1:A:371:ALA:O	2.27	0.68
1:A:711:ILE:O	1:A:715:ILE:HG13	1.94	0.67
1:A:226:PHE:O	1:A:230:ILE:HG13	1.94	0.67
1:B:262:PRO:O	1:B:266:GLN:HG3	1.94	0.67
1:A:406:LEU:HD13	1:A:407:PRO:HD3	1.75	0.67
1:B:247:LEU:HD13	1:B:248:HIS:H	1.58	0.67
1:B:130:PRO:HA	1:B:690:ARG:HH22	1.59	0.67
1:B:229:ILE:HG23	1:B:241:LEU:HD21	1.76	0.67
1:B:184:ARG:HH12	1:B:639:GLU:CD	2.03	0.67
1:A:325:GLN:H	1:A:337:ARG:CZ	2.08	0.66
1:A:295:MET:HA	1:A:319:GLY:HA3	1.77	0.66
1:B:50:MET:HE3	1:B:82:MET:HA	1.77	0.66
1:A:295:MET:HE1	1:A:321:VAL:HB	1.78	0.65
1:B:266:GLN:HA	1:B:269:ARG:HB2	1.77	0.65
1:A:126:GLU:OE2	1:A:129:MET:HE2	1.97	0.65
1:A:140:LEU:HD21	1:A:185:TYR:O	1.96	0.65
1:B:476:SER:HB3	1:B:621:SER:OG	1.97	0.65
1:A:290:ASP:OD1	1:A:293:GLY:N	2.29	0.64
1:B:502:TYR:CD1	1:B:584:LYS:HG3	2.31	0.64
1:A:655:LEU:HD12	1:A:655:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:O	1:A:335:LYS:HD3	1.98	0.64
1:A:161:LYS:HG2	1:A:161:LYS:O	1.98	0.64
1:B:96:ILE:HD13	1:B:115:ILE:HG22	1.80	0.63
1:A:332:THR:OG1	1:A:373:GLU:OE2	2.15	0.63
1:B:226:PHE:O	1:B:230:ILE:HG13	1.98	0.63
1:A:197:LYS:HB3	1:A:200:ASP:OD1	1.99	0.63
1:A:96:ILE:HD12	1:A:115:ILE:HG22	1.81	0.63
1:B:446:VAL:O	1:B:450:LYS:HG3	1.99	0.62
1:A:432:GLY:N	1:A:433:GLN:HA	2.14	0.62
1:A:109:THR:HG23	1:A:141:ARG:NE	2.14	0.62
1:A:432:GLY:H	1:A:433:GLN:HA	1.63	0.62
1:B:32:HIS:HA	1:B:131:GLN:HE21	1.64	0.62
1:B:143:TYR:O	1:B:269:ARG:NH2	2.30	0.62
1:A:337:ARG:NH1	1:A:338:ILE:HB	2.14	0.62
1:A:433:GLN:OE1	1:A:434:HIS:N	2.32	0.62
1:B:189:GLU:OE1	1:B:189:GLU:N	2.25	0.62
1:A:176:MET:O	1:A:180:ARG:HG3	2.00	0.62
1:B:523:LYS:NZ	1:B:532:TYR:OH	2.32	0.62
1:A:338:ILE:C	1:A:339:GLN:HE21	2.08	0.62
1:B:396:VAL:HG22	1:B:444:LEU:HD13	1.82	0.61
1:A:313:THR:OG1	1:A:344:TYR:OH	2.18	0.61
1:A:338:ILE:HG21	1:A:341:VAL:HG23	1.82	0.61
1:A:570:GLN:OE1	1:A:611:ARG:NH1	2.34	0.61
1:B:14:ILE:HD11	1:B:92:LEU:HD13	1.81	0.61
1:B:326:GLU:HA	1:B:337:ARG:HB2	1.82	0.61
1:A:636:ILE:HD13	1:A:644:VAL:HG21	1.81	0.61
1:A:530:MET:HE2	1:A:535:ALA:HA	1.83	0.61
1:B:405:ASP:OD1	1:B:408:ARG:NH1	2.34	0.60
1:B:710:GLN:O	1:B:714:GLN:HG3	2.01	0.60
1:A:474:LYS:O	1:A:621:SER:HB3	2.00	0.60
1:B:32:HIS:HB2	1:B:132:THR:CG2	2.31	0.60
1:A:45:LEU:HG	1:A:82:MET:HB2	1.84	0.60
1:B:180:ARG:O	1:B:183:GLN:HB3	2.02	0.60
1:A:125:VAL:HG13	1:A:160:LEU:HD11	1.84	0.60
1:A:138:GLN:HE21	1:A:692:LEU:HG	1.66	0.60
1:A:274:TRP:HB3	1:A:383:PHE:CD2	2.36	0.60
1:A:429:GLU:O	1:A:433:GLN:NE2	2.34	0.60
1:A:338:ILE:HG12	1:A:366:LEU:HD21	1.84	0.59
1:A:29:ILE:HD13	1:A:40:LEU:HD23	1.84	0.59
1:A:109:THR:O	1:A:113:ARG:HG2	2.03	0.59
1:B:325:GLN:NE2	1:B:377:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:O	1:A:269:ARG:NH2	2.36	0.59
1:A:23:ARG:HG2	1:A:23:ARG:HH21	1.66	0.59
1:A:332:THR:HG21	1:A:368:ASP:O	2.02	0.59
1:A:659:LYS:O	1:A:665:MET:HE3	2.03	0.58
1:A:218:PHE:CZ	1:A:246:PRO:HD2	2.38	0.58
1:A:131:GLN:O	1:A:134:THR:OG1	2.17	0.58
1:A:624:VAL:HG11	1:A:702:ARG:HH21	1.69	0.58
1:B:599:VAL:HG13	1:B:600:HIS:ND1	2.19	0.58
1:A:330:ILE:O	1:A:331:ASN:ND2	2.37	0.58
1:B:84:HIS:NE2	1:B:253:ASP:OD2	2.35	0.58
1:A:190:TYR:O	1:A:194:TRP:HB2	2.03	0.57
1:B:329:LEU:HD23	1:B:369:ALA:HB2	1.86	0.57
1:A:470:GLU:OE1	1:A:577:LEU:HB2	2.04	0.57
1:B:165:GLN:HB2	1:B:168:MET:HE2	1.85	0.57
1:B:332:THR:O	1:B:334:ARG:HG3	2.05	0.57
1:B:620:LYS:NZ	1:B:728:GLU:OE1	2.37	0.57
1:B:171:PHE:O	1:B:175:ILE:HG13	2.05	0.57
1:A:141:ARG:NE	1:A:142:GLU:HG2	2.19	0.57
1:A:113:ARG:HA	1:A:269:ARG:HH12	1.70	0.56
1:B:247:LEU:HD13	1:B:248:HIS:N	2.19	0.56
1:A:282:ILE:HD13	1:A:294:LYS:NZ	2.17	0.56
1:B:279:SER:HA	1:B:284:GLN:HE22	1.71	0.56
1:B:290:ASP:OD2	1:B:293:GLY:N	2.37	0.56
1:A:216:VAL:HG22	1:A:217:PRO:HD3	1.87	0.56
1:A:186:ALA:HB3	1:A:191:LYS:HG2	1.88	0.56
1:A:727:THR:HG22	1:A:730:ASP:OD2	2.06	0.56
1:A:266:GLN:HE21	1:A:317:TRP:HE3	1.51	0.56
1:A:411:GLU:O	1:A:415:GLN:HG3	2.06	0.56
1:B:423:LEU:HD22	1:B:447:LYS:HE3	1.88	0.56
1:B:266:GLN:HB3	1:B:270:ILE:HG12	1.88	0.56
1:B:505:ILE:HD11	1:B:546:MET:HE3	1.87	0.56
1:B:143:TYR:CE2	1:B:272:HIS:CD2	2.80	0.55
1:B:414:ARG:HG3	1:B:418:LYS:NZ	2.22	0.55
1:B:225:LYS:O	1:B:229:ILE:HD12	2.05	0.55
1:A:340:GLN:HE21	1:A:341:VAL:N	2.04	0.55
1:A:32:HIS:ND1	1:A:33:ILE:N	2.54	0.55
1:B:274:TRP:HZ2	1:B:380:ILE:HG21	1.71	0.55
1:A:521:VAL:O	1:A:525:LEU:HD12	2.07	0.55
1:A:270:ILE:HA	1:A:273:LEU:HD12	1.89	0.54
1:B:156:LEU:HA	1:B:160:LEU:HD21	1.89	0.54
1:A:34:ASP:H	3:A:801:GCP:H3B2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LYS:HE3	1:A:458:ASP:OD1	2.07	0.54
1:B:164:PRO:HB3	2:G:107:PHE:HD2	1.72	0.54
1:A:337:ARG:HD2	1:A:338:ILE:N	2.22	0.54
1:B:15:LYS:HD2	1:B:352:MET:HE2	1.88	0.54
1:B:32:HIS:HB2	1:B:132:THR:HG22	1.89	0.54
1:A:135:VAL:HA	1:A:138:GLN:OE1	2.08	0.54
1:A:413:LEU:HD13	1:A:425:VAL:HG11	1.90	0.54
1:B:614:ILE:O	1:B:618:MET:HG3	2.06	0.54
1:A:370:MET:HE1	1:A:389:VAL:HG22	1.90	0.53
1:B:533:GLU:OE1	1:B:536:ARG:NH2	2.40	0.53
1:A:266:GLN:HA	1:A:269:ARG:HB2	1.90	0.53
1:A:294:LYS:NZ	1:A:378:GLU:HB3	2.24	0.53
1:A:13:LYS:HA	1:A:15:LYS:HE2	1.90	0.53
1:A:483:SER:HB2	1:A:605:GLN:HB3	1.90	0.53
1:B:102:VAL:HG23	1:B:104:PHE:O	2.09	0.53
1:A:505:ILE:HD11	1:A:546:MET:HE3	1.89	0.53
1:A:378:GLU:OE1	1:A:380:ILE:HG23	2.08	0.53
1:B:152:LYS:HE3	3:B:801:GCP:C4	2.39	0.53
1:B:640:TYR:CE2	1:B:690:ARG:HD2	2.43	0.53
1:A:188:GLU:HA	1:A:191:LYS:HE2	1.91	0.53
1:A:476:SER:HB3	1:A:621:SER:OG	2.08	0.53
1:A:34:ASP:H	3:A:801:GCP:C3B	2.22	0.53
1:A:334:ARG:HH11	1:A:367:ARG:HE	1.56	0.53
1:A:138:GLN:NE2	1:A:692:LEU:HG	2.24	0.52
1:B:25:ARG:NE	1:B:259:LEU:O	2.42	0.52
1:A:15:LYS:O	1:A:18:MET:HE3	2.10	0.52
1:A:530:MET:HE2	1:A:535:ALA:CA	2.39	0.52
1:B:332:THR:OG1	1:B:334:ARG:NH1	2.43	0.52
1:A:416:LEU:HD22	1:A:419:GLU:HG2	1.91	0.52
1:A:528:LEU:O	1:A:530:MET:N	2.38	0.52
1:B:50:MET:HE3	1:B:83:VAL:H	1.75	0.52
1:A:428:ASP:CG	1:A:429:GLU:H	2.18	0.52
1:B:473:THR:HB	1:B:622:ASN:HB3	1.91	0.52
1:A:410:ILE:HG22	1:A:434:HIS:NE2	2.25	0.52
1:B:86:TYR:HB3	1:B:91:TYR:CE1	2.44	0.52
1:B:50:MET:CE	1:B:83:VAL:H	2.22	0.52
1:A:327:VAL:HG13	1:A:337:ARG:HD3	1.92	0.51
1:A:163:THR:OG1	1:A:166:GLN:HG3	2.10	0.51
1:B:14:ILE:HD12	1:B:17:LEU:HD12	1.91	0.51
1:B:503:ASN:O	1:B:507:GLU:HG2	2.11	0.51
1:A:494:VAL:HG22	1:A:617:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:TYR:CZ	1:B:583:MET:HE3	2.46	0.51
1:A:129:MET:N	1:A:132:THR:OG1	2.42	0.51
1:A:218:PHE:CZ	1:A:245:ALA:HA	2.46	0.51
1:A:416:LEU:CD1	1:A:450:LYS:HD2	2.40	0.51
1:B:101:HIS:CE1	1:B:131:GLN:HB2	2.46	0.51
1:A:206:GLY:HA2	1:A:212:TRP:CZ3	2.46	0.51
1:B:125:VAL:HG21	1:B:155:ARG:HE	1.75	0.51
1:A:340:GLN:NE2	1:A:341:VAL:O	2.44	0.51
1:A:266:GLN:NE2	1:A:317:TRP:CE3	2.71	0.50
1:B:27:ILE:O	1:B:95:LEU:HA	2.11	0.50
1:A:141:ARG:CZ	1:A:142:GLU:HG2	2.41	0.50
1:B:97:ASP:OD2	1:B:301:LYS:NZ	2.44	0.50
1:A:708:ALA:O	1:A:712:ILE:HG13	2.11	0.50
1:A:277:ASP:OD1	1:A:280:SER:OG	2.26	0.50
1:A:583:MET:HE2	1:A:584:LYS:HD3	1.93	0.50
1:B:414:ARG:HG3	1:B:418:LYS:HZ3	1.77	0.50
1:A:182:ILE:HD13	1:A:194:TRP:O	2.12	0.50
1:A:396:VAL:HG12	1:A:464:PRO:HA	1.94	0.50
1:A:452:LYS:HB2	1:A:457:ILE:H	1.76	0.50
1:A:639:GLU:CD	1:A:639:GLU:H	2.18	0.49
1:B:345:MET:N	1:B:349:ARG:HB2	2.25	0.49
1:A:413:LEU:HD11	1:A:425:VAL:HG21	1.94	0.49
1:B:115:ILE:HG13	1:B:144:VAL:HG11	1.93	0.49
1:B:715:ILE:O	1:B:719:LYS:HG3	2.13	0.49
1:A:339:GLN:HE21	1:A:339:GLN:CA	2.25	0.49
1:A:426:LYS:HG3	1:A:435:LEU:HD11	1.94	0.49
1:B:183:GLN:O	1:B:191:LYS:HD3	2.12	0.49
1:A:426:LYS:O	1:A:434:HIS:HD2	1.96	0.49
1:A:494:VAL:HG12	1:A:587:VAL:HG22	1.94	0.49
1:A:706:GLU:H	1:A:706:GLU:CD	2.16	0.49
1:B:706:GLU:HG2	1:B:707:LEU:HD13	1.94	0.49
1:B:523:LYS:O	1:B:527:GLU:HG3	2.11	0.49
1:A:21:PRO:O	1:A:262:PRO:HD2	2.12	0.49
1:B:179:ASN:HB3	1:B:195:MET:HE2	1.95	0.49
1:A:641:MET:SD	1:A:665:MET:HG2	2.53	0.48
1:B:32:HIS:ND1	1:B:33:ILE:N	2.61	0.48
1:A:184:ARG:HD3	1:A:185:TYR:CZ	2.47	0.48
1:A:340:GLN:H	1:A:364:THR:HG22	1.77	0.48
1:A:625:LEU:HD22	1:A:712:ILE:HG12	1.95	0.48
1:A:397:ALA:H	1:A:462:SER:HG	1.61	0.48
1:B:179:ASN:OD1	1:B:196:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:OD1	1:A:152:LYS:N	2.39	0.48
1:A:207:SER:HB3	1:A:212:TRP:NE1	2.28	0.48
1:A:282:ILE:HG21	1:A:294:LYS:NZ	2.28	0.48
1:B:197:LYS:HB2	1:B:200:ASP:OD1	2.13	0.48
1:B:211:ASN:HA	1:B:247:LEU:HG	1.94	0.48
1:B:125:VAL:HG11	1:B:155:ARG:HH21	1.79	0.48
1:A:420:ASP:OD2	1:A:443:HIS:NE2	2.41	0.48
1:B:488:ASN:HA	1:B:593:GLN:O	2.13	0.48
1:A:495:GLU:OE2	1:A:588:ARG:NH2	2.46	0.48
1:A:647:GLU:OE2	1:A:682:SER:HB3	2.13	0.48
1:B:160:LEU:HD23	1:B:162:LEU:CD1	2.37	0.48
1:A:610:ILE:O	1:A:614:ILE:HG13	2.14	0.48
1:B:286:MET:SD	1:B:296:VAL:HG11	2.54	0.48
1:B:512:GLU:OE1	1:B:543:ASN:N	2.34	0.47
1:B:154:ASP:OD1	1:B:155:ARG:N	2.47	0.47
1:B:297:MET:HE2	1:B:375:VAL:HG11	1.95	0.47
1:A:448:LEU:O	1:A:451:LEU:HB2	2.14	0.47
1:A:416:LEU:HD13	1:A:447:LYS:HE3	1.97	0.47
1:B:78:ALA:HA	1:B:301:LYS:HZ1	1.80	0.47
1:B:501:ILE:O	1:B:505:ILE:HG13	2.14	0.47
1:B:331:ASN:HB2	1:B:373:GLU:HG2	1.97	0.47
1:A:13:LYS:NZ	1:A:16:GLU:HG2	2.30	0.47
1:A:141:ARG:CG	1:A:142:GLU:HG2	2.45	0.47
1:A:340:GLN:H	1:A:364:THR:CG2	2.27	0.47
1:A:679:PHE:O	1:A:683:ILE:HG22	2.14	0.47
1:B:349:ARG:HA	1:B:349:ARG:HD2	1.56	0.47
1:A:504:ALA:HA	1:A:509:ILE:HD12	1.96	0.47
1:A:140:LEU:HD23	1:A:140:LEU:C	2.40	0.47
1:A:133:GLU:HG2	1:A:181:LEU:HD11	1.96	0.47
1:A:168:MET:HB3	1:A:168:MET:HE2	1.73	0.47
1:A:226:PHE:CD1	2:E:106:LEU:HB3	2.50	0.46
1:A:469:ARG:HH12	1:A:506:LYS:HZ3	1.62	0.46
1:A:658:MET:HG2	1:A:665:MET:HE2	1.97	0.46
1:A:660:GLN:HB2	1:A:665:MET:HE1	1.97	0.46
1:A:16:GLU:HB2	1:A:19:LEU:HD11	1.96	0.46
1:A:716:ARG:HD3	1:A:723:PRO:O	2.15	0.46
1:B:32:HIS:HB3	1:B:35:HIS:CG	2.50	0.46
1:B:313:THR:HG23	1:B:344:TYR:HE2	1.81	0.46
1:B:381:GLU:HG3	1:B:382:PRO:HD2	1.97	0.46
1:B:501:ILE:HD13	1:B:530:MET:HE2	1.97	0.46
1:A:505:ILE:HD11	1:A:546:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:HIS:HB2	1:B:132:THR:HG23	1.97	0.46
1:B:408:ARG:NH2	1:B:455:TRP:O	2.49	0.46
1:A:300:THR:HG23	1:A:314:GLY:HA2	1.96	0.46
1:B:32:HIS:CD2	1:B:131:GLN:HG2	2.50	0.46
1:A:436:LEU:HG	1:A:444:LEU:HD22	1.97	0.46
1:A:143:TYR:CD1	1:A:190:TYR:HE2	2.34	0.46
1:B:659:LYS:HD2	1:B:659:LYS:HA	1.73	0.46
1:A:541:ILE:CD1	1:A:546:MET:HE2	2.46	0.46
1:B:240:THR:O	1:B:244:LYS:HB2	2.15	0.46
1:B:280:SER:OG	1:B:282:ILE:HG22	2.16	0.46
1:B:164:PRO:HB3	2:G:107:PHE:CD2	2.50	0.46
1:A:113:ARG:HD3	1:A:141:ARG:HH11	1.81	0.46
1:A:537:GLY:O	1:A:549:ASP:N	2.37	0.46
1:B:177:ASP:O	1:B:181:LEU:HD13	2.16	0.46
1:B:327:VAL:CG1	1:B:375:VAL:HG13	2.46	0.46
1:A:140:LEU:HD21	1:A:185:TYR:C	2.41	0.45
1:A:631:LYS:O	1:A:695:THR:HA	2.16	0.45
1:B:107:ASP:O	1:B:110:ARG:HG2	2.16	0.45
1:A:25:ARG:NE	1:A:259:LEU:O	2.49	0.45
1:B:339:GLN:HB2	1:B:364:THR:HG23	1.97	0.45
1:A:414:ARG:HA	1:A:417:ALA:HB3	1.98	0.45
1:A:715:ILE:O	1:A:719:LYS:HG3	2.17	0.45
1:B:178:VAL:O	1:B:182:ILE:HG13	2.16	0.45
1:B:455:TRP:N	1:B:456:GLY:HA2	2.32	0.45
1:B:349:ARG:HD2	1:B:350:ILE:H	1.81	0.45
1:B:661:GLU:O	1:B:664:VAL:HG12	2.17	0.45
1:A:24:ILE:HG21	1:A:358:GLY:O	2.17	0.45
1:B:79:ASN:HD22	1:B:344:TYR:HD2	1.65	0.45
1:A:260:PRO:HB2	1:A:264:GLU:HB3	1.99	0.45
1:B:417:ALA:HB2	1:B:425:VAL:HG12	1.99	0.45
1:B:490:PHE:CE1	1:B:564:LEU:HD21	2.52	0.45
1:A:226:PHE:HD1	2:E:106:LEU:HB3	1.82	0.44
1:B:31:ALA:HB2	1:B:121:VAL:HB	1.97	0.44
1:B:20:GLN:OE1	1:B:20:GLN:N	2.50	0.44
1:B:82:MET:HE3	1:B:82:MET:HB2	1.86	0.44
1:B:272:HIS:HD1	1:B:272:HIS:C	2.17	0.44
1:A:134:THR:O	1:A:137:ARG:N	2.51	0.44
1:A:454:ASP:OD2	1:A:455:TRP:NE1	2.50	0.44
1:A:561:MET:O	1:A:565:ILE:HG12	2.17	0.44
1:A:265:ALA:HA	1:A:268:TYR:CE2	2.52	0.44
1:A:283:GLY:O	1:A:287:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:HG21	1:B:382:PRO:HD3	1.99	0.44
1:B:370:MET:O	1:B:373:GLU:HB2	2.18	0.44
1:B:519:LYS:HB3	1:B:519:LYS:HE3	1.59	0.44
1:B:633:ILE:O	1:B:693:TRP:HA	2.18	0.44
1:B:537:GLY:HA3	1:B:549:ASP:O	2.18	0.44
1:A:124:ALA:HB2	1:A:150:ILE:HG22	1.99	0.44
1:A:165:GLN:HA	1:A:168:MET:HG3	2.00	0.44
1:A:337:ARG:HH11	1:A:338:ILE:HB	1.82	0.44
1:B:521:VAL:O	1:B:525:LEU:HD13	2.18	0.44
1:A:141:ARG:HG2	1:A:142:GLU:H	1.80	0.44
1:B:484:PRO:HD2	1:B:605:GLN:HA	1.99	0.44
1:A:414:ARG:NH2	1:A:425:VAL:HG22	2.33	0.43
1:A:447:LYS:O	1:A:451:LEU:HD23	2.18	0.43
1:B:295:MET:HA	1:B:318:SER:O	2.18	0.43
1:A:328:TYR:HA	1:A:335:LYS:HD2	1.99	0.43
1:A:500:GLU:H	1:A:500:GLU:CD	2.26	0.43
1:B:80:VAL:HG23	1:B:95:LEU:HD13	2.00	0.43
1:B:265:ALA:HA	1:B:268:TYR:CE2	2.53	0.43
1:B:619:MET:HE2	1:B:727:THR:C	2.42	0.43
1:A:343:ILE:O	1:A:350:ILE:HG22	2.18	0.43
1:B:151:ASN:O	1:B:152:LYS:HB2	2.17	0.43
1:B:455:TRP:H	1:B:456:GLY:HA2	1.82	0.43
1:A:495:GLU:CD	1:A:588:ARG:HH21	2.26	0.43
1:B:640:TYR:HE2	1:B:690:ARG:HD2	1.80	0.43
1:B:274:TRP:CZ2	1:B:276:GLY:HA3	2.53	0.43
1:A:661:GLU:O	1:A:664:VAL:HG12	2.18	0.43
1:B:619:MET:HG3	1:B:731:VAL:CG2	2.45	0.43
1:A:606:ILE:O	1:A:610:ILE:HG22	2.19	0.43
1:A:213:ALA:HB3	1:A:250:VAL:HB	2.01	0.43
1:A:261:SER:N	1:A:264:GLU:HB2	2.34	0.43
1:A:413:LEU:CD1	1:A:425:VAL:HG21	2.49	0.43
1:B:343:ILE:HG22	1:B:344:TYR:N	2.34	0.43
1:B:417:ALA:HB3	1:B:418:LYS:NZ	2.33	0.43
1:B:93:ILE:HD12	1:B:252:LEU:HD22	2.00	0.43
1:B:101:HIS:CD2	1:B:101:HIS:C	2.97	0.43
1:B:474:LYS:O	1:B:621:SER:HB3	2.18	0.43
1:B:641:MET:HE3	1:B:641:MET:HB2	1.74	0.43
1:B:658:MET:HG2	1:B:665:MET:HE2	2.00	0.43
1:A:165:GLN:O	1:A:169:GLU:HG3	2.19	0.43
1:A:454:ASP:HB3	1:A:455:TRP:HD1	1.83	0.43
1:B:339:GLN:OE1	1:B:365:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ASP:HA	1:B:421:PRO:HD2	1.94	0.43
1:A:133:GLU:HA	1:A:181:LEU:HD21	2.01	0.42
1:A:141:ARG:HG2	1:A:142:GLU:HG2	2.00	0.42
1:A:423:LEU:C	1:A:424:HIS:HD1	2.27	0.42
1:B:173:LYS:NZ	1:B:177:ASP:OD1	2.40	0.42
1:B:470:GLU:OE1	1:B:577:LEU:HB2	2.19	0.42
1:B:729:LYS:HE3	1:B:729:LYS:HB3	1.44	0.42
1:A:143:TYR:HB3	1:A:268:TYR:CE1	2.54	0.42
1:A:154:ASP:OD2	1:A:154:ASP:N	2.53	0.42
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.75	0.42
1:A:125:VAL:HG21	1:A:155:ARG:HD3	2.01	0.42
1:A:139:ALA:O	1:A:144:VAL:HB	2.19	0.42
1:A:288:ASN:OD1	1:A:290:ASP:HB2	2.19	0.42
1:A:416:LEU:HD12	1:A:450:LYS:HD2	2.01	0.42
1:A:595:HIS:CD2	1:A:600:HIS:HD1	2.38	0.42
1:A:637:PRO:HB2	1:A:639:GLU:OE1	2.20	0.42
1:B:413:LEU:HD21	1:B:451:LEU:HD11	2.01	0.42
1:B:505:ILE:HD11	1:B:546:MET:CE	2.49	0.42
1:A:112:MET:HE1	1:A:138:GLN:HB2	2.01	0.42
1:B:143:TYR:C	1:B:269:ARG:NH2	2.77	0.42
1:B:537:GLY:O	1:B:549:ASP:N	2.36	0.42
1:B:711:ILE:O	1:B:715:ILE:HG13	2.20	0.42
1:A:197:LYS:HB3	1:A:200:ASP:CG	2.45	0.42
1:A:291:PRO:O	1:A:319:GLY:HA2	2.18	0.42
1:A:340:GLN:NE2	1:A:341:VAL:H	2.17	0.42
1:A:367:ARG:C	1:A:367:ARG:HD2	2.45	0.42
1:A:416:LEU:HD11	1:A:450:LYS:HD2	2.02	0.42
1:B:625:LEU:HD23	1:B:625:LEU:HA	1.77	0.42
1:A:402:ASN:HB2	1:A:405:ASP:OD2	2.20	0.42
1:B:20:GLN:HA	1:B:21:PRO:HD3	1.62	0.42
1:B:321:VAL:HG13	1:B:341:VAL:HG21	2.02	0.42
1:A:138:GLN:HA	1:A:141:ARG:HB3	2.02	0.41
1:A:141:ARG:CZ	1:A:142:GLU:CG	2.98	0.41
1:A:270:ILE:HD13	1:A:286:MET:C	2.45	0.41
1:B:349:ARG:C	1:B:350:ILE:HD13	2.45	0.41
1:B:527:GLU:C	1:B:529:GLY:H	2.28	0.41
1:A:420:ASP:HA	1:A:421:PRO:HD2	1.83	0.41
1:A:495:GLU:OE1	1:A:588:ARG:HD3	2.20	0.41
1:A:638:TYR:HB2	1:A:641:MET:HE3	2.03	0.41
1:B:298:VAL:HB	1:B:317:TRP:HE1	1.85	0.41
1:B:403:VAL:HG23	1:B:406:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ILE:O	1:B:37:LYS:HD2	2.21	0.41
1:B:101:HIS:NE2	1:B:134:THR:HG21	2.34	0.41
1:A:418:LYS:O	1:A:418:LYS:HG3	2.13	0.41
1:B:23:ARG:HD2	1:B:90:ASP:O	2.20	0.41
1:B:86:TYR:OH	1:B:257:ARG:HD2	2.21	0.41
1:A:143:TYR:HD1	1:A:190:TYR:HE2	1.69	0.41
1:A:367:ARG:HG3	1:A:368:ASP:HB2	2.02	0.41
1:A:566:ASP:HB2	1:A:607:TYR:CE2	2.56	0.41
1:A:724:ASN:HA	1:A:725:PRO:HD3	1.82	0.41
1:B:408:ARG:O	1:B:412:ALA:N	2.43	0.41
1:B:546:MET:HE2	1:B:546:MET:HB3	1.92	0.41
1:B:457:ILE:H	1:B:457:ILE:HG13	1.59	0.41
1:B:551:THR:HG22	1:B:591:ASP:HA	2.03	0.41
1:A:130:PRO:O	1:A:133:GLU:HB2	2.21	0.41
1:A:212:TRP:CH2	1:A:229:ILE:HG21	2.56	0.41
1:A:517:ASN:O	1:A:521:VAL:HG23	2.21	0.41
1:A:683:ILE:HD12	1:A:683:ILE:HA	1.91	0.41
1:B:154:ASP:OD1	1:B:155:ARG:HG2	2.21	0.41
1:B:156:LEU:HA	1:B:160:LEU:CD2	2.50	0.41
1:B:423:LEU:HD12	1:B:437:SER:O	2.21	0.41
1:B:494:VAL:HG22	1:B:617:ALA:HB1	2.02	0.41
1:A:707:LEU:O	1:A:711:ILE:HG12	2.20	0.41
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.75	0.41
1:B:160:LEU:H	1:B:160:LEU:HD13	1.86	0.41
1:A:93:ILE:HD12	1:A:252:LEU:HD22	2.03	0.40
1:A:151:ASN:CG	1:A:152:LYS:N	2.79	0.40
1:A:638:TYR:CD1	1:A:638:TYR:C	2.98	0.40
1:B:38:THR:OG1	3:B:801:GCP:O1B	2.25	0.40
1:A:148:LEU:HD12	1:A:149:PHE:H	1.87	0.40
1:A:227:ASN:OD1	1:A:227:ASN:N	2.53	0.40
1:A:401:LYS:HE2	1:A:402:ASN:HD21	1.80	0.40
1:A:497:MET:HA	1:A:498:PRO:HD3	1.91	0.40
1:A:557:LEU:HA	1:A:594:VAL:HG21	2.02	0.40
1:B:156:LEU:O	1:B:160:LEU:HD22	2.21	0.40
1:A:274:TRP:CH2	1:A:381:GLU:HB3	2.56	0.40
1:A:401:LYS:HE2	1:A:402:ASN:HD22	1.77	0.40
1:A:479:VAL:HG21	1:A:617:ALA:HA	2.04	0.40
1:A:480:GLU:HG3	1:A:491:TYR:CE1	2.56	0.40
1:A:517:ASN:OD1	1:A:519:LYS:NZ	2.48	0.40
1:B:690:ARG:NH2	1:B:690:ARG:HG2	2.37	0.40
1:A:439:MET:HB2	1:A:443:HIS:ND1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:ILE:HD13	1:B:669:ALA:CB	2.52	0.40
1:A:246:PRO:O	1:A:250:VAL:HG23	2.22	0.40
1:A:394:VAL:O	1:A:437:SER:HA	2.22	0.40
1:B:349:ARG:CD	1:B:350:ILE:H	2.34	0.40
1:B:380:ILE:HG22	1:B:381:GLU:N	2.30	0.40
1:B:417:ALA:HB3	1:B:418:LYS:HZ2	1.86	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	688/743 (93%)	643 (94%)	41 (6%)	4 (1%)	21	52
1	B	685/743 (92%)	641 (94%)	44 (6%)	0	100	100
2	E	7/11 (64%)	7 (100%)	0	0	100	100
2	G	8/11 (73%)	8 (100%)	0	0	100	100
All	All	1388/1508 (92%)	1299 (94%)	85 (6%)	4 (0%)	36	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	GLU
1	A	529	GLY
1	A	367	ARG
1	A	428	ASP

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	595/638 (93%)	550 (92%)	45 (8%)	12	39
1	B	593/638 (93%)	541 (91%)	52 (9%)	9	33
2	E	5/6 (83%)	5 (100%)	0	100	100
2	G	5/6 (83%)	4 (80%)	1 (20%)	1	6
All	All	1198/1288 (93%)	1100 (92%)	98 (8%)	10	36

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	33	ILE
1	A	45	LEU
1	A	140	LEU
1	A	141	ARG
1	A	160	LEU
1	A	165	GLN
1	A	173	LYS
1	A	192	LYS
1	A	198	VAL
1	A	228	GLU
1	A	229	ILE
1	A	241	LEU
1	A	261	SER
1	A	274	TRP
1	A	282	ILE
1	A	322	LYS
1	A	327	VAL
1	A	333	LYS
1	A	334	ARG
1	A	337	ARG
1	A	339	GLN
1	A	340	GLN
1	A	341	VAL
1	A	349	ARG
1	A	350	ILE
1	A	355	VAL
1	A	377	GLU

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Mol	Chain	Res	Type
1	A	384	GLU
1	A	390	SER
1	A	391	GLU
1	A	399	GLU
1	A	406	LEU
1	A	408	ARG
1	A	418	LYS
1	A	425	VAL
1	A	433	GLN
1	A	435	LEU
1	A	445	GLU
1	A	528	LEU
1	A	577	LEU
1	A	639	GLU
1	A	655	LEU
1	A	692	LEU
1	A	721	LEU
1	B	15	LYS
1	B	19	LEU
1	B	27	ILE
1	B	33	ILE
1	B	95	LEU
1	B	131	GLN
1	B	133	GLU
1	B	134	THR
1	B	160	LEU
1	B	165	GLN
1	B	188	GLU
1	B	198	VAL
1	B	216	VAL
1	B	229	ILE
1	B	241	LEU
1	B	244	LYS
1	B	247	LEU
1	B	272	HIS
1	B	301	LYS
1	B	304	ILE
1	B	322	LYS
1	B	326	GLU
1	B	329	LEU
1	B	333	LYS
1	B	335	LYS

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Mol	Chain	Res	Type
1	B	337	ARG
1	B	340	GLN
1	B	349	ARG
1	B	350	ILE
1	B	389	VAL
1	B	391	GLU
1	B	401	LYS
1	B	402	ASN
1	B	406	LEU
1	B	429	GLU
1	B	448	LEU
1	B	449	TYR
1	B	473	THR
1	B	480	GLU
1	B	482	LYS
1	B	486	ARG
1	B	519	LYS
1	B	524	LYS
1	B	528	LEU
1	B	577	LEU
1	B	596	GLU
1	B	625	LEU
1	B	654	GLN
1	B	655	LEU
1	B	707	LEU
1	B	721	LEU
1	B	729	LYS
2	G	100	LEU

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

Mol	Chain	Res	Type
1	A	272	HIS
1	A	331	ASN
1	A	339	GLN
1	A	340	GLN
1	A	402	ASN
1	A	434	HIS
1	A	654	GLN
1	B	79	ASN
1	B	94	ASN
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	650	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	GCP	B	801	-	32,34,34	1.95	9 (28%)	49,54,54	1.83	10 (20%)
3	GCP	A	801	-	32,34,34	1.73	6 (18%)	49,54,54	1.94	11 (22%)

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	GCP	B	801	-	-	7/19/38/38	0/3/3/3
3	GCP	A	801	-	-	3/19/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	GCP	PG-O1G	5.71	1.61	1.50
3	A	801	GCP	PG-O1G	5.52	1.61	1.50
3	B	801	GCP	PB-O1B	4.10	1.61	1.51
3	B	801	GCP	PB-O2B	-3.47	1.47	1.56
3	A	801	GCP	PG-O3G	3.20	1.62	1.55
3	A	801	GCP	C5-C4	3.17	1.47	1.38
3	B	801	GCP	PG-O2G	3.07	1.61	1.55
3	B	801	GCP	C5-C4	3.03	1.47	1.38
3	A	801	GCP	PG-O2G	-2.80	1.48	1.55
3	B	801	GCP	C6-N1	-2.64	1.33	1.38
3	B	801	GCP	PG-O3G	-2.35	1.49	1.55
3	B	801	GCP	C4-N9	-2.18	1.32	1.38
3	A	801	GCP	C6-N1	-2.11	1.34	1.38
3	B	801	GCP	PB-O3A	2.09	1.60	1.58
3	A	801	GCP	PA-O3A	2.06	1.61	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	GCP	C5-C4-N3	-5.59	119.49	128.39
3	A	801	GCP	C2-N3-C4	5.14	121.15	112.30
3	B	801	GCP	C5-C4-N3	-4.71	120.89	128.39
3	B	801	GCP	C6-C5-N7	4.25	138.03	130.29
3	B	801	GCP	C2-N3-C4	4.22	119.56	112.30
3	A	801	GCP	PB-O3A-PA	-4.13	118.89	132.37
3	A	801	GCP	C6-C5-N7	3.88	137.35	130.29
3	A	801	GCP	N9-C4-N3	3.86	133.67	125.95
3	B	801	GCP	N9-C4-N3	3.22	132.40	125.95
3	B	801	GCP	O4'-C4'-C3'	3.17	111.44	105.15
3	A	801	GCP	O3G-PG-C3B	3.12	113.97	106.40
3	B	801	GCP	C4-C5-N7	-2.99	105.93	110.67
3	A	801	GCP	C4-C5-N7	-2.92	106.05	110.67
3	B	801	GCP	C5'-C4'-C3'	-2.76	105.26	115.21
3	B	801	GCP	PB-O3A-PA	-2.59	123.91	132.37
3	A	801	GCP	O3G-PG-O1G	-2.39	106.20	112.39
3	A	801	GCP	O4'-C1'-N9	2.38	113.75	108.36
3	A	801	GCP	C2'-C3'-C4'	2.20	106.86	102.61
3	B	801	GCP	C8-N7-C5	2.09	107.99	104.26
3	B	801	GCP	PA-O5'-C5'	-2.03	109.72	121.35
3	A	801	GCP	C2'-C1'-N9	-2.03	107.60	113.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

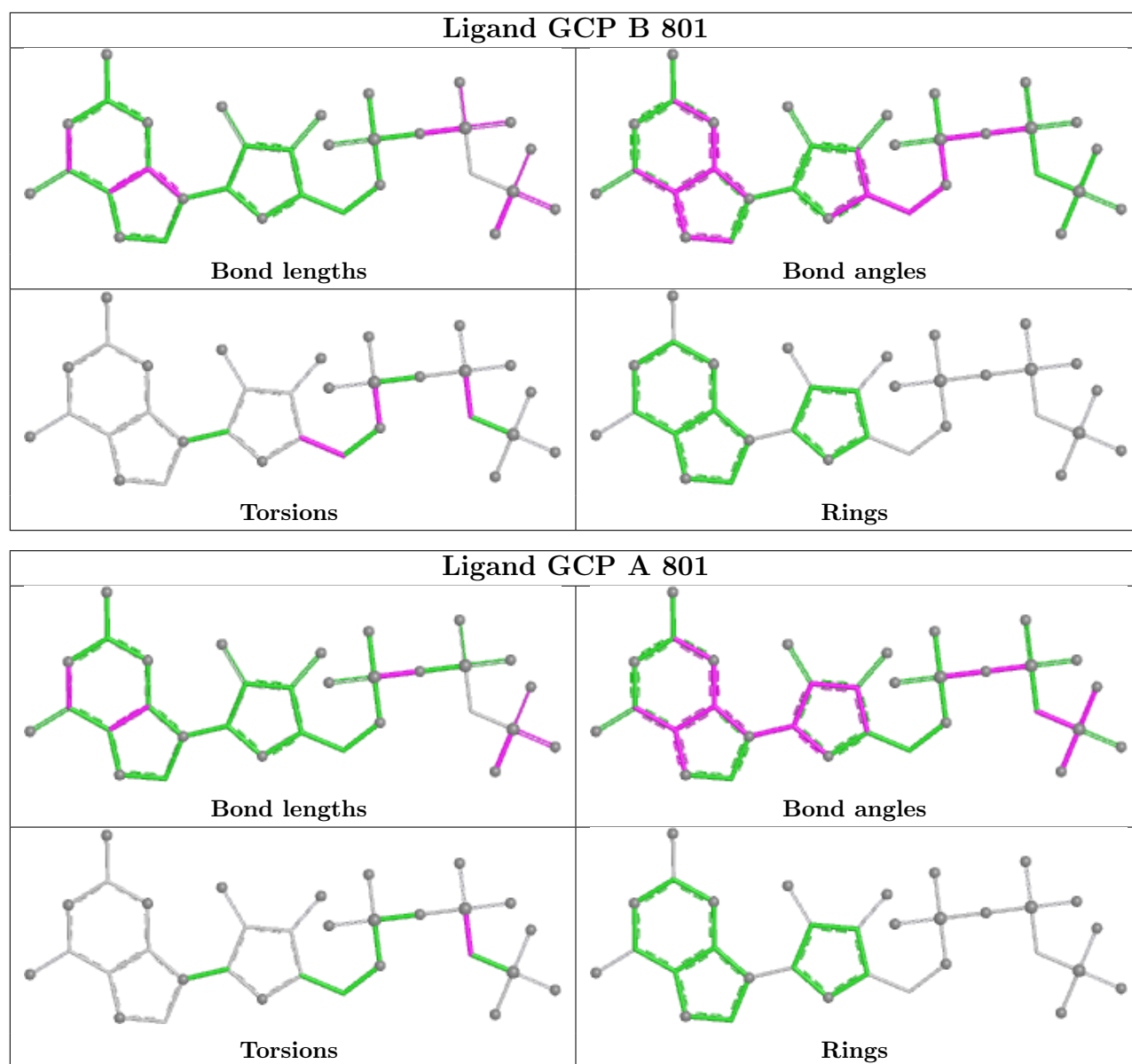
Mol	Chain	Res	Type	Atoms
3	A	801	GCP	PG-C3B-PB-O1B
3	A	801	GCP	PG-C3B-PB-O2B
3	A	801	GCP	PG-C3B-PB-O3A
3	B	801	GCP	PG-C3B-PB-O1B
3	B	801	GCP	PG-C3B-PB-O3A
3	B	801	GCP	C5'-O5'-PA-O3A
3	B	801	GCP	C5'-O5'-PA-O2A
3	B	801	GCP	C3'-C4'-C5'-O5'
3	B	801	GCP	O4'-C4'-C5'-O5'
3	B	801	GCP	PG-C3B-PB-O2B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	GCP	2	0
3	A	801	GCP	3	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	694/743 (93%)	-0.02	21 (3%)	52	31	66, 104, 158, 170	0
1	B	691/743 (93%)	-0.09	4 (0%)	85	70	55, 106, 152, 160	0
2	E	9/11 (81%)	0.06	0	100	100	105, 114, 128, 140	0
2	G	10/11 (90%)	0.45	0	100	100	123, 133, 145, 151	0
All	All	1404/1508 (93%)	-0.05	25 (1%)	67	47	55, 105, 155, 170	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	GLY	5.6
1	B	11	ILE	4.5
1	B	366	LEU	4.4
1	A	383	PHE	3.1
1	B	338	ILE	2.9
1	A	14	ILE	2.8
1	A	380	ILE	2.8
1	A	282	ILE	2.6
1	A	331	ASN	2.6
1	A	12	ALA	2.6
1	A	382	PRO	2.6
1	A	300	THR	2.6
1	A	274	TRP	2.5
1	A	271	PRO	2.4
1	A	31	ALA	2.3
1	A	376	ALA	2.3
1	A	386	LEU	2.3
1	A	82	MET	2.3
1	A	385	ALA	2.2
1	A	427	ILE	2.2
1	A	138	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	343	ILE	2.2
1	A	451	LEU	2.1
1	B	347	PRO	2.0
1	A	409	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

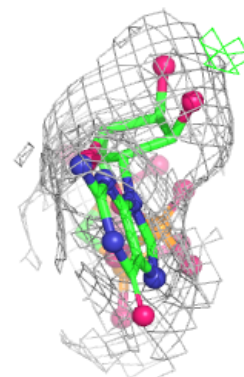
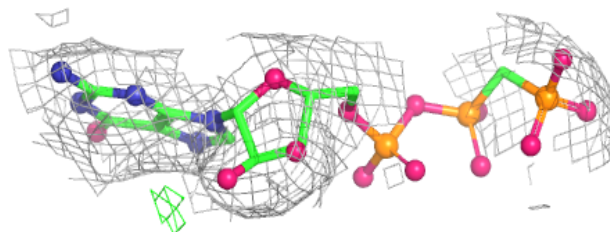
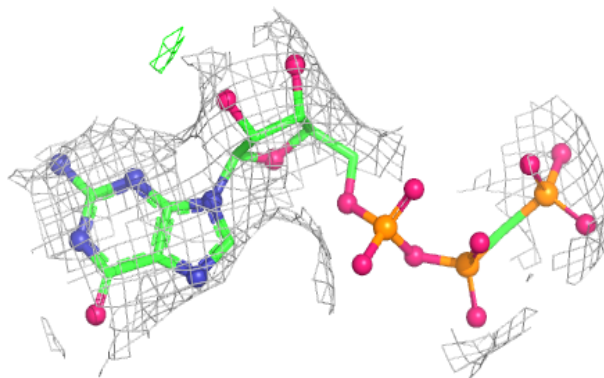
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GCP	A	801	32/32	0.87	0.08	82,106,123,135	0
3	GCP	B	801	32/32	0.91	0.07	95,107,134,137	0

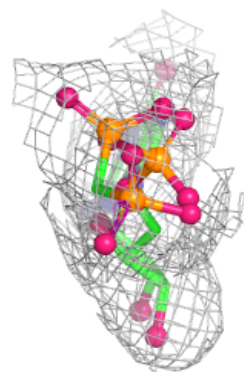
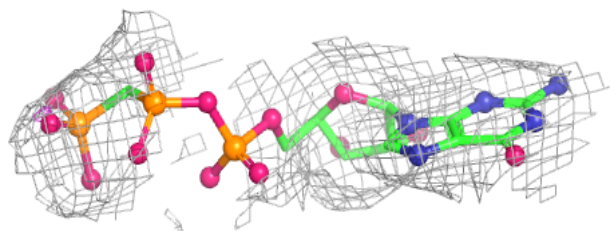
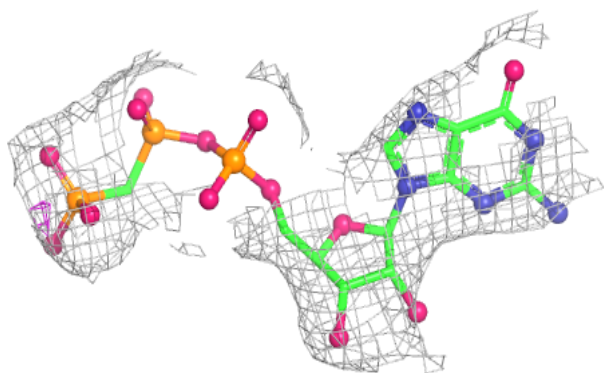
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GCP A 801:

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

**Electron density around GCP B 801:**

$2mF_o-DF_c$ (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.