



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:20 PM UTC

PDB ID : 2GVZ / pdb_00002gvz
Title : Crystal Structure of Complex of Gs- with The Catalytic Domains of Mammalian Adenylyl Cyclase: Complex with MANT-ATP and Mn
Authors : Mou, T.-C.; Sprang, S.R.
Deposited on : 2006-05-03
Resolution : 3.27 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

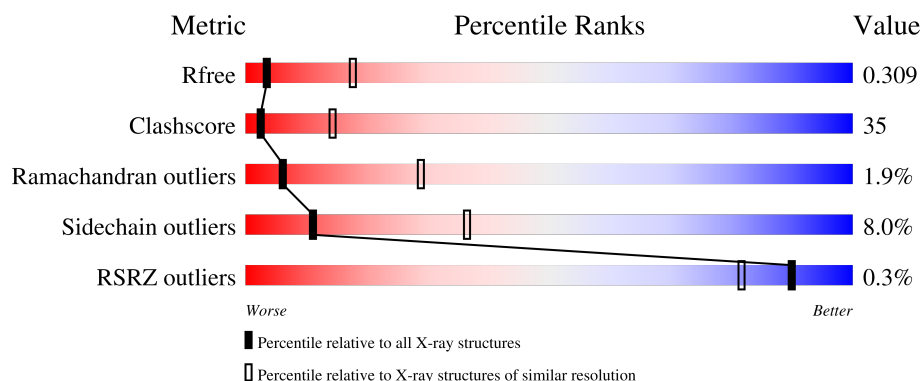
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	225	% 32% 40% 10% • 16%
2	B	212	39% 43% 7% 11%
3	C	394	35% 43% 6% 16%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5751 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 Adenylate cyclase type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1476	929	259	271	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	MET	-	initiating methionine	UNP P30803
A	357	HIS	-	expression tag	UNP P30803
A	358	HIS	-	expression tag	UNP P30803
A	359	HIS	-	expression tag	UNP P30803
A	360	HIS	-	expression tag	UNP P30803
A	361	HIS	-	expression tag	UNP P30803
A	362	HIS	-	expression tag	UNP P30803
A	476	MET	VAL	engineered mutation	UNP P30803

- Molecule 2 is a protein called Adenylate cyclase type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1457	930	239	278	10			

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s), alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	330	Total	C	N	O	S	0	0	0
			2702	1714	470	505	13			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

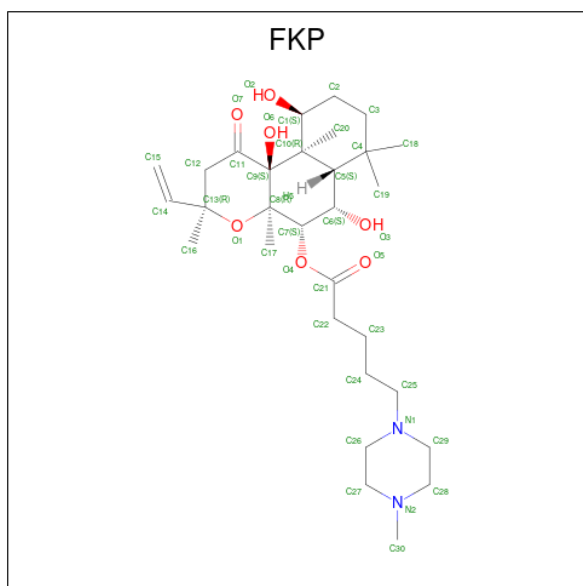
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

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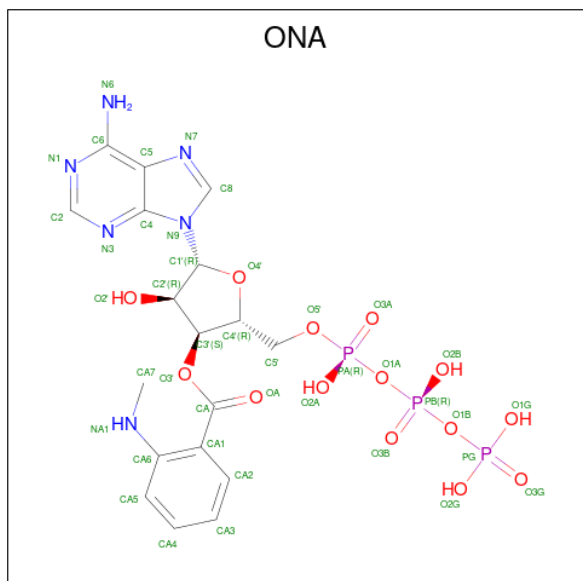
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is METHYLPIPERAZINOFORSKOLIN (CCD ID: FKP) (formula: $C_{30}H_{50}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			39	30	2	7		

- Molecule 6 is 3'-O-[2-(METHYLAMINO)BENZOYL]ADENOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE) (CCD ID: ONA) (formula: $C_{18}H_{23}N_6O_{14}P_3$).

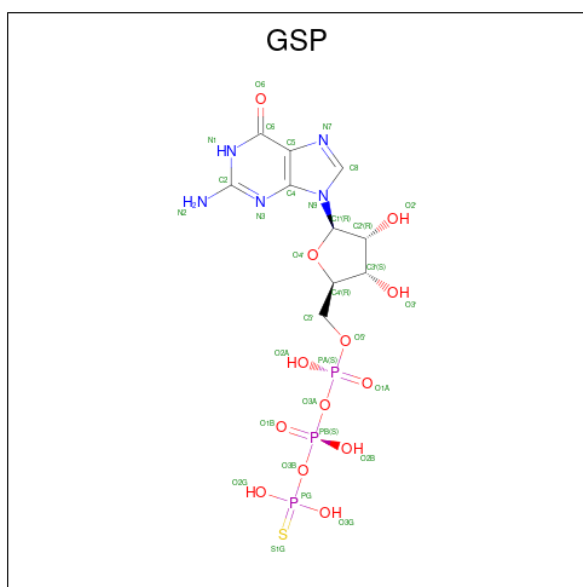


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			41	18	6	14	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).

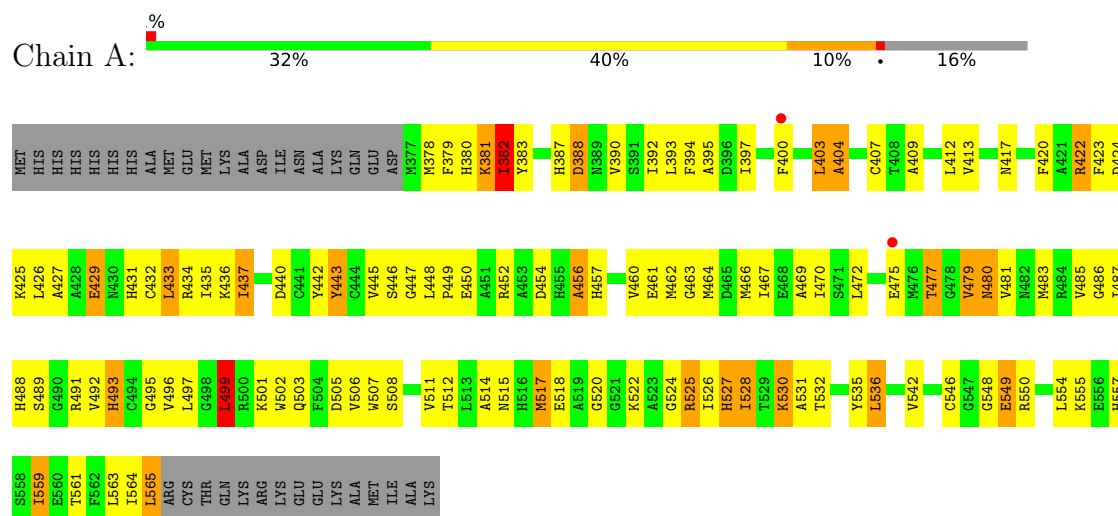


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

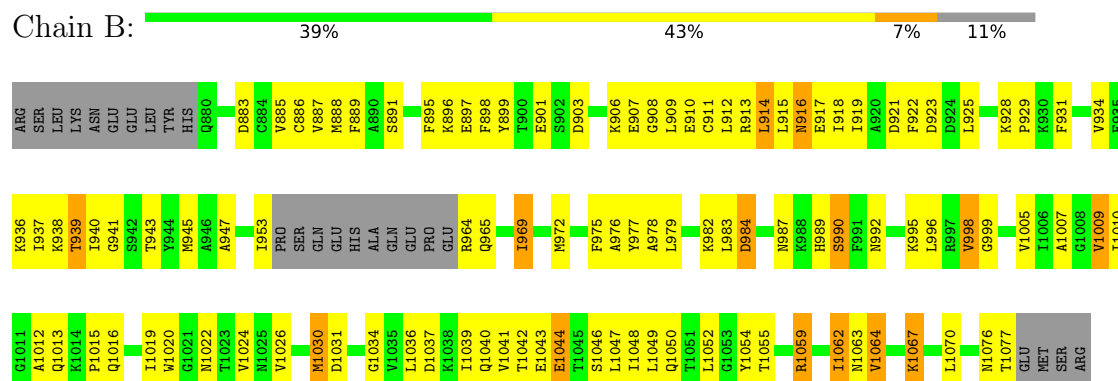
3 Residue-property plots

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.

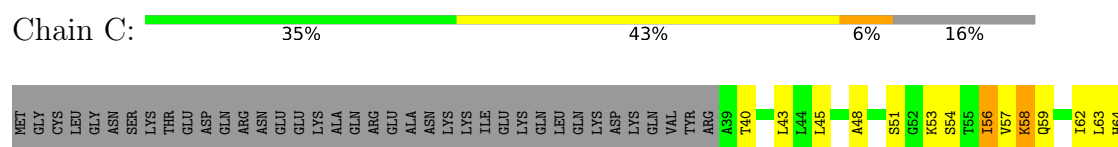
• Molecule 1: Adenylate cyclase type 5



• Molecule 2: Adenylate cyclase type 2



• Molecule 3: Guanine nucleotide-binding protein G(s), alpha subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.80Å 132.10Å 69.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 3.27 14.97 – 3.27	Depositor EDS
% Data completeness (in resolution range)	85.8 (14.97-3.27) 75.1 (14.97-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 3.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.330 0.260 , 0.309	Depositor DCC
R_{free} test set	774 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	1.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5751	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: MN, GSP, CL, ONA, FKP

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	0.54	0/1504	1.12	12/2027 (0.6%)
2	B	0.70	0/1481	1.08	9/1999 (0.5%)
3	C	0.62	0/2759	1.10	18/3733 (0.5%)
All	All	0.63	0/5744	1.10	39/7759 (0.5%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ASP	N-CA-C	14.41	131.10	113.23
3	C	327	GLU	CA-C-N	14.34	137.77	119.84
3	C	327	GLU	C-N-CA	14.34	137.77	119.84
1	A	525	ARG	N-CA-C	-13.59	88.34	109.95
2	B	912	LEU	N-CA-C	-9.50	100.00	111.69
2	B	969	ILE	N-CA-C	-9.20	101.88	110.53
2	B	976	ALA	N-CA-C	-8.09	102.42	111.07
3	C	182	ILE	N-CA-C	-7.88	102.59	110.62
2	B	998	VAL	N-CA-C	7.67	120.66	108.85
2	B	916	ASN	N-CA-C	-7.58	102.15	111.40
3	C	364	THR	N-CA-C	7.49	120.11	108.96
1	A	477	THR	N-CA-C	7.40	121.75	112.87
1	A	549	GLU	N-CA-C	-7.06	103.34	112.23
3	C	378	ASP	N-CA-C	-7.06	103.60	111.71
1	A	559	ILE	N-CA-C	6.97	118.04	108.84
3	C	320	THR	CA-C-N	6.55	126.52	120.03
3	C	320	THR	C-N-CA	6.55	126.52	120.03
2	B	1059	ARG	N-CA-C	-6.27	104.45	111.28
1	A	404	ALA	N-CA-C	6.09	117.59	111.07
3	C	244	ILE	N-CA-C	6.09	116.58	107.51
2	B	1064	VAL	N-CA-C	-5.79	98.69	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	330	GLU	N-CA-C	-5.79	97.72	108.02
1	A	517	MET	N-CA-C	-5.78	105.11	111.82
1	A	479	VAL	N-CA-C	5.77	121.33	109.34
2	B	1067	LYS	N-CA-C	-5.70	106.33	113.28
3	C	218	ASN	N-CA-C	5.63	118.61	110.28
3	C	310	ASP	N-CA-C	-5.58	106.64	113.50
1	A	407	CYS	N-CA-C	5.50	118.94	110.42
3	C	178	PHE	N-CA-C	5.31	116.75	111.07
3	C	139	ASP	N-CA-C	5.23	121.94	110.80
3	C	160	ARG	N-CA-C	-5.21	105.29	111.69
3	C	337	ALA	N-CA-C	5.16	117.31	111.02
3	C	58	LYS	N-CA-C	-5.13	105.38	111.69
3	C	348	ILE	CB-CA-C	-5.13	105.48	111.94
1	A	381	LYS	N-CA-C	5.12	121.71	110.80
1	A	499	LEU	N-CA-C	-5.11	106.98	114.39
1	A	443	TYR	N-CA-C	5.09	116.71	108.41
3	C	92	VAL	N-CA-C	-5.09	105.43	110.62
2	B	945	MET	N-CA-C	5.00	117.74	107.69

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	1476	0	1450	132	0
2	B	1457	0	1463	102	0
3	C	2702	0	2650	187	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	39	0	50	6	0
6	A	41	0	19	2	0
7	C	1	0	0	1	0
8	C	32	0	12	1	0
All	All	5751	0	5644	397	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 35.

All (397) 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)
2:B:925:LEU:HG	2:B:982:LYS:HZ2	1.23	1.00
3:C:231:ARG:HH21	3:C:272:LEU:HD22	1.26	0.98
3:C:63:LEU:HD13	3:C:373:ARG:HE	1.31	0.94
5:A:1:FKP:H173	5:A:1:FKP:H201	1.51	0.90
3:C:119:LEU:H	3:C:119:LEU:HD12	1.37	0.88
1:A:378:MET:HE2	3:C:284:THR:HG22	1.54	0.88
3:C:228:ARG:HA	3:C:231:ARG:HH11	1.41	0.84
1:A:517:MET:HE1	1:A:561:THR:HG23	1.61	0.82
3:C:183:ASP:HA	3:C:186:LYS:HE2	1.60	0.82
1:A:395:ALA:HB1	1:A:483:MET:HE3	1.59	0.81
3:C:373:ARG:HH12	3:C:376:PHE:HD2	1.29	0.81
1:A:381:LYS:O	1:A:382:ILE:HG13	1.80	0.81
1:A:542:VAL:HG12	1:A:564:ILE:HD13	1.63	0.81
3:C:207:ILE:HG12	3:C:224:VAL:HG12	1.61	0.81
1:A:404:ALA:HA	1:A:412:LEU:HD11	1.62	0.81
2:B:914:LEU:HD22	3:C:235:ILE:HD11	1.61	0.79
2:B:1026:VAL:HG22	2:B:1064:VAL:HG11	1.65	0.79
2:B:953:ILE:HD12	2:B:953:ILE:H	1.47	0.78
3:C:333:ARG:HA	3:C:336:ARG:HH12	1.50	0.77
1:A:403:LEU:HD12	1:A:412:LEU:HD21	1.67	0.75
2:B:998:VAL:HB	2:B:1039:ILE:HG23	1.69	0.75
1:A:435:ILE:HD11	1:A:445:VAL:HB	1.67	0.75
3:C:269:ALA:HB2	7:C:397:CL:CL	2.25	0.73
3:C:250:SER:HB3	3:C:297:LEU:HD22	1.71	0.72
2:B:1007:ALA:HB2	2:B:1019:ILE:HG22	1.73	0.70
3:C:59:GLN:HG3	3:C:372:ILE:HG13	1.74	0.70
1:A:508:SER:OG	1:A:511:VAL:HG23	1.91	0.70
1:A:378:MET:HE3	3:C:281:TRP:C	2.17	0.69
2:B:917:GLU:HG2	3:C:281:TRP:CZ2	2.28	0.68
3:C:380:ARG:O	3:C:384:GLN:HG2	1.94	0.68
1:A:530:LYS:HD2	1:A:531:ALA:N	2.08	0.68
3:C:107:VAL:HA	3:C:110:MET:HE2	1.77	0.67
1:A:528:ILE:HD12	1:A:564:ILE:HG12	1.76	0.67
2:B:1043:GLU:O	2:B:1046:SER:HB3	1.94	0.67
2:B:964:ARG:HE	2:B:964:ARG:HA	1.60	0.66
3:C:373:ARG:NH1	3:C:376:PHE:HD2	1.94	0.66
2:B:989:HIS:HD2	3:C:280:ARG:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:VAL:HB	1:A:446:SER:O	1.96	0.65
1:A:392:ILE:HG12	1:A:445:VAL:HG23	1.78	0.65
1:A:546:CYS:O	1:A:549:GLU:HG2	1.96	0.65
1:A:527:HIS:NE2	1:A:561:THR:HG21	2.10	0.65
2:B:887:VAL:HG21	2:B:1024:VAL:HG22	1.78	0.65
3:C:172:ILE:HD12	3:C:174:CYS:SG	2.37	0.65
1:A:445:VAL:HG22	1:A:446:SER:H	1.61	0.64
1:A:493:HIS:HB2	1:A:507:TRP:O	1.96	0.64
3:C:53:LYS:HG2	3:C:247:VAL:HG21	1.79	0.64
3:C:163:TYR:OH	3:C:176:GLN:HB2	1.97	0.64
3:C:63:LEU:HD13	3:C:373:ARG:NE	2.10	0.63
3:C:245:ILE:HA	3:C:288:ILE:HG23	1.80	0.63
1:A:475:GLU:HB3	1:A:477:THR:HG23	1.81	0.63
3:C:59:GLN:HE22	3:C:369:THR:N	1.96	0.63
3:C:144:PRO:O	3:C:148:GLU:HG3	1.99	0.63
1:A:417:ASN:HA	2:B:1010:ILE:HD11	1.81	0.63
1:A:460:VAL:HG21	1:A:536:LEU:HD11	1.80	0.63
3:C:277:TRP:CE2	3:C:349:SER:HA	2.34	0.63
3:C:297:LEU:O	3:C:301:VAL:HG23	1.99	0.62
3:C:277:TRP:NE1	3:C:349:SER:HA	2.15	0.62
1:A:456:ALA:O	1:A:460:VAL:HG23	1.99	0.62
2:B:1059:ARG:HH12	2:B:1062:ILE:HG13	1.65	0.62
3:C:63:LEU:CD1	3:C:373:ARG:HH21	2.12	0.62
3:C:87:GLU:O	3:C:90:THR:HG22	2.00	0.62
2:B:1062:ILE:HD13	2:B:1063:ASN:N	2.14	0.61
3:C:366:ALA:HB3	8:C:395:GSP:N7	2.15	0.61
1:A:470:ILE:HD11	1:A:483:MET:SD	2.40	0.61
1:A:488:HIS:HB3	1:A:514:ALA:HB2	1.83	0.61
1:A:397:ILE:HG12	1:A:440:ASP:HB2	1.81	0.61
2:B:914:LEU:HD13	3:C:235:ILE:HD12	1.83	0.60
3:C:63:LEU:HD12	3:C:373:ARG:HH21	1.65	0.60
3:C:386:MET:HB2	3:C:388:LEU:HG	1.83	0.60
2:B:917:GLU:HG2	3:C:281:TRP:HZ2	1.64	0.60
3:C:45:LEU:HA	3:C:245:ILE:O	2.01	0.60
3:C:246:PHE:O	3:C:290:PHE:HB2	2.01	0.60
6:A:100:ONA:HA72	2:B:1022:ASN:HB2	1.83	0.60
3:C:43:LEU:HB2	3:C:221:MET:HE3	1.84	0.59
2:B:990:SER:HA	3:C:235:ILE:HG21	1.83	0.59
3:C:353:GLY:HA2	3:C:357:HIS:CD2	2.37	0.59
3:C:166:SER:HB2	3:C:171:LEU:HD23	1.84	0.59
5:A:1:FKP:H201	5:A:1:FKP:C17	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:ALA:C	3:C:326:PRO:HD3	2.27	0.59
1:A:487:ILE:HG22	1:A:488:HIS:H	1.66	0.58
2:B:915:LEU:O	2:B:919:ILE:HG12	2.02	0.58
2:B:1030:MET:HE1	2:B:1041:VAL:HA	1.85	0.58
3:C:95:ILE:HG23	3:C:178:PHE:CE1	2.39	0.58
3:C:244:ILE:HB	3:C:287:VAL:HG12	1.84	0.58
2:B:917:GLU:O	2:B:921:ASP:HB2	2.04	0.57
3:C:124:ASN:O	3:C:128:VAL:HG23	2.03	0.57
1:A:487:ILE:HG22	1:A:488:HIS:N	2.20	0.57
2:B:1010:ILE:HB	2:B:1020:TRP:HH2	1.69	0.57
1:A:461:GLU:HA	1:A:464:MET:HB2	1.86	0.57
2:B:886:CYS:HB2	2:B:969:ILE:HD13	1.87	0.57
3:C:102:ALA:O	3:C:106:ILE:HG13	2.05	0.57
2:B:937:ILE:HD11	2:B:947:ALA:HB3	1.86	0.57
3:C:171:LEU:HD12	3:C:172:ILE:H	1.70	0.57
3:C:249:ALA:HB3	3:C:252:SER:HB2	1.86	0.56
3:C:252:SER:HB3	3:C:265:ARG:HD2	1.87	0.56
2:B:964:ARG:CZ	2:B:965:GLN:HE21	2.18	0.56
3:C:92:VAL:O	3:C:95:ILE:HB	2.06	0.56
1:A:436:LYS:HE2	1:A:503:GLN:HB3	1.88	0.56
2:B:888:MET:SD	2:B:972:MET:HE2	2.45	0.56
2:B:964:ARG:NH2	2:B:965:GLN:HE21	2.04	0.56
2:B:1067:LYS:HD3	2:B:1070:LEU:HD11	1.88	0.56
1:A:445:VAL:HG11	1:A:448:LEU:HD12	1.87	0.55
2:B:1030:MET:HE2	2:B:1042:THR:HG23	1.88	0.55
3:C:248:VAL:HG12	3:C:249:ALA:N	2.21	0.55
2:B:922:PHE:CD2	2:B:979:LEU:HD22	2.42	0.55
2:B:936:LYS:HE3	2:B:939:THR:HG23	1.88	0.55
3:C:143:PRO:HB2	3:C:145:GLU:OE2	2.05	0.55
3:C:366:ALA:HA	3:C:372:ILE:HD11	1.88	0.55
2:B:897:GLU:HG3	2:B:898:PHE:N	2.22	0.55
1:A:486:GLY:HA3	1:A:518:GLU:HA	1.88	0.55
3:C:99:LEU:HD11	3:C:179:LEU:HD23	1.89	0.55
3:C:205:SER:HA	3:C:230:GLU:OE2	2.06	0.55
3:C:166:SER:HA	3:C:169:TYR:CE2	2.41	0.55
1:A:530:LYS:HE3	1:A:559:ILE:HG23	1.88	0.55
5:A:1:FKP:H221	2:B:896:LYS:HE2	1.87	0.54
1:A:382:ILE:HG22	2:B:916:ASN:ND2	2.22	0.54
1:A:392:ILE:HD13	1:A:511:VAL:HG22	1.89	0.54
1:A:424:ASP:HB2	2:B:1012:ALA:HB3	1.87	0.54
2:B:895:PHE:CZ	2:B:915:LEU:HB2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:SER:C	3:C:253:TYR:H	2.15	0.54
1:A:526:ILE:N	1:A:526:ILE:HD12	2.23	0.54
2:B:1034:GLY:HA2	2:B:1040:GLN:NE2	2.22	0.54
3:C:238:PHE:CZ	3:C:282:LEU:HD11	2.43	0.54
2:B:1030:MET:HE1	2:B:1042:THR:N	2.23	0.54
3:C:99:LEU:HD11	3:C:182:ILE:CD1	2.37	0.54
1:A:491:ARG:HH21	2:B:901:GLU:HG2	1.73	0.54
2:B:891:SER:HB3	2:B:943:THR:HG23	1.90	0.53
2:B:914:LEU:HD22	3:C:235:ILE:CD1	2.37	0.53
2:B:914:LEU:O	2:B:918:ILE:HG13	2.08	0.53
2:B:1050:GLN:HA	2:B:1054:TYR:O	2.09	0.53
1:A:392:ILE:HD11	1:A:492:VAL:CG1	2.39	0.53
2:B:885:VAL:HG21	2:B:1005:VAL:HG22	1.91	0.53
3:C:124:ASN:OD1	3:C:127:ARG:HD2	2.09	0.53
3:C:181:LYS:O	3:C:185:ILE:HG13	2.09	0.52
3:C:324:ALA:HB1	3:C:326:PRO:HD3	1.91	0.52
3:C:360:TYR:OH	3:C:386:MET:HG3	2.09	0.52
1:A:528:ILE:N	1:A:528:ILE:HD13	2.24	0.52
2:B:1049:LEU:HD22	2:B:1054:TYR:HD1	1.73	0.52
1:A:515:ASN:O	1:A:518:GLU:HB3	2.10	0.52
3:C:304:GLY:C	3:C:306:SER:H	2.18	0.52
3:C:353:GLY:HA2	3:C:357:HIS:NE2	2.25	0.52
1:A:520:GLY:O	1:A:550:ARG:HD2	2.09	0.51
1:A:548:GLY:O	1:A:555:LYS:HB2	2.10	0.51
1:A:447:GLY:O	1:A:448:LEU:HD23	2.10	0.51
3:C:315:PHE:HB2	3:C:340:PHE:CE2	2.45	0.51
1:A:462:MET:O	1:A:466:MET:HG3	2.09	0.51
1:A:461:GLU:O	1:A:464:MET:HB2	2.09	0.51
3:C:376:PHE:O	3:C:380:ARG:HG3	2.11	0.51
3:C:325:THR:N	3:C:326:PRO:HD3	2.25	0.51
2:B:1007:ALA:CB	2:B:1019:ILE:HG22	2.40	0.51
2:B:903:ASP:HA	2:B:907:GLU:OE2	2.11	0.51
3:C:376:PHE:HA	3:C:379:CYS:HB2	1.93	0.51
2:B:940:ILE:H	2:B:940:ILE:HD12	1.75	0.51
3:C:250:SER:O	3:C:297:LEU:HD13	2.11	0.51
1:A:436:LYS:HG2	1:A:437:ILE:H	1.76	0.51
1:A:445:VAL:HG22	1:A:446:SER:N	2.24	0.51
3:C:128:VAL:O	3:C:132:LEU:HG	2.11	0.51
2:B:1049:LEU:O	2:B:1054:TYR:HB2	2.11	0.50
3:C:103:ILE:HG23	3:C:104:GLU:N	2.27	0.50
3:C:160:ARG:O	3:C:163:TYR:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ILE:HG22	2:B:916:ASN:CG	2.36	0.50
1:A:528:ILE:HG22	1:A:532:THR:HG21	1.93	0.50
3:C:59:GLN:HB3	3:C:372:ILE:HG21	1.92	0.50
1:A:422:ARG:O	1:A:426:LEU:HG	2.12	0.50
2:B:1010:ILE:O	2:B:1015:PRO:HA	2.11	0.50
3:C:324:ALA:C	3:C:326:PRO:CD	2.85	0.50
1:A:456:ALA:HB1	1:A:536:LEU:HD12	1.93	0.50
1:A:548:GLY:HA3	1:A:555:LYS:HD3	1.94	0.50
2:B:925:LEU:CG	2:B:982:LYS:HZ2	2.11	0.50
2:B:995:LYS:HB2	2:B:1036:LEU:HD13	1.94	0.50
1:A:397:ILE:HD13	1:A:483:MET:SD	2.52	0.50
3:C:165:ARG:HB3	3:C:168:GLU:OE2	2.12	0.50
3:C:318:TYR:CE2	3:C:340:PHE:HB2	2.47	0.50
1:A:512:THR:HA	5:A:1:FKP:H203	1.93	0.49
2:B:1009:VAL:HG12	2:B:1010:ILE:H	1.75	0.49
3:C:134:VAL:HA	3:C:137:VAL:HG23	1.93	0.49
3:C:292:ASN:CG	3:C:293:LYS:H	2.20	0.49
2:B:922:PHE:HZ	2:B:983:LEU:HB2	1.77	0.49
2:B:987:ASN:HB3	2:B:992:ASN:O	2.11	0.49
3:C:99:LEU:CD1	3:C:179:LEU:HD23	2.42	0.49
2:B:964:ARG:NH1	2:B:965:GLN:HE21	2.11	0.49
3:C:45:LEU:HD11	3:C:221:MET:HE2	1.94	0.49
2:B:931:PHE:HB3	2:B:934:VAL:CG2	2.43	0.49
3:C:233:LYS:O	3:C:236:GLN:HB2	2.13	0.49
1:A:403:LEU:HD12	1:A:412:LEU:CD2	2.42	0.49
2:B:889:PHE:O	2:B:998:VAL:HG13	2.12	0.49
2:B:923:ASP:C	2:B:925:LEU:H	2.20	0.49
3:C:107:VAL:HG23	3:C:108:ALA:N	2.28	0.49
2:B:928:LYS:HG2	2:B:929:PRO:HD2	1.95	0.49
3:C:57:VAL:HG21	3:C:223:ASP:HB2	1.94	0.49
3:C:100:LYS:HG3	3:C:146:PHE:CZ	2.48	0.49
1:A:378:MET:HE1	3:C:283:ARG:H	1.78	0.48
1:A:417:ASN:ND2	2:B:1010:ILE:HG13	2.28	0.48
1:A:466:MET:O	1:A:469:ALA:HB3	2.13	0.48
3:C:334:VAL:O	3:C:335:THR:C	2.56	0.48
1:A:393:LEU:C	1:A:393:LEU:HD23	2.38	0.48
1:A:435:ILE:CG2	1:A:505:ASP:HA	2.44	0.48
1:A:527:HIS:CE1	1:A:561:THR:HG21	2.48	0.48
2:B:1030:MET:CE	2:B:1042:THR:HG23	2.43	0.48
1:A:392:ILE:HD11	1:A:492:VAL:HG12	1.95	0.48
3:C:203:LEU:HD11	3:C:227:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:VAL:HG11	3:C:380:ARG:HD2	1.95	0.48
3:C:336:ARG:HB3	3:C:336:ARG:NH1	2.28	0.48
1:A:456:ALA:HB2	1:A:535:TYR:HB3	1.96	0.48
3:C:274:LYS:HG3	3:C:348:ILE:HD13	1.95	0.48
1:A:463:GLY:O	1:A:467:ILE:HG12	2.13	0.48
1:A:470:ILE:O	1:A:470:ILE:HG22	2.13	0.48
2:B:909:LEU:O	2:B:911:CYS:N	2.47	0.48
2:B:1055:THR:HB	2:B:1076:ASN:HD22	1.78	0.48
1:A:382:ILE:HG22	2:B:916:ASN:CB	2.44	0.48
3:C:343:ASP:HA	3:C:346:LEU:HB2	1.95	0.48
3:C:288:ILE:HG13	3:C:360:TYR:O	2.14	0.47
1:A:382:ILE:HG12	2:B:913:ARG:NH1	2.29	0.47
3:C:110:MET:HG2	3:C:162:CYS:SG	2.54	0.47
1:A:470:ILE:HG21	1:A:481:VAL:HG23	1.97	0.47
3:C:58:LYS:O	3:C:62:ILE:HG12	2.14	0.47
3:C:325:THR:N	3:C:326:PRO:CD	2.78	0.47
1:A:548:GLY:HA2	1:A:554:LEU:HB2	1.95	0.47
3:C:250:SER:CB	3:C:297:LEU:HD22	2.41	0.47
1:A:409:ALA:O	1:A:413:VAL:HG23	2.15	0.47
3:C:64:HIS:NE2	3:C:373:ARG:NH1	2.62	0.47
3:C:248:VAL:HG12	3:C:249:ALA:H	1.79	0.47
3:C:266:LEU:HD23	3:C:312:PHE:CZ	2.49	0.47
1:A:528:ILE:HG12	1:A:528:ILE:O	2.13	0.47
3:C:207:ILE:CG1	3:C:224:VAL:HG12	2.39	0.47
3:C:59:GLN:OE1	3:C:369:THR:HG23	2.14	0.47
3:C:228:ARG:HA	3:C:231:ARG:NH1	2.20	0.47
3:C:368:ASP:C	3:C:370:GLU:N	2.70	0.47
1:A:485:VAL:HG11	1:A:526:ILE:HG13	1.97	0.47
3:C:100:LYS:NZ	3:C:140:PHE:HB2	2.30	0.47
3:C:355:GLY:HA2	3:C:358:TYR:CE1	2.50	0.47
1:A:495:GLY:O	1:A:496:VAL:HG13	2.14	0.47
3:C:276:ILE:HG23	3:C:282:LEU:HD13	1.97	0.47
1:A:472:LEU:HD11	1:A:481:VAL:HG22	1.97	0.46
3:C:99:LEU:HD11	3:C:182:ILE:HD13	1.97	0.46
3:C:257:ILE:HG13	3:C:260:ASP:OD1	2.15	0.46
3:C:246:PHE:HB3	3:C:289:LEU:HA	1.97	0.46
3:C:308:ILE:HB	3:C:315:PHE:CD2	2.50	0.46
1:A:400:PHE:N	6:A:100:ONA:O2G	2.48	0.46
2:B:931:PHE:HB3	2:B:934:VAL:HG21	1.97	0.46
3:C:51:SER:HB3	3:C:247:VAL:HG12	1.97	0.46
3:C:131:ILE:HG13	3:C:153:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:SER:O	3:C:253:TYR:N	2.48	0.46
3:C:253:TYR:CZ	3:C:308:ILE:HG12	2.50	0.46
3:C:203:LEU:HD21	3:C:227:GLN:HG3	1.96	0.46
1:A:506:VAL:HG23	1:A:511:VAL:HG11	1.97	0.46
3:C:98:ASN:O	3:C:99:LEU:C	2.59	0.46
3:C:231:ARG:HG2	3:C:234:TRP:CZ2	2.51	0.46
3:C:248:VAL:HG21	3:C:345:PHE:CZ	2.51	0.46
3:C:54:SER:O	3:C:58:LYS:HG3	2.15	0.46
3:C:134:VAL:HA	3:C:137:VAL:CG2	2.45	0.46
3:C:379:CYS:O	3:C:383:ILE:HG13	2.16	0.46
1:A:550:ARG:HB2	1:A:550:ARG:NH1	2.31	0.46
2:B:887:VAL:HG11	2:B:1024:VAL:HG13	1.97	0.46
1:A:491:ARG:HH22	2:B:907:GLU:HG3	1.81	0.45
1:A:505:ASP:HB3	1:A:507:TRP:CZ2	2.51	0.45
3:C:279:ASN:O	3:C:283:ARG:HG3	2.16	0.45
1:A:434:ARG:HG3	1:A:442:TYR:CZ	2.51	0.45
2:B:998:VAL:HG12	2:B:999:GLY:N	2.30	0.45
3:C:382:ILE:HG23	3:C:386:MET:HG2	1.97	0.45
1:A:378:MET:CE	3:C:283:ARG:H	2.29	0.45
1:A:393:LEU:HD13	1:A:462:MET:HB3	1.99	0.45
1:A:394:PHE:HB3	1:A:518:GLU:HB2	1.98	0.45
2:B:1062:ILE:HD13	2:B:1062:ILE:C	2.42	0.45
3:C:341:ILE:O	3:C:341:ILE:HG22	2.16	0.45
1:A:491:ARG:HH22	2:B:907:GLU:CG	2.30	0.45
2:B:984:ASP:O	2:B:987:ASN:HB2	2.17	0.45
1:A:507:TRP:O	1:A:508:SER:HB3	2.16	0.45
1:A:518:GLU:C	1:A:520:GLY:H	2.25	0.45
2:B:975:PHE:O	2:B:978:ALA:HB3	2.17	0.45
1:A:436:LYS:HG2	1:A:437:ILE:N	2.31	0.45
2:B:922:PHE:CG	2:B:979:LEU:HD22	2.51	0.45
3:C:249:ALA:C	3:C:251:SER:N	2.75	0.45
1:A:382:ILE:HG13	1:A:382:ILE:O	2.17	0.44
1:A:397:ILE:HB	1:A:400:PHE:HB2	1.99	0.44
1:A:429:GLU:C	1:A:431:HIS:H	2.24	0.44
3:C:100:LYS:HA	3:C:146:PHE:HZ	1.81	0.44
1:A:470:ILE:HD11	1:A:483:MET:HG2	1.99	0.44
1:A:527:HIS:CD2	1:A:561:THR:HG21	2.52	0.44
3:C:59:GLN:CB	3:C:372:ILE:HG21	2.47	0.44
3:C:101:GLU:O	3:C:102:ALA:C	2.60	0.44
1:A:423:PHE:HB3	1:A:442:TYR:CZ	2.53	0.44
1:A:548:GLY:C	1:A:555:LYS:HD3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:HA	1:A:502:TRP:HE1	1.81	0.44
1:A:522:LYS:C	1:A:524:GLY:N	2.76	0.44
1:A:457:HIS:O	1:A:460:VAL:HB	2.17	0.44
1:A:488:HIS:CG	1:A:489:SER:N	2.86	0.44
3:C:104:GLU:HA	3:C:107:VAL:HG22	2.00	0.44
3:C:253:TYR:CE1	3:C:308:ILE:HG12	2.52	0.44
1:A:436:LYS:HD3	2:B:938:LYS:NZ	2.33	0.44
2:B:925:LEU:HD12	2:B:979:LEU:HD23	1.99	0.44
3:C:150:ALA:O	3:C:153:LEU:HB2	2.17	0.44
3:C:287:VAL:O	3:C:287:VAL:HG23	2.17	0.44
1:A:420:PHE:HD2	2:B:1010:ILE:HD11	1.83	0.44
1:A:435:ILE:HD13	1:A:506:VAL:CG2	2.48	0.44
3:C:100:LYS:O	3:C:104:GLU:HG2	2.18	0.44
2:B:906:LYS:O	2:B:907:GLU:HB2	2.18	0.43
2:B:1050:GLN:HG2	2:B:1054:TYR:O	2.16	0.43
3:C:179:LEU:O	3:C:182:ILE:HG12	2.18	0.43
3:C:107:VAL:HG11	3:C:153:LEU:HD13	2.01	0.43
3:C:292:ASN:CG	3:C:293:LYS:N	2.75	0.43
3:C:364:THR:CG2	3:C:375:VAL:HG11	2.48	0.43
1:A:449:PRO:HG2	1:A:450:GLU:H	1.83	0.43
3:C:228:ARG:HB2	3:C:259:GLU:HG2	2.00	0.43
1:A:435:ILE:HD12	1:A:443:TYR:CD2	2.54	0.43
3:C:95:ILE:HG12	3:C:178:PHE:CZ	2.53	0.43
3:C:368:ASP:HB3	3:C:371:ASN:HB3	1.99	0.43
2:B:922:PHE:CZ	2:B:983:LEU:HB2	2.53	0.43
2:B:984:ASP:HA	2:B:987:ASN:ND2	2.34	0.43
3:C:277:TRP:O	3:C:357:HIS:HE1	2.01	0.43
1:A:496:VAL:HG12	1:A:503:GLN:O	2.19	0.43
1:A:517:MET:HE3	1:A:527:HIS:HB3	2.01	0.43
1:A:526:ILE:N	1:A:526:ILE:CD1	2.82	0.43
2:B:1044:GLU:HA	2:B:1047:LEU:HD12	2.01	0.43
3:C:230:GLU:C	3:C:232:ARG:H	2.26	0.43
2:B:886:CYS:SG	2:B:969:ILE:HA	2.59	0.43
3:C:234:TRP:C	3:C:236:GLN:N	2.77	0.43
3:C:337:ALA:O	3:C:341:ILE:HG13	2.19	0.43
3:C:372:ILE:HA	3:C:375:VAL:HG23	2.01	0.43
3:C:372:ILE:O	3:C:375:VAL:HG23	2.19	0.43
1:A:425:LYS:C	1:A:427:ALA:N	2.77	0.43
1:A:433:LEU:HD23	1:A:448:LEU:HB2	2.00	0.43
2:B:1009:VAL:HG13	2:B:1016:GLN:C	2.44	0.43
3:C:119:LEU:HA	3:C:158:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ILE:CG2	1:A:481:VAL:HG23	2.49	0.42
2:B:1050:GLN:C	2:B:1052:LEU:H	2.25	0.42
3:C:59:GLN:OE1	3:C:59:GLN:HA	2.19	0.42
3:C:147:TYR:CD1	3:C:186:LYS:HB3	2.55	0.42
3:C:251:SER:HB3	3:C:297:LEU:N	2.34	0.42
1:A:382:ILE:O	1:A:382:ILE:CG1	2.66	0.42
1:A:525:ARG:NH2	1:A:565:LEU:HG	2.34	0.42
3:C:45:LEU:HD12	3:C:222:PHE:O	2.19	0.42
1:A:381:LYS:HD3	1:A:383:TYR:CE2	2.55	0.42
1:A:420:PHE:HA	1:A:423:PHE:HB2	2.00	0.42
1:A:501:LYS:HB2	2:B:936:LYS:HD2	2.02	0.42
3:C:201:ARG:HD3	3:C:201:ARG:C	2.44	0.42
3:C:260:ASP:O	3:C:261:ASN:HB2	2.19	0.42
1:A:527:HIS:ND1	1:A:563:LEU:HD21	2.34	0.42
2:B:1009:VAL:HA	2:B:1016:GLN:O	2.19	0.42
1:A:497:LEU:HA	2:B:916:ASN:OD1	2.20	0.42
2:B:899:TYR:HE1	2:B:908:GLY:O	2.03	0.42
3:C:368:ASP:C	3:C:370:GLU:H	2.26	0.42
1:A:378:MET:HE1	3:C:283:ARG:HB2	2.02	0.42
2:B:940:ILE:HB	2:B:943:THR:HB	2.01	0.42
2:B:983:LEU:HD22	2:B:996:LEU:HD13	2.02	0.42
3:C:331:ASP:OD1	3:C:333:ARG:HG3	2.20	0.42
3:C:376:PHE:O	3:C:376:PHE:CG	2.72	0.42
1:A:460:VAL:CG2	1:A:536:LEU:HD11	2.49	0.42
1:A:501:LYS:O	1:A:502:TRP:C	2.62	0.42
3:C:304:GLY:C	3:C:306:SER:N	2.76	0.42
3:C:343:ASP:O	3:C:347:ARG:HG3	2.20	0.42
1:A:378:MET:CE	3:C:283:ARG:N	2.83	0.42
3:C:242:THR:HG21	3:C:383:ILE:HG23	2.01	0.42
1:A:392:ILE:CD1	1:A:511:VAL:HG22	2.49	0.41
2:B:1036:LEU:O	2:B:1037:ASP:HB2	2.20	0.41
3:C:320:THR:HA	3:C:321:PRO:HD3	1.79	0.41
3:C:230:GLU:C	3:C:232:ARG:N	2.78	0.41
3:C:244:ILE:O	3:C:288:ILE:N	2.44	0.41
3:C:95:ILE:HG12	3:C:178:PHE:HZ	1.85	0.41
3:C:373:ARG:NE	3:C:373:ARG:HA	2.34	0.41
2:B:977:TYR:CE1	2:B:1039:ILE:HD11	2.55	0.41
3:C:385:ARG:C	3:C:387:HIS:H	2.29	0.41
1:A:452:ARG:HG2	1:A:454:ASP:HB3	2.02	0.41
2:B:1042:THR:HB	2:B:1044:GLU:OE2	2.20	0.41
3:C:56:ILE:O	3:C:59:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:LEU:HD21	3:C:168:GLU:HB2	2.02	0.41
3:C:157:GLU:O	3:C:157:GLU:HG2	2.19	0.41
3:C:372:ILE:HA	3:C:375:VAL:CG2	2.51	0.41
3:C:378:ASP:O	3:C:381:ASP:HB3	2.20	0.41
2:B:1048:ILE:O	2:B:1052:LEU:HG	2.19	0.41
1:A:435:ILE:HD12	1:A:443:TYR:HD2	1.84	0.41
1:A:449:PRO:HG2	1:A:450:GLU:N	2.35	0.41
1:A:548:GLY:HA2	1:A:555:LYS:N	2.35	0.41
3:C:225:GLY:HA3	3:C:230:GLU:HB3	2.03	0.41
3:C:251:SER:C	3:C:253:TYR:N	2.79	0.41
1:A:452:ARG:C	1:A:454:ASP:H	2.29	0.41
5:A:1:FKP:H202	5:A:1:FKP:H22	1.72	0.41
5:A:1:FKP:H162	2:B:896:LYS:HA	2.03	0.41
3:C:171:LEU:HD12	3:C:172:ILE:N	2.35	0.41
1:A:532:THR:O	1:A:536:LEU:HD13	2.21	0.41
2:B:923:ASP:C	2:B:925:LEU:N	2.78	0.41
3:C:337:ALA:O	3:C:340:PHE:HB3	2.20	0.41
1:A:423:PHE:CE1	1:A:483:MET:HE2	2.55	0.40
1:A:557:HIS:HB2	1:A:559:ILE:HD11	2.02	0.40
3:C:87:GLU:C	3:C:89:ALA:H	2.28	0.40
3:C:296:LEU:O	3:C:297:LEU:C	2.65	0.40
1:A:381:LYS:O	1:A:382:ILE:C	2.63	0.40
1:A:422:ARG:O	1:A:422:ARG:HG3	2.22	0.40
2:B:995:LYS:HB3	2:B:1036:LEU:HB3	2.03	0.40
3:C:103:ILE:HG23	3:C:104:GLU:H	1.85	0.40
3:C:219:PHE:CZ	3:C:380:ARG:HG2	2.57	0.40
3:C:371:ASN:O	3:C:375:VAL:HG22	2.21	0.40
1:A:379:PHE:O	1:A:380:HIS:C	2.64	0.40
2:B:990:SER:C	2:B:992:ASN:N	2.79	0.40
2:B:1043:GLU:O	2:B:1047:LEU:HG	2.21	0.40
3:C:235:ILE:HA	3:C:238:PHE:CG	2.57	0.40
3:C:245:ILE:HG12	3:C:288:ILE:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	187/225 (83%)	153 (82%)	30 (16%)	4 (2%)	5	26
2	B	184/212 (87%)	156 (85%)	26 (14%)	2 (1%)	11	39
3	C	326/394 (83%)	270 (83%)	49 (15%)	7 (2%)	5	26
All	All	697/831 (84%)	579 (83%)	105 (15%)	13 (2%)	6	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	351	ALA
1	A	382	ILE
1	A	456	ALA
1	A	479	VAL
1	A	480	ASN
2	B	910	GLU
3	C	48	ALA
3	C	252	SER
3	C	328	PRO
2	B	941	GLY
3	C	242	THR
3	C	148	GLU
3	C	175	ALA

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	158/189 (84%)	141 (89%)	17 (11%)	6	24
2	B	161/184 (88%)	149 (92%)	12 (8%)	12	38
3	C	297/351 (85%)	277 (93%)	20 (7%)	15	42
All	All	616/724 (85%)	567 (92%)	49 (8%)	11	36

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	ILE
1	A	387	HIS
1	A	388	ASP
1	A	403	LEU
1	A	422	ARG
1	A	429	GLU
1	A	432	CYS
1	A	433	LEU
1	A	437	ILE
1	A	480	ASN
1	A	493	HIS
1	A	499	LEU
1	A	527	HIS
1	A	528	ILE
1	A	530	LYS
1	A	536	LEU
1	A	565	LEU
2	B	883	ASP
2	B	914	LEU
2	B	939	THR
2	B	984	ASP
2	B	990	SER
2	B	1009	VAL
2	B	1013	GLN
2	B	1030	MET
2	B	1031	ASP
2	B	1044	GLU
2	B	1062	ILE
2	B	1077	THR
3	C	40	THR
3	C	56	ILE
3	C	87	GLU
3	C	119	LEU
3	C	155	GLU
3	C	195	GLN
3	C	200	CYS
3	C	218	ASN
3	C	227	GLN
3	C	229	ASP
3	C	255	MET
3	C	257	ILE
3	C	295	ASP

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Mol	Chain	Res	Type
3	C	314	GLU
3	C	326	PRO
3	C	327	GLU
3	C	328	PRO
3	C	370	GLU
3	C	374	ARG
3	C	375	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	410	GLN
1	A	493	HIS
1	A	503	GLN
1	A	509	ASN
1	A	515	ASN
2	B	965	GLN
2	B	989	HIS
2	B	992	ASN
2	B	1001	ASN
2	B	1013	GLN
2	B	1016	GLN
2	B	1050	GLN
2	B	1076	ASN
3	C	93	GLN
3	C	124	ASN
3	C	176	GLN
3	C	213	GLN
3	C	220	HIS
3	C	371	ASN
3	C	377	ASN
3	C	384	GLN
3	C	387	HIS

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](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
6	ONA	A	100	4	43,44,44	4.12	18 (41%)	63,67,67	2.62	26 (41%)
5	FKP	A	1	-	40,42,42	2.73	20 (50%)	52,68,68	2.74	21 (40%)
8	GSP	C	395	4	33,34,34	1.67	6 (18%)	47,54,54	1.52	6 (12%)

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
6	ONA	A	100	4	-	6/32/48/48	0/4/4/4
5	FKP	A	1	-	-	12/14/97/97	0/4/4/4
8	GSP	C	395	4	-	3/21/38/38	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	100	ONA	CA4-CA5	12.12	1.59	1.38
6	A	100	ONA	CA5-CA6	12.09	1.59	1.39
6	A	100	ONA	CA3-CA2	10.52	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	100	ONA	CA3-CA4	8.60	1.57	1.38
6	A	100	ONA	OA-CA	7.72	1.44	1.22
5	A	1	FKP	C2-C1	7.31	1.63	1.52
5	A	1	FKP	C10-C5	6.58	1.67	1.56
8	C	395	GSP	PB-O3B	5.97	1.65	1.59
5	A	1	FKP	C9-C10	5.22	1.71	1.57
5	A	1	FKP	C12-C11	5.11	1.58	1.50
6	A	100	ONA	C2-N1	5.02	1.42	1.33
6	A	100	ONA	PB-O1B	-4.60	1.54	1.59
6	A	100	ONA	PG-O3G	4.30	1.63	1.50
5	A	1	FKP	C17-C8	4.22	1.58	1.51
6	A	100	ONA	O5'-C5'	-4.18	1.28	1.44
5	A	1	FKP	C3-C2	3.52	1.60	1.53
6	A	100	ONA	PB-O3B	3.37	1.62	1.50
6	A	100	ONA	C5-N7	-3.35	1.33	1.39
6	A	100	ONA	C6-N1	3.28	1.44	1.35
5	A	1	FKP	C5-C6	3.27	1.64	1.54
6	A	100	ONA	PB-O1A	-3.23	1.56	1.59
5	A	1	FKP	O4-C7	3.19	1.50	1.45
5	A	1	FKP	C22-C21	3.11	1.59	1.50
8	C	395	GSP	PA-O3A	-3.03	1.56	1.59
5	A	1	FKP	C20-C10	2.93	1.59	1.53
5	A	1	FKP	C9-C11	2.86	1.57	1.54
5	A	1	FKP	C23-C22	2.83	1.62	1.52
6	A	100	ONA	O3'-C3'	2.65	1.48	1.44
5	A	1	FKP	C25-N1	2.59	1.53	1.47
8	C	395	GSP	C3'-C4'	2.50	1.59	1.53
5	A	1	FKP	C29-N1	2.47	1.53	1.46
5	A	1	FKP	C26-N1	2.36	1.53	1.46
6	A	100	ONA	CA7-NA1	2.33	1.49	1.45
8	C	395	GSP	PG-O2G	-2.22	1.47	1.54
5	A	1	FKP	C4-C5	2.21	1.59	1.56
6	A	100	ONA	C5'-C4'	2.17	1.58	1.51
6	A	100	ONA	CA1-CA	2.10	1.54	1.50
6	A	100	ONA	PG-O1G	2.10	1.62	1.54
8	C	395	GSP	O3'-C3'	2.09	1.48	1.43
5	A	1	FKP	C3-C4	2.08	1.57	1.54
5	A	1	FKP	C29-C28	2.06	1.59	1.51
8	C	395	GSP	C2'-C3'	2.06	1.59	1.53
5	A	1	FKP	C24-C25	2.02	1.59	1.51
5	A	1	FKP	C6-C7	2.02	1.57	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	FKP	C19-C4-C18	-10.98	91.89	107.87
6	A	100	ONA	N1-C2-N3	-7.02	117.95	128.58
6	A	100	ONA	O2B-PB-O1A	6.79	125.63	107.27
6	A	100	ONA	O2B-PB-O1B	6.58	125.05	107.27
5	A	1	FKP	O1-C8-C7	5.99	108.83	103.16
6	A	100	ONA	C3'-O3'-CA	5.41	125.88	117.24
5	A	1	FKP	O1-C8-C17	-5.01	103.70	110.17
6	A	100	ONA	O1A-PB-O3B	-4.92	95.89	110.70
6	A	100	ONA	C2-N3-C4	4.75	123.44	111.83
6	A	100	ONA	O5'-C5'-C4'	4.71	125.04	108.99
5	A	1	FKP	C2-C3-C4	-4.68	106.34	113.40
5	A	1	FKP	C3-C2-C1	-4.64	104.70	111.48
6	A	100	ONA	CA7-NA1-CA6	4.37	129.26	122.37
8	C	395	GSP	O2B-PB-O3B	3.99	118.06	107.27
8	C	395	GSP	PB-O3B-PG	-3.94	118.76	133.17
6	A	100	ONA	CA3-CA2-CA1	3.88	126.81	119.80
8	C	395	GSP	O3B-PB-O1B	-3.79	99.31	110.70
5	A	1	FKP	C7-O4-C21	3.78	125.57	118.00
8	C	395	GSP	O6-C6-N1	3.73	127.14	120.11
5	A	1	FKP	C17-C8-C7	-3.70	103.78	111.56
6	A	100	ONA	CA4-CA3-CA2	-3.70	115.68	120.24
6	A	100	ONA	CA1-CA6-NA1	-3.62	117.40	121.36
5	A	1	FKP	C4-C5-C6	-3.62	110.47	115.09
5	A	1	FKP	C19-C4-C5	3.59	124.44	111.92
5	A	1	FKP	C2-C1-C10	-3.58	107.59	112.18
6	A	100	ONA	C5-C4-N3	-3.58	121.79	126.72
6	A	100	ONA	CA3-CA4-CA5	-3.34	116.12	120.24
5	A	1	FKP	C20-C10-C1	-3.08	102.20	107.40
5	A	1	FKP	C10-C5-C6	-3.04	106.54	112.48
5	A	1	FKP	C3-C4-C5	2.92	112.02	107.89
6	A	100	ONA	O5'-PA-O3A	-2.86	97.60	108.94
5	A	1	FKP	C8-C7-C6	2.81	118.45	115.09
6	A	100	ONA	N3-C4-N9	2.81	131.94	127.17
6	A	100	ONA	N9-C8-N7	-2.73	110.06	113.94
5	A	1	FKP	C17-C8-C9	2.72	118.20	115.19
6	A	100	ONA	C5-N7-C8	2.67	107.65	103.45
5	A	1	FKP	O4-C7-C6	2.58	113.07	107.71
5	A	1	FKP	C23-C22-C21	2.48	122.78	113.69
8	C	395	GSP	O4'-C1'-C2'	-2.41	101.45	106.62
6	A	100	ONA	O2A-PA-O1A	2.41	113.79	107.27
6	A	100	ONA	PA-O5'-C5'	-2.41	107.56	121.35
6	A	100	ONA	CA5-CA6-CA1	2.33	122.42	119.37
6	A	100	ONA	O1A-PA-O3A	2.33	117.72	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	FKP	O4-C7-C8	-2.33	104.31	108.31
8	C	395	GSP	C1'-N9-C8	2.30	133.28	126.73
6	A	100	ONA	O4'-C1'-N9	2.21	112.33	108.09
6	A	100	ONA	C4-C5-N7	-2.16	108.11	110.58
6	A	100	ONA	O3'-CA-CA1	2.13	115.10	111.71
6	A	100	ONA	C5'-C4'-C3'	2.13	121.46	114.38
5	A	1	FKP	C16-C13-C14	-2.12	104.51	109.46
5	A	1	FKP	C13-O1-C8	2.11	123.17	119.86
6	A	100	ONA	C4-N9-C8	2.07	107.91	105.74
5	A	1	FKP	O4-C21-C22	2.06	115.93	111.48

There are no chirality outliers.

All (21) torsion outliers are listed below:

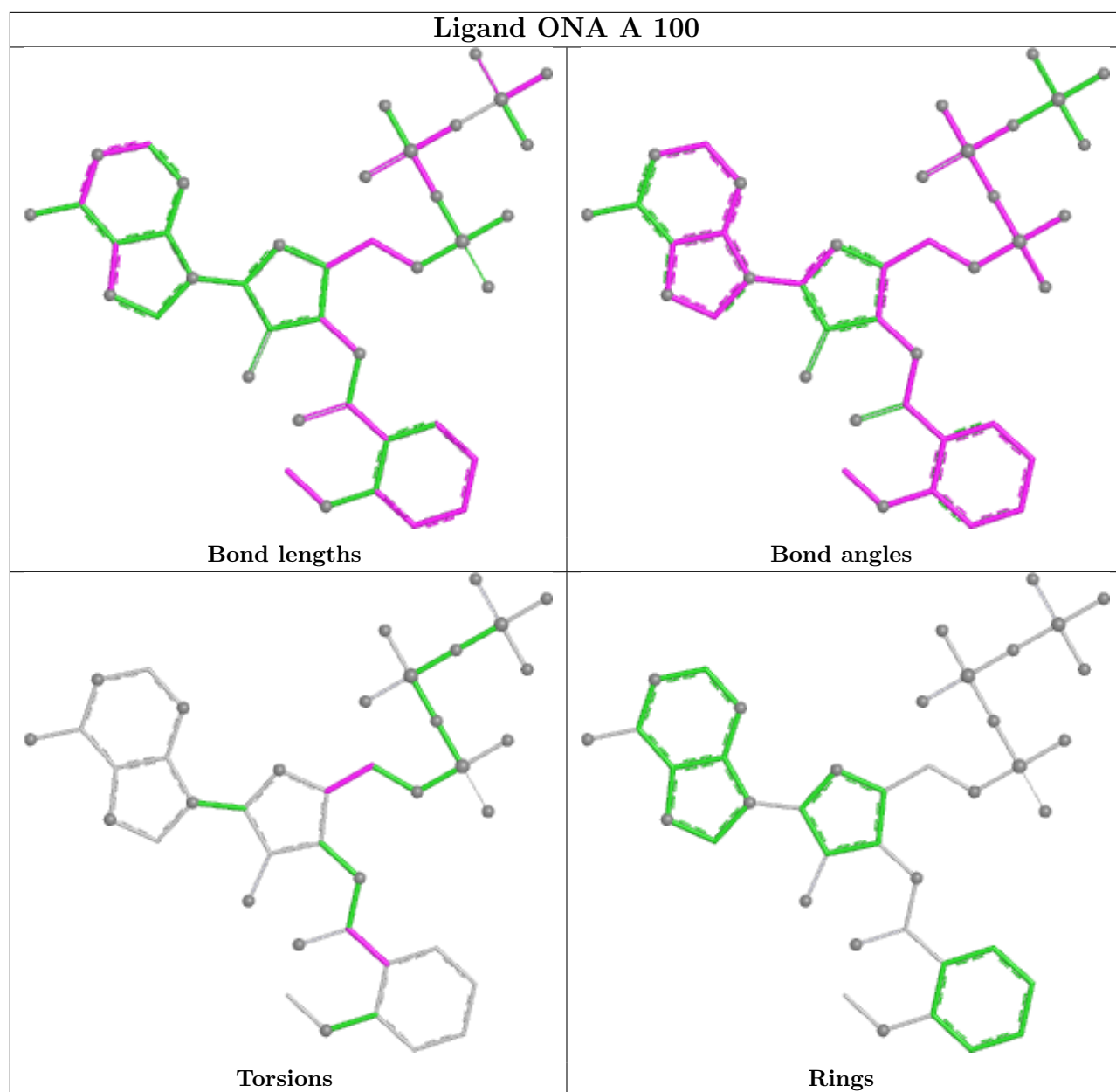
Mol	Chain	Res	Type	Atoms
5	A	1	FKP	C6-C7-O4-C21
5	A	1	FKP	C16-C13-C14-C15
5	A	1	FKP	C22-C21-O4-C7
5	A	1	FKP	O5-C21-O4-C7
5	A	1	FKP	C23-C24-C25-N1
5	A	1	FKP	C8-C7-O4-C21
6	A	100	ONA	C3'-C4'-C5'-O5'
6	A	100	ONA	O4'-C4'-C5'-O5'
8	C	395	GSP	PA-O3A-PB-O1B
5	A	1	FKP	C24-C25-N1-C29
6	A	100	ONA	O3'-CA-CA1-CA6
5	A	1	FKP	C24-C25-N1-C26
5	A	1	FKP	O1-C13-C14-C15
6	A	100	ONA	O3'-CA-CA1-CA2
6	A	100	ONA	OA-CA-CA1-CA6
8	C	395	GSP	PG-O3B-PB-O2B
8	C	395	GSP	PA-O3A-PB-O2B
5	A	1	FKP	C22-C23-C24-C25
6	A	100	ONA	OA-CA-CA1-CA2
5	A	1	FKP	O4-C21-C22-C23
5	A	1	FKP	C12-C13-C14-C15

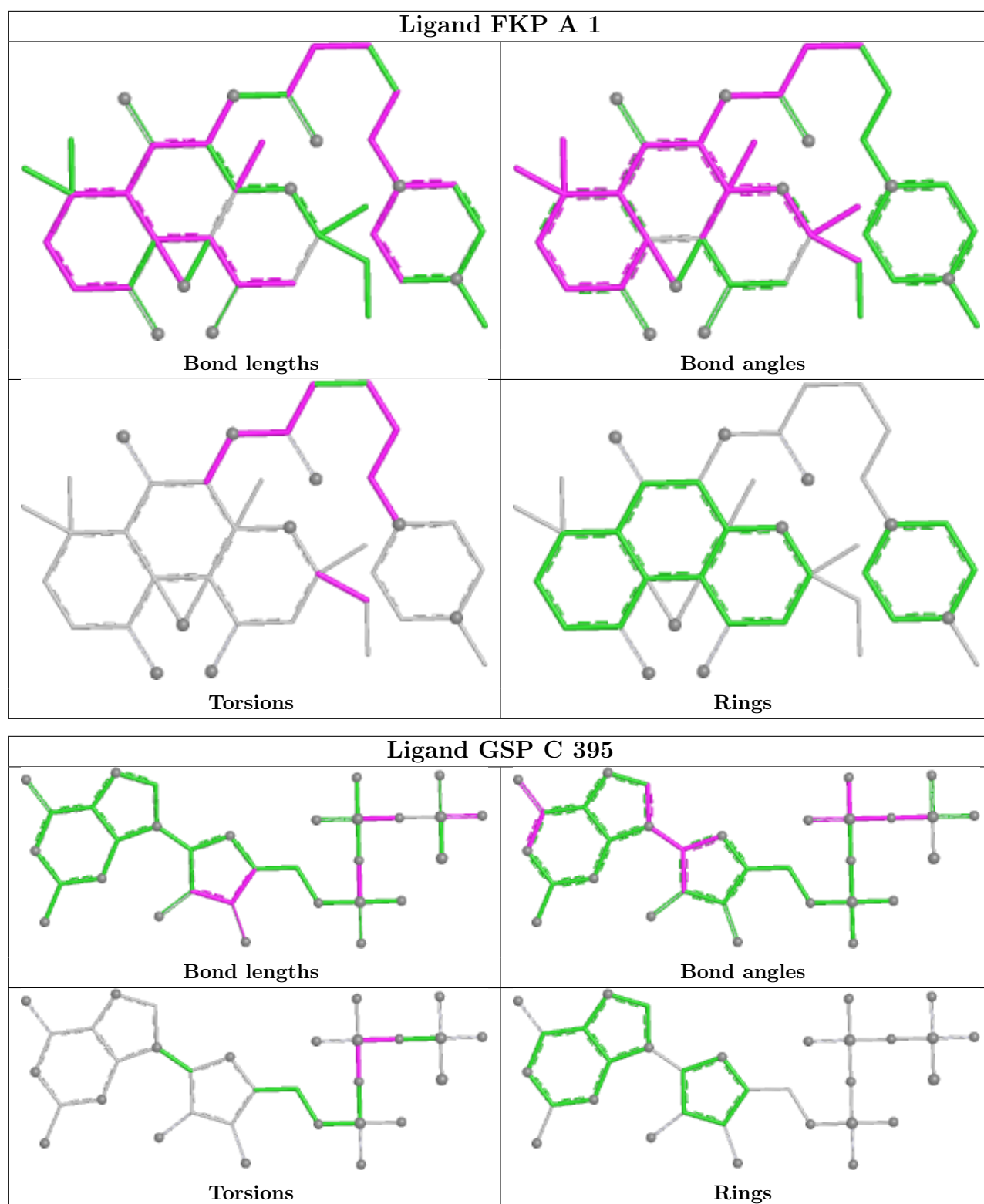
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	100	ONA	2	0
5	A	1	FKP	6	0
8	C	395	GSP	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 ⓘ

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	189/225 (84%)	0.03	2 (1%) 78 61	30, 87, 99, 116	0
2	B	188/212 (88%)	-0.36	0 100 100	13, 49, 96, 98	0
3	C	330/394 (83%)	-0.34	0 100 100	19, 55, 93, 100	0
All	All	707/831 (85%)	-0.25	2 (0%) 90 82	13, 59, 97, 116	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	PHE	3.9
1	A	475	GLU	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
6	ONA	A	100	41/41	0.91	0.11	53,88,97,100	0

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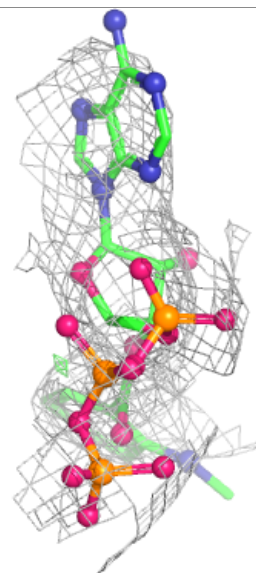
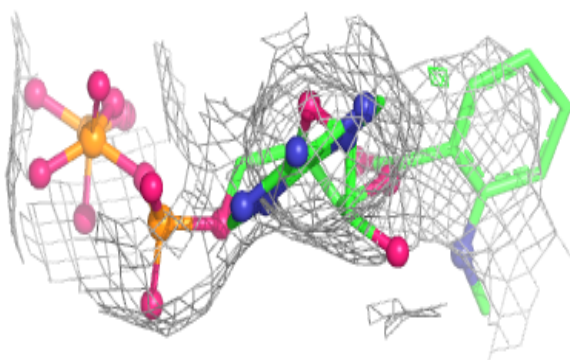
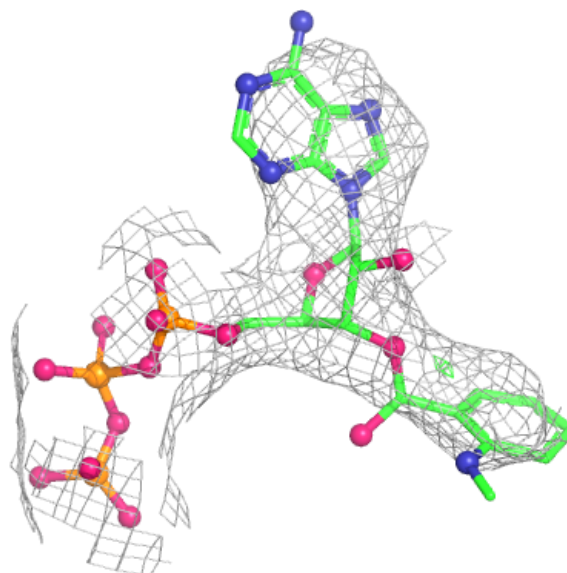
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MN	A	581	1/1	0.93	0.09	64,64,64,64	0
5	FKP	A	1	39/39	0.94	0.09	13,23,87,89	0
7	CL	C	397	1/1	0.95	0.35	59,59,59,59	0
8	GSP	C	395	32/32	0.95	0.08	31,41,73,76	0
4	MN	A	582	1/1	0.97	0.06	31,31,31,31	0
4	MN	C	396	1/1	0.99	0.04	17,17,17,17	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.

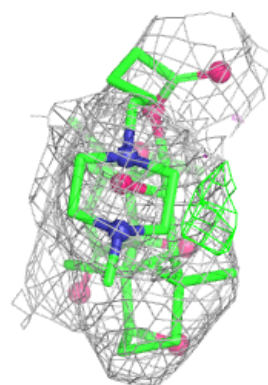
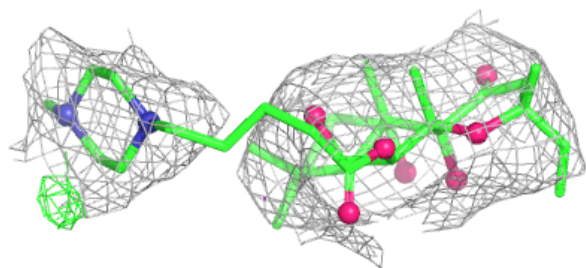
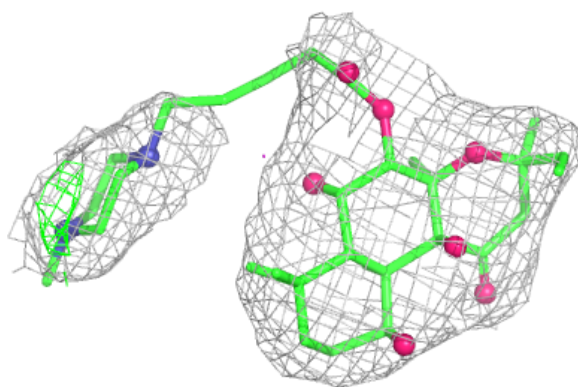
Electron density around ONA A 100:

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

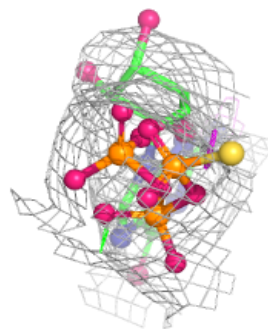
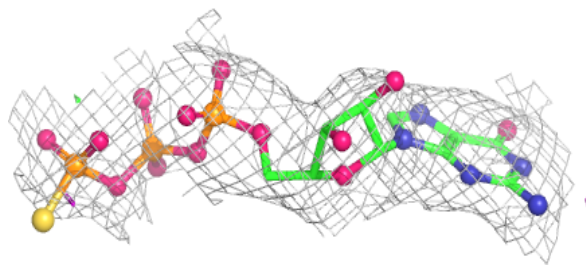
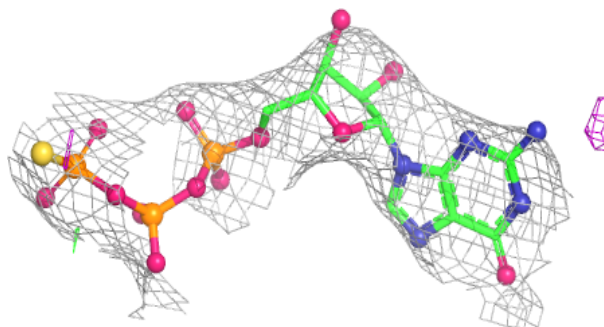


Electron density around FKP A 1:

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

**Electron density around GSP C 395:**

$2mF_o - DF_c$ (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.