



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:22 PM UTC

PDB ID : 1TND / pdb_00001tnd
Title : THE 2.2 ANGSTROMS CRYSTAL STRUCTURE OF TRANSDUCIN-
ALPHA COMPLEXED WITH GTP GAMMA S
Authors : Noel, J.P.; Hamm, H.E.; Sigler, P.B.
Deposited on : 1994-03-31
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

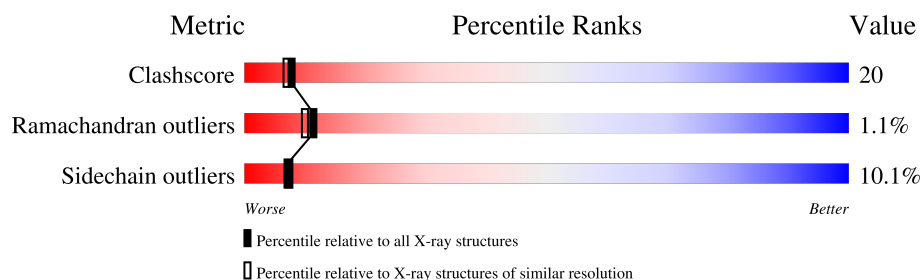
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	324	 60% 33% 6% •
1	B	324	 49% 39% 9% •
1	C	324	 63% 27% 6% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8599 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.

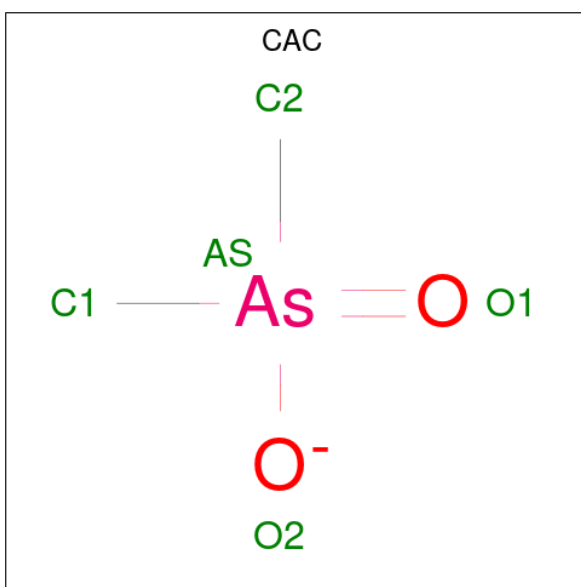
- Molecule 1 is a protein called TRANSDUCIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2590	1641	437	493	19			
1	B	316	Total	C	N	O	S	0	0	0
			2539	1610	428	483	18			
1	C	316	Total	C	N	O	S	0	0	0
			2539	1610	428	483	18			

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

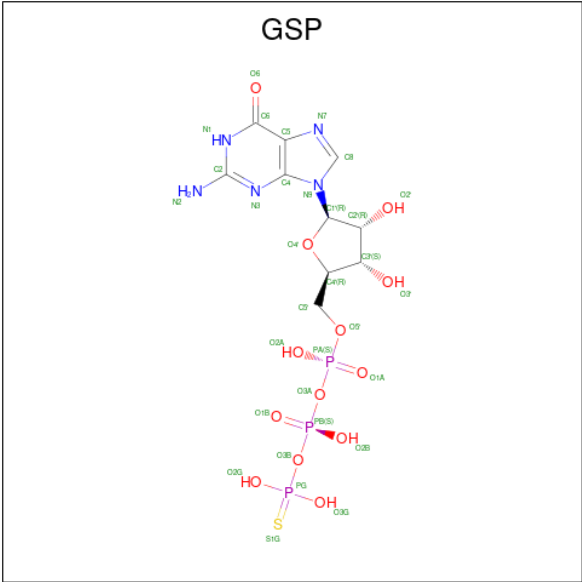
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	As 1	0	0
3	A	1	Total 1	As 1	0	0
3	B	1	Total 1	As 1	0	0
3	B	1	Total 1	As 1	0	0
3	C	1	Total 1	As 1	0	0
3	C	1	Total 1	As 1	0	0

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	305	Total O	0	0
			305 305		
5	B	225	Total O	0	0
			225 225		
5	C	296	Total O	0	0
			296 296		



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.50 Å 108.30 Å 79.00 Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8599	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, CAC, MG

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	0.86	1/2635 (0.0%)	1.21	18/3552 (0.5%)
1	B	0.79	2/2584 (0.1%)	1.24	23/3484 (0.7%)
1	C	0.82	2/2584 (0.1%)	1.17	18/3484 (0.5%)
All	All	0.82	5/7803 (0.1%)	1.21	59/10520 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	ILE	CA-CB	6.23	1.61	1.54
1	B	197	VAL	CA-CB	5.70	1.61	1.55
1	C	264	LEU	CA-C	5.39	1.59	1.52
1	A	49	MET	SD-CE	-5.32	1.66	1.79
1	C	331	VAL	CA-CB	5.03	1.60	1.54

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	TYR	N-CA-C	9.35	124.03	110.10
1	B	207	TRP	N-CA-C	8.74	120.42	111.07
1	B	115	MET	CA-C-N	8.46	128.50	119.78
1	B	115	MET	C-N-CA	8.46	128.50	119.78
1	A	287	ASN	N-CA-C	7.47	122.49	111.96
1	C	255	PHE	N-CA-C	7.42	122.04	112.92
1	B	92	GLY	N-CA-C	-7.30	104.64	113.99
1	B	125	ARG	N-CA-C	-7.19	103.05	111.03
1	B	84	MET	N-CA-C	-7.09	102.75	111.40
1	B	134	ALA	N-CA-C	-6.92	103.35	111.03
1	C	99	ASP	N-CA-C	-6.86	103.42	111.03
1	B	178	THR	N-CA-C	-6.85	99.06	109.95
1	B	314	GLU	N-CA-C	6.63	118.51	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	LEU	N-CA-C	6.60	118.48	111.28
1	B	277	ALA	N-CA-C	6.43	119.42	109.07
1	C	230	LEU	N-CA-C	6.40	118.56	110.24
1	C	52	ILE	N-CA-C	6.34	116.49	110.53
1	A	92	GLY	N-CA-C	-6.30	107.50	115.31
1	B	230	LEU	N-CA-C	6.29	118.91	110.35
1	C	320	THR	N-CA-C	6.27	119.24	109.52
1	A	288	GLY	N-CA-C	6.26	125.12	112.34
1	A	292	TYR	N-CA-C	6.22	117.73	111.07
1	B	89	ILE	CB-CA-C	-6.11	102.85	111.28
1	A	212	GLU	N-CA-C	6.08	118.69	108.23
1	C	155	LEU	N-CA-C	6.03	117.85	111.28
1	A	283	PHE	CA-C-N	5.92	127.24	119.84
1	A	283	PHE	C-N-CA	5.92	127.24	119.84
1	B	90	GLN	N-CA-C	5.84	117.48	109.18
1	A	281	ILE	CB-CA-C	-5.83	103.13	112.16
1	C	319	MET	N-CA-C	-5.79	100.55	109.76
1	C	294	ASP	N-CA-C	5.79	117.39	111.14
1	B	319	MET	N-CA-C	-5.69	100.02	109.46
1	A	315	ILE	N-CA-C	5.66	116.25	107.99
1	B	52	ILE	N-CA-C	5.63	116.28	110.82
1	A	311	ASP	N-CA-C	-5.61	98.85	110.80
1	A	216	CYS	N-CA-C	5.58	117.75	108.99
1	B	58	SER	N-CA-C	-5.57	102.28	110.52
1	A	273	LYS	N-CA-C	5.53	117.11	111.14
1	A	166	THR	N-CA-C	-5.48	102.36	110.46
1	B	268	ASP	N-CA-C	-5.45	105.24	111.07
1	C	211	PHE	N-CA-C	5.43	119.66	113.19
1	C	285	ASP	N-CA-C	5.41	119.87	113.16
1	A	81	VAL	N-CA-C	-5.40	105.06	110.30
1	C	80	ILE	N-CA-C	-5.39	105.47	110.53
1	C	84	MET	N-CA-C	-5.34	105.36	111.07
1	B	264	LEU	N-CA-C	-5.32	97.98	107.98
1	B	231	VAL	CB-CA-C	-5.30	104.91	112.22
1	C	231	VAL	N-CA-C	-5.29	105.38	110.72
1	A	53	HIS	N-CA-C	5.27	120.37	113.30
1	C	236	VAL	N-CA-C	5.26	115.43	107.80
1	A	164	VAL	N-CA-C	-5.24	97.57	108.88
1	C	58	SER	N-CA-C	-5.18	103.08	110.59
1	C	333	ASP	N-CA-C	-5.18	105.71	111.36
1	B	99	ASP	N-CA-C	-5.16	105.31	111.03
1	C	111	GLU	N-CA-C	-5.14	102.67	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ILE	N-CA-C	5.09	115.29	108.17
1	C	212	GLU	N-CA-C	5.05	117.85	109.46
1	B	108	ASP	N-CA-C	-5.04	107.62	112.97
1	A	255	PHE	N-CA-C	5.03	119.14	113.15

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	2590	0	2572	87	0
1	B	2539	0	2518	121	0
1	C	2539	0	2520	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	2	0
4	A	32	0	12	1	0
4	B	32	0	12	4	0
4	C	32	0	12	0	0
5	A	305	0	0	11	0
5	B	225	0	0	16	0
5	C	296	0	0	14	0
All	All	8599	0	7646	299	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 (299) 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:308:MET:HB3	1:A:309:ARG:HH21	1.26	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:MET:HB3	1:A:309:ARG:NH2	1.85	0.92
1:B:252:HIS:HE1	1:B:254:TYR:HD2	1.14	0.91
1:C:84:MET:HA	1:C:89:ILE:HG22	1.57	0.87
1:B:168:GLN:O	1:B:172:ARG:HG2	1.75	0.85
1:B:90:GLN:HB2	5:B:477:HOH:O	1.77	0.84
1:A:170:VAL:O	1:A:173:SER:HB2	1.78	0.84
1:B:96:ARG:HD2	1:B:96:ARG:N	1.95	0.80
1:C:74:LEU:HD22	1:C:78:LEU:HD22	1.63	0.79
1:B:84:MET:HE3	1:B:135:CYS:HB2	1.66	0.77
1:A:307:ASN:OD1	1:A:309:ARG:HG2	1.84	0.77
1:A:54:GLN:HE22	1:A:183:THR:HG23	1.50	0.77
1:B:53:HIS:HD2	5:B:384:HOH:O	1.68	0.74
1:A:54:GLN:NE2	1:A:183:THR:HG23	2.04	0.73
1:C:229:VAL:HG13	1:C:234:ASP:HA	1.70	0.72
1:C:251:ASN:HD21	1:C:308:MET:H	1.36	0.71
1:B:101:ARG:HH12	1:B:105:HIS:HB2	1.55	0.71
1:A:48:GLN:HE21	1:A:48:GLN:HA	1.55	0.71
1:A:212:GLU:O	1:A:348:GLY:HA3	1.89	0.71
1:A:99:ASP:HB3	1:A:122:ILE:HG23	1.74	0.70
1:A:213:GLY:HA3	1:A:348:GLY:HA2	1.74	0.70
1:C:98:ASP:O	1:C:102:LYS:HG3	1.92	0.70
1:C:168:GLN:O	1:C:172:ARG:HG2	1.90	0.70
1:C:309:ARG:N	1:C:309:ARG:HD2	2.07	0.69
1:C:223:LEU:HD21	1:C:319:MET:CE	2.22	0.69
1:C:185:PHE:HZ	1:C:332:PHE:CZ	2.11	0.69
1:B:193:ARG:HD2	5:B:505:HOH:O	1.92	0.69
1:A:78:LEU:O	1:A:82:ARG:HG3	1.93	0.68
1:B:280:SER:HB2	5:B:441:HOH:O	1.92	0.68
1:B:129:ASP:HB3	1:B:132:ILE:HB	1.76	0.68
1:A:229:VAL:HG13	1:A:234:ASP:HA	1.74	0.67
1:C:310:ARG:HD2	5:C:545:HOH:O	1.94	0.67
1:B:229:VAL:HG13	1:B:234:ASP:HA	1.77	0.67
1:A:47:LYS:HG2	1:A:57:TYR:OH	1.95	0.66
1:B:322:ALA:HB3	4:B:351:GSP:N7	2.11	0.66
1:A:201:ARG:HD3	1:A:241:GLU:OE2	1.96	0.66
1:B:168:GLN:OE1	1:B:172:ARG:HD3	1.96	0.65
1:C:298:TYR:O	1:C:302:GLN:HG2	1.96	0.65
1:A:31:LYS:HE2	1:A:214:VAL:HG22	1.78	0.65
1:B:252:HIS:CE1	1:B:254:TYR:HD2	2.06	0.65
1:B:265:ASN:OD1	1:B:320:THR:HG22	1.98	0.65
1:B:255:PHE:HA	1:B:258:THR:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:MET:SD	1:C:89:ILE:HG23	2.38	0.63
1:C:84:MET:SD	1:C:89:ILE:CG2	2.87	0.63
1:B:79:ALA:HB3	1:B:144:LEU:HD12	1.79	0.63
1:B:208:ILE:HD11	5:B:359:HOH:O	1.98	0.63
1:A:162:GLY:HA2	1:B:182:GLU:O	1.99	0.63
1:A:349:LEU:HD11	5:C:366:HOH:O	1.97	0.63
1:B:225:ALA:HB1	1:B:238:ARG:HB3	1.81	0.63
1:C:139:ALA:HA	1:C:142:TYR:CE1	2.34	0.63
1:A:164:VAL:HB	5:A:549:HOH:O	1.99	0.63
1:C:265:ASN:OD1	1:C:320:THR:HG22	1.99	0.62
1:C:223:LEU:HD21	1:C:319:MET:HE1	1.80	0.62
1:A:332:PHE:O	1:A:336:THR:HG23	2.00	0.62
1:A:308:MET:HE3	1:A:308:MET:HA	1.81	0.62
1:A:215:THR:HG23	1:A:345:LYS:O	2.00	0.61
1:B:157:ARG:NH2	1:B:163:TYR:HE1	1.98	0.61
1:A:50:LYS:HE2	5:A:428:HOH:O	2.00	0.61
1:C:315:ILE:N	1:C:315:ILE:HD12	2.15	0.61
1:B:197:VAL:HG23	1:B:206:LYS:HZ1	1.64	0.61
1:C:229:VAL:CG1	1:C:234:ASP:HA	2.31	0.61
1:C:119:MET:O	1:C:123:ILE:HG13	1.99	0.61
1:C:197:VAL:HG23	1:C:206:LYS:NZ	2.16	0.61
1:A:213:GLY:HA3	1:A:348:GLY:CA	2.31	0.61
1:C:197:VAL:HG23	1:C:206:LYS:HZ1	1.65	0.61
1:A:174:ARG:HD3	5:A:629:HOH:O	2.01	0.61
1:B:252:HIS:HE1	1:B:254:TYR:CD2	2.07	0.60
1:C:27:ALA:HB3	1:C:191:ASN:HD21	1.66	0.60
1:C:260:ILE:O	1:C:315:ILE:HG23	2.02	0.60
1:C:257:THR:HG23	5:C:631:HOH:O	2.02	0.60
1:A:215:THR:OG1	1:A:346:ASP:HA	2.01	0.60
1:A:282:CYS:O	1:A:284:PRO:HD3	2.03	0.59
1:A:318:HIS:HE1	5:A:573:HOH:O	1.86	0.59
1:B:47:LYS:HG2	1:B:57:TYR:OH	2.03	0.59
1:C:82:ARG:HG2	1:C:104:MET:HE1	1.84	0.58
1:B:291:THR:OG1	1:B:293:GLU:HG3	2.03	0.58
1:C:74:LEU:HD22	1:C:78:LEU:CD2	2.33	0.58
1:A:252:HIS:HB3	1:A:255:PHE:CD2	2.39	0.58
1:A:59:LEU:O	1:A:63:LEU:HG	2.03	0.58
1:A:218:ILE:HA	1:A:261:VAL:HG22	1.86	0.58
1:B:41:GLY:O	1:B:45:ILE:HD12	2.04	0.58
1:C:244:HIS:HB3	5:C:540:HOH:O	2.04	0.57
1:A:230:LEU:HD23	1:A:238:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD12	1:B:33:LEU:N	2.19	0.57
1:B:148:ALA:O	1:B:152:LEU:HB2	2.04	0.57
1:B:187:PHE:CD2	1:B:336:THR:HG21	2.40	0.57
1:A:229:VAL:CG1	1:A:234:ASP:HA	2.35	0.57
1:B:197:VAL:HG23	1:B:206:LYS:NZ	2.20	0.57
1:B:84:MET:CE	1:B:135:CYS:HB2	2.34	0.57
1:B:99:ASP:HB3	1:B:122:ILE:HG23	1.87	0.56
1:B:244:HIS:CD2	5:B:491:HOH:O	2.57	0.56
1:C:180:ILE:HG13	1:C:206:LYS:HZ3	1.69	0.56
1:C:265:ASN:HA	1:C:320:THR:HG22	1.87	0.56
1:A:252:HIS:HB3	1:A:255:PHE:HD2	1.70	0.56
1:A:254:TYR:H	1:A:254:TYR:HD1	1.54	0.56
1:C:252:HIS:HE1	1:C:254:TYR:CD1	2.24	0.56
1:C:48:GLN:HA	1:C:48:GLN:HE21	1.71	0.56
1:C:89:ILE:HB	5:C:570:HOH:O	2.06	0.55
1:A:96:ARG:HG3	1:A:129:ASP:OD1	2.06	0.55
1:A:262:LEU:O	1:A:317:SER:HA	2.05	0.55
1:C:258:THR:HG22	5:C:631:HOH:O	2.07	0.55
1:B:78:LEU:CD2	1:B:104:MET:SD	2.95	0.55
1:A:305:GLU:HB2	5:A:467:HOH:O	2.06	0.55
1:B:279:LEU:HD22	1:B:295:ALA:HB1	1.89	0.55
1:B:307:ASN:ND2	1:B:310:ARG:HA	2.22	0.55
1:A:120:SER:O	1:A:124:GLN:HG3	2.07	0.54
1:B:48:GLN:HA	1:B:48:GLN:HE21	1.72	0.54
1:A:48:GLN:O	1:A:52:ILE:HG13	2.08	0.54
1:B:274:ILE:HD12	1:B:277:ALA:O	2.07	0.54
1:C:310:ARG:HA	1:C:313:LYS:O	2.07	0.54
1:B:188:LYS:HD2	1:B:336:THR:OG1	2.08	0.54
1:A:301:VAL:O	1:A:305:GLU:HG2	2.07	0.54
1:B:103:LEU:HD12	1:B:119:MET:HE2	1.90	0.53
1:B:274:ILE:O	1:B:290:ASN:ND2	2.41	0.53
1:A:298:TYR:O	1:A:302:GLN:HG2	2.09	0.53
1:B:31:LYS:HE2	1:B:214:VAL:HG22	1.89	0.53
1:C:297:ASN:HD21	1:C:300:LYS:NZ	2.06	0.53
1:B:146:ASP:OD1	4:B:351:GSP:H4'	2.08	0.53
1:C:285:ASP:HB2	5:C:552:HOH:O	2.08	0.53
1:C:96:ARG:O	1:C:99:ASP:HB2	2.09	0.53
1:A:335:VAL:O	1:A:338:ILE:HB	2.09	0.53
1:C:185:PHE:CZ	1:C:332:PHE:CZ	2.96	0.53
1:C:251:ASN:HD22	1:C:309:ARG:CD	2.22	0.53
1:A:82:ARG:NH1	5:A:507:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HH21	1:B:163:TYR:HE1	1.57	0.52
1:C:222:ALA:HB1	1:C:266:LYS:HD2	1.92	0.52
1:B:231:VAL:HG23	5:B:371:HOH:O	2.09	0.52
1:C:180:ILE:CG1	1:C:206:LYS:HZ3	2.21	0.52
1:A:211:PHE:CD1	1:A:255:PHE:HZ	2.28	0.52
1:B:106:MET:O	1:B:110:ILE:HG23	2.10	0.52
1:B:74:LEU:O	1:B:74:LEU:HD22	2.10	0.51
1:C:83:ALA:O	1:C:87:LEU:HB2	2.10	0.51
1:B:135:CYS:O	1:B:138:ARG:N	2.43	0.51
1:A:162:GLY:HA3	1:B:181:ILE:HG23	1.93	0.51
1:B:170:VAL:O	1:B:173:SER:OG	2.28	0.51
1:B:96:ARG:HA	1:B:96:ARG:HH11	1.75	0.51
1:C:265:ASN:OD1	1:C:320:THR:CG2	2.58	0.51
1:B:229:VAL:CG1	1:B:234:ASP:HA	2.41	0.51
1:C:230:LEU:HD12	1:C:238:ARG:HG2	1.92	0.51
1:C:278:HIS:CD2	5:C:641:HOH:O	2.64	0.51
1:B:95:ALA:C	1:B:96:ARG:HH11	2.19	0.51
1:B:79:ALA:HB3	1:B:144:LEU:CD1	2.40	0.50
1:B:204:ARG:NH2	1:B:241:GLU:OE2	2.44	0.50
1:A:54:GLN:NE2	1:A:183:THR:CG2	2.73	0.50
1:B:55:ASP:HB2	5:B:470:HOH:O	2.10	0.50
1:A:326:GLN:O	1:A:330:PHE:HD1	1.94	0.50
1:B:289:PRO:HB2	1:B:291:THR:HG23	1.92	0.50
1:A:156:GLU:HG3	5:A:393:HOH:O	2.11	0.50
1:B:225:ALA:HB1	1:B:238:ARG:HG2	1.94	0.50
1:C:210:CYS:CB	3:C:354:CAC:AS	3.20	0.50
1:A:61:GLU:O	1:A:64:GLU:HB2	2.12	0.50
1:B:226:TYR:OH	1:B:277:ALA:HB3	2.12	0.50
1:B:78:LEU:HD22	1:B:104:MET:SD	2.52	0.49
1:B:83:ALA:O	1:B:87:LEU:HB2	2.11	0.49
1:C:289:PRO:O	1:C:291:THR:N	2.43	0.49
1:A:310:ARG:HD3	1:A:310:ARG:C	2.37	0.49
1:B:307:ASN:HD21	1:B:313:LYS:HB3	1.78	0.49
1:C:35:LEU:HD12	1:C:217:ILE:HG21	1.93	0.49
1:C:75:GLN:CD	5:C:404:HOH:O	2.55	0.49
1:B:334:ALA:O	1:B:337:ASP:HB2	2.13	0.49
1:C:185:PHE:HZ	1:C:332:PHE:HZ	1.58	0.48
1:C:278:HIS:HA	1:C:290:ASN:ND2	2.28	0.48
1:B:131:GLY:O	1:B:134:ALA:HB3	2.13	0.48
1:B:226:TYR:O	1:B:282:CYS:HB2	2.13	0.48
1:A:291:THR:OG1	1:A:294:ASP:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:CYS:SG	1:B:307:ASN:HB2	2.54	0.48
1:C:258:THR:O	1:C:313:LYS:NZ	2.47	0.48
1:B:252:HIS:HB3	1:B:255:PHE:CD2	2.49	0.48
1:C:252:HIS:HE1	1:C:254:TYR:HD1	1.61	0.48
1:A:244:HIS:HD2	5:A:561:HOH:O	1.97	0.47
1:A:289:PRO:O	1:A:291:THR:N	2.43	0.47
1:A:344:LEU:HD22	1:A:345:LYS:N	2.29	0.47
1:B:96:ARG:NH2	1:B:125:ARG:HD2	2.29	0.47
1:B:111:GLU:HB3	5:B:521:HOH:O	2.13	0.47
1:B:312:VAL:HG23	1:B:313:LYS:N	2.29	0.47
1:B:201:ARG:HA	1:B:204:ARG:HG3	1.95	0.47
1:B:283:PHE:CZ	1:B:302:GLN:HG3	2.49	0.47
1:A:102:LYS:CE	1:A:122:ILE:HD11	2.45	0.47
1:B:172:ARG:HA	4:B:351:GSP:O2'	2.14	0.47
1:A:344:LEU:HD22	1:A:345:LYS:H	1.79	0.47
1:C:223:LEU:HB3	1:C:270:PHE:HB2	1.95	0.47
1:B:62:CYS:O	1:B:65:PHE:HB2	2.14	0.47
1:B:222:ALA:HB1	1:B:266:LYS:HD2	1.96	0.47
1:B:132:ILE:HG22	1:B:133:GLN:HE21	1.80	0.47
1:A:327:ASN:O	1:A:331:VAL:HG23	2.14	0.46
1:C:111:GLU:O	1:C:114:THR:OG1	2.30	0.46
1:B:226:TYR:OH	1:B:274:ILE:HA	2.15	0.46
1:C:83:ALA:HB3	1:C:135:CYS:SG	2.55	0.46
1:C:255:PHE:O	1:C:258:THR:HG23	2.15	0.46
1:B:202:SER:HA	1:B:205:LYS:HE2	1.96	0.46
1:B:117:LYS:HA	1:B:120:SER:OG	2.16	0.46
1:B:142:TYR:HE1	1:B:144:LEU:HB2	1.80	0.46
1:B:38:GLY:O	1:B:39:GLU:HB2	2.16	0.46
1:B:101:ARG:NH1	1:B:105:HIS:HB2	2.27	0.46
1:B:187:PHE:CE2	1:B:336:THR:HG21	2.50	0.46
1:B:283:PHE:CE2	1:B:302:GLN:HG3	2.51	0.46
1:C:331:VAL:O	1:C:335:VAL:HG23	2.16	0.46
1:A:30:VAL:HG13	1:A:215:THR:HB	1.97	0.46
1:C:335:VAL:O	1:C:338:ILE:HB	2.16	0.46
1:B:207:TRP:HB2	5:B:547:HOH:O	2.16	0.46
1:A:82:ARG:HD2	5:A:507:HOH:O	2.15	0.46
1:B:78:LEU:HD23	1:B:78:LEU:HA	1.77	0.46
1:B:96:ARG:HD2	1:B:96:ARG:H	1.76	0.46
1:A:251:ASN:HD22	1:A:309:ARG:HD2	1.81	0.45
1:B:273:LYS:O	1:B:277:ALA:N	2.45	0.45
1:B:202:SER:O	1:B:205:LYS:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:HD23	1:B:264:LEU:HA	1.75	0.45
1:A:254:TYR:CD1	1:A:254:TYR:N	2.84	0.45
1:C:332:PHE:O	1:C:336:THR:HG23	2.16	0.45
1:B:131:GLY:O	1:B:134:ALA:N	2.43	0.45
1:B:316:TYR:HB2	5:B:576:HOH:O	2.15	0.45
1:A:251:ASN:HD21	1:A:308:MET:H	1.65	0.45
1:C:62:CYS:CB	3:C:353:CAC:AS	3.25	0.45
1:A:262:LEU:HB3	1:A:317:SER:HB3	1.99	0.45
1:B:42:LYS:NZ	4:B:351:GSP:O3G	2.50	0.45
1:B:228:MET:O	1:B:238:ARG:HB2	2.16	0.45
1:C:80:ILE:HG21	1:C:132:ILE:HG23	1.98	0.45
1:C:214:VAL:O	1:C:258:THR:HB	2.16	0.45
1:B:142:TYR:CE1	1:B:144:LEU:HB2	2.52	0.44
1:B:278:HIS:HA	1:B:290:ASN:OD1	2.17	0.44
1:C:267:LYS:HG2	1:C:320:THR:O	2.18	0.44
1:A:96:ARG:HA	1:A:96:ARG:NE	2.32	0.44
1:B:39:GLU:HG2	1:B:174:ARG:CZ	2.48	0.44
1:B:305:GLU:HA	1:B:310:ARG:NH1	2.33	0.44
1:C:84:MET:HA	1:C:89:ILE:CG2	2.40	0.44
1:C:252:HIS:CE1	1:C:254:TYR:CD1	3.04	0.44
1:B:159:VAL:CG1	5:B:529:HOH:O	2.66	0.44
1:B:194:MET:HE3	1:B:194:MET:HB2	1.88	0.44
1:B:272:GLU:HB3	5:B:573:HOH:O	2.18	0.44
1:A:279:LEU:HB3	1:A:286:TYR:CD2	2.53	0.44
1:C:96:ARG:HA	1:C:96:ARG:HD3	1.61	0.44
1:B:53:HIS:CD2	5:B:384:HOH:O	2.55	0.43
1:A:29:THR:O	1:A:346:ASP:HB3	2.19	0.43
1:A:274:ILE:HD12	1:A:290:ASN:ND2	2.33	0.43
1:B:118:GLU:O	1:B:122:ILE:HG13	2.18	0.43
1:B:143:GLN:NE2	1:B:238:ARG:NH1	2.67	0.43
1:C:35:LEU:HD12	1:C:217:ILE:CG2	2.48	0.43
1:A:349:LEU:HD21	5:C:366:HOH:O	2.19	0.43
1:C:252:HIS:CE1	1:C:254:TYR:HD1	2.35	0.43
1:A:78:LEU:HD23	1:A:103:LEU:HD13	2.00	0.43
1:A:164:VAL:HG23	5:A:549:HOH:O	2.18	0.43
1:C:46:VAL:HG13	1:C:183:THR:HG21	2.01	0.43
1:C:252:HIS:HB3	1:C:255:PHE:CD2	2.54	0.42
1:A:281:ILE:O	1:A:281:ILE:HG22	2.18	0.42
1:A:291:THR:HG1	1:A:294:ASP:HB3	1.84	0.42
1:A:266:LYS:HG2	4:A:351:GSP:C6	2.54	0.42
1:B:258:THR:O	1:B:313:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LYS:HA	1:C:54:GLN:HB2	2.01	0.42
1:C:99:ASP:HB3	1:C:122:ILE:HG23	2.00	0.42
1:C:278:HIS:HD2	5:C:641:HOH:O	2.02	0.42
1:A:199:GLY:HA2	1:A:207:TRP:HZ2	1.83	0.42
1:C:27:ALA:HB3	1:C:191:ASN:ND2	2.33	0.42
1:B:255:PHE:HD1	1:B:258:THR:HG21	1.85	0.42
1:C:83:ALA:HA	1:C:86:THR:OG1	2.19	0.42
1:B:255:PHE:HA	1:B:258:THR:CG2	2.46	0.42
1:A:346:ASP:O	1:A:347:CYS:C	2.62	0.42
1:C:305:GLU:HA	5:C:545:HOH:O	2.20	0.42
1:A:102:LYS:HE3	1:A:122:ILE:HD11	2.02	0.42
1:B:57:TYR:CE2	1:B:65:PHE:HE2	2.37	0.42
1:C:139:ALA:HA	1:C:142:TYR:CZ	2.54	0.42
1:B:188:LYS:NZ	1:B:333:ASP:OD1	2.49	0.42
1:C:33:LEU:HD22	1:C:214:VAL:HG21	2.01	0.42
1:B:248:SER:O	1:B:252:HIS:HB2	2.20	0.41
1:A:265:ASN:OD1	1:A:320:THR:HG23	2.20	0.41
1:C:29:THR:HG23	1:C:193:ARG:HH11	1.85	0.41
1:C:338:ILE:HD11	5:C:487:HOH:O	2.19	0.41
1:A:203:GLU:HG3	5:A:433:HOH:O	2.20	0.41
1:A:278:HIS:HB3	1:A:280:SER:OG	2.20	0.41
1:A:326:GLN:O	1:A:330:PHE:CD1	2.73	0.41
1:B:223:LEU:HD22	1:B:264:LEU:C	2.45	0.41
1:C:322:ALA:HA	1:C:328:VAL:CG2	2.50	0.41
1:A:150:TYR:CE1	1:A:172:ARG:HG3	2.55	0.41
1:B:300:LYS:HG2	1:B:304:LEU:HD12	2.02	0.41
1:B:41:GLY:O	1:B:45:ILE:CD1	2.69	0.41
1:B:139:ALA:HA	1:B:142:TYR:CZ	2.55	0.41
1:B:175:VAL:O	5:B:372:HOH:O	2.21	0.41
1:B:159:VAL:HG13	5:B:529:HOH:O	2.21	0.41
1:C:307:ASN:ND2	1:C:310:ARG:HA	2.35	0.41
1:A:341:LYS:O	1:A:343:ASN:N	2.53	0.41
1:B:197:VAL:CG2	1:B:206:LYS:NZ	2.83	0.41
1:B:48:GLN:CB	1:B:328:VAL:HG11	2.51	0.41
1:C:110:ILE:HD13	1:C:119:MET:SD	2.61	0.41
1:C:251:ASN:ND2	1:C:308:MET:H	2.11	0.41
1:A:234:ASP:OD1	1:A:235:GLU:HG2	2.20	0.41
1:A:289:PRO:HD2	1:A:294:ASP:OD2	2.21	0.41
1:B:57:TYR:HE2	1:B:65:PHE:HE2	1.67	0.41
1:C:33:LEU:HD22	1:C:214:VAL:CG2	2.51	0.41
1:C:82:ARG:CG	1:C:104:MET:HE1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LYS:HE3	1:C:117:LYS:HB3	1.78	0.41
1:C:274:ILE:HD12	1:C:274:ILE:HA	1.86	0.41
1:A:233:ASP:OD2	1:A:236:VAL:HG23	2.21	0.40
1:C:48:GLN:O	1:C:52:ILE:HG13	2.21	0.40
1:A:81:VAL:CG1	1:A:104:MET:HE3	2.50	0.40
1:B:145:ASN:OD1	1:B:145:ASN:N	2.54	0.40
1:C:132:ILE:HD13	1:C:132:ILE:HA	1.98	0.40
1:C:251:ASN:HD22	1:C:309:ARG:HD3	1.86	0.40
1:A:279:LEU:HD22	1:A:295:ALA:HB1	2.04	0.40
1:B:166:THR:OG1	1:B:169:ASP:CG	2.64	0.40
1:C:276:LYS:HE3	5:C:481:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/324 (99%)	294 (92%)	22 (7%)	5 (2%)	7	6
1	B	314/324 (97%)	292 (93%)	18 (6%)	4 (1%)	9	8
1	C	314/324 (97%)	301 (96%)	12 (4%)	1 (0%)	36	42
All	All	949/972 (98%)	887 (94%)	52 (6%)	10 (1%)	11	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	A	347	CYS
1	A	258	THR
1	B	311	ASP
1	B	312	VAL
1	B	315	ILE

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Mol	Chain	Res	Type
1	C	290	ASN
1	B	253	ARG
1	A	94	SER
1	A	288	GLY

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	287/288 (100%)	261 (91%)	26 (9%)	9	9
1	B	281/288 (98%)	248 (88%)	33 (12%)	5	5
1	C	281/288 (98%)	254 (90%)	27 (10%)	8	8
All	All	849/864 (98%)	763 (90%)	86 (10%)	7	7

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	33	LEU
1	A	48	GLN
1	A	55	ASP
1	A	59	LEU
1	A	74	LEU
1	A	88	ASN
1	A	103	LEU
1	A	140	SER
1	A	144	LEU
1	A	152	LEU
1	A	164	VAL
1	A	173	SER
1	A	174	ARG
1	A	229	VAL
1	A	235	GLU
1	A	257	THR
1	A	287	ASN

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Mol	Chain	Res	Type
1	A	293	GLU
1	A	308	MET
1	A	309	ARG
1	A	312	VAL
1	A	343	ASN
1	A	344	LEU
1	A	347	CYS
1	A	349	LEU
1	B	32	LEU
1	B	33	LEU
1	B	48	GLN
1	B	74	LEU
1	B	90	GLN
1	B	96	ARG
1	B	130	SER
1	B	132	ILE
1	B	135	CYS
1	B	137	ASP
1	B	145	ASN
1	B	152	LEU
1	B	161	PRO
1	B	176	LYS
1	B	186	SER
1	B	189	ASP
1	B	205	LYS
1	B	208	ILE
1	B	223	LEU
1	B	224	SER
1	B	229	VAL
1	B	238	ARG
1	B	253	ARG
1	B	258	THR
1	B	259	SER
1	B	260	ILE
1	B	280	SER
1	B	285	ASP
1	B	291	THR
1	B	293	GLU
1	B	308	MET
1	B	331	VAL
1	B	336	THR
1	C	32	LEU

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Mol	Chain	Res	Type
1	C	33	LEU
1	C	48	GLN
1	C	74	LEU
1	C	78	LEU
1	C	80	ILE
1	C	89	ILE
1	C	96	ARG
1	C	101	ARG
1	C	120	SER
1	C	124	GLN
1	C	145	ASN
1	C	152	LEU
1	C	154	ASP
1	C	158	LEU
1	C	159	VAL
1	C	172	ARG
1	C	205	LYS
1	C	223	LEU
1	C	229	VAL
1	C	230	LEU
1	C	258	THR
1	C	271	SER
1	C	290	ASN
1	C	297	ASN
1	C	309	ARG
1	C	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	53	HIS
1	A	54	GLN
1	A	97	GLN
1	A	105	HIS
1	A	145	ASN
1	A	191	ASN
1	A	251	ASN
1	A	252	HIS
1	A	318	HIS
1	A	343	ASN
1	B	48	GLN

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Mol	Chain	Res	Type
1	B	53	HIS
1	B	88	ASN
1	B	133	GLN
1	B	143	GLN
1	B	247	ASN
1	B	307	ASN
1	B	318	HIS
1	C	48	GLN
1	C	53	HIS
1	C	124	GLN
1	C	145	ASN
1	C	191	ASN
1	C	247	ASN
1	C	251	ASN
1	C	287	ASN
1	C	297	ASN
1	C	307	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic and 6 are modelled with single atom - 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	$\# Z > 2$
4	GSP	C	351	2	33,34,34	1.90	5 (15%)	47,54,54	1.18	5 (10%)
4	GSP	A	351	2	33,34,34	1.55	7 (21%)	47,54,54	1.13	4 (8%)
4	GSP	B	351	2	33,34,34	1.75	6 (18%)	47,54,54	1.42	8 (17%)

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
4	GSP	C	351	2	-	3/21/38/38	0/3/3/3
4	GSP	A	351	2	-	1/21/38/38	0/3/3/3
4	GSP	B	351	2	-	3/21/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	351	GSP	PB-O3A	8.28	1.68	1.59
4	B	351	GSP	PA-O3A	6.20	1.66	1.59
4	A	351	GSP	PB-O3A	4.05	1.63	1.59
4	A	351	GSP	PG-O2G	-3.00	1.45	1.54
4	B	351	GSP	C5'-C4'	2.77	1.59	1.51
4	A	351	GSP	PA-O3A	2.67	1.62	1.59
4	C	351	GSP	PA-O3A	2.59	1.62	1.59
4	C	351	GSP	PG-O2G	-2.53	1.46	1.54
4	A	351	GSP	C4-N3	2.53	1.40	1.34
4	C	351	GSP	PG-O3G	-2.33	1.47	1.54
4	A	351	GSP	C5'-C4'	2.28	1.58	1.51
4	B	351	GSP	O4'-C1'	2.25	1.47	1.42
4	A	351	GSP	O4'-C4'	-2.23	1.40	1.45
4	B	351	GSP	PA-O5'	2.20	1.68	1.59
4	B	351	GSP	PB-O3A	2.15	1.61	1.59
4	A	351	GSP	PB-O2B	-2.07	1.45	1.55
4	B	351	GSP	C6-N1	2.04	1.42	1.38
4	C	351	GSP	PB-O3B	2.04	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	351	GSP	C2'-C3'-C4'	3.70	109.76	102.61
4	B	351	GSP	O2B-PB-O3B	3.58	116.96	107.27
4	B	351	GSP	O2'-C2'-C1'	3.33	121.57	110.10
4	C	351	GSP	O4'-C1'-N9	-2.74	102.15	108.36
4	B	351	GSP	O2A-PA-O1A	2.56	124.34	112.44
4	B	351	GSP	O3A-PB-O1B	-2.48	103.25	110.70
4	C	351	GSP	C1'-N9-C8	2.35	133.40	126.73
4	C	351	GSP	O3A-PB-O1B	-2.33	103.69	110.70
4	A	351	GSP	O2'-C2'-C3'	2.31	119.22	111.82
4	C	351	GSP	O4'-C1'-C2'	2.28	111.50	106.62
4	B	351	GSP	N9-C8-N7	2.28	117.63	113.40
4	A	351	GSP	O4'-C1'-C2'	-2.22	101.87	106.62
4	A	351	GSP	O3A-PB-O1B	-2.21	104.05	110.70
4	B	351	GSP	O2A-PA-O3A	-2.20	101.32	107.27
4	C	351	GSP	PB-O3B-PG	2.08	140.78	133.17
4	A	351	GSP	O4'-C4'-C5'	-2.03	102.84	109.33
4	B	351	GSP	O2B-PB-O3A	-2.01	101.83	107.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	351	GSP	C5'-O5'-PA-O2A
4	C	351	GSP	C5'-O5'-PA-O2A
4	C	351	GSP	C5'-O5'-PA-O3A
4	B	351	GSP	PA-O3A-PB-O1B
4	B	351	GSP	PA-O3A-PB-O2B
4	A	351	GSP	C4'-C5'-O5'-PA
4	C	351	GSP	PA-O3A-PB-O1B

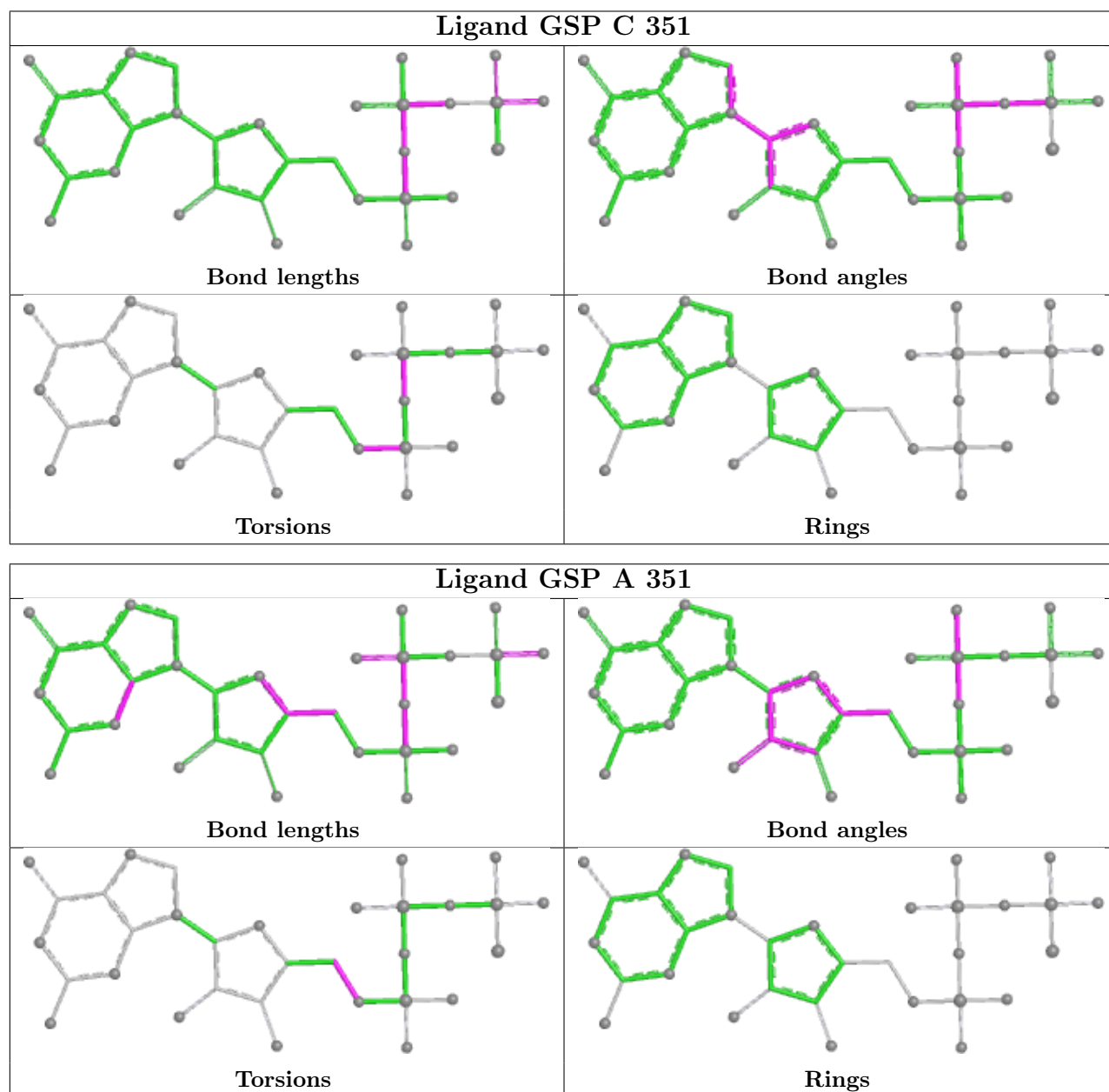
There are no ring outliers.

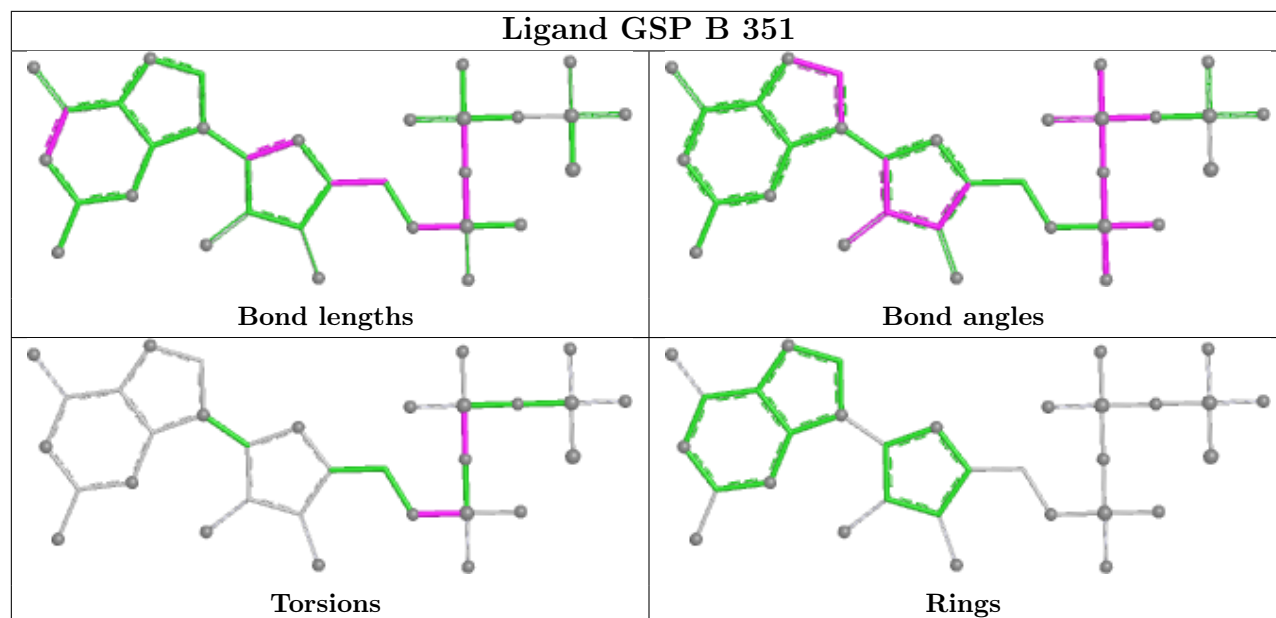
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	351	GSP	1	0
4	B	351	GSP	4	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.