Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 03:20 AM EST

PDB ID	:	1TND
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 (i) 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 (1)) were used in the production of this report:

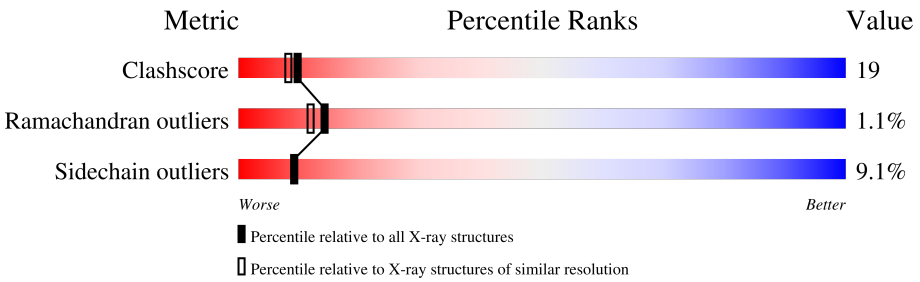
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	324	64% 31% 5%
1	B	324	55% 37% 6% ·
1	C	324	66% 27% · ·

2 Entry composition (i)

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.

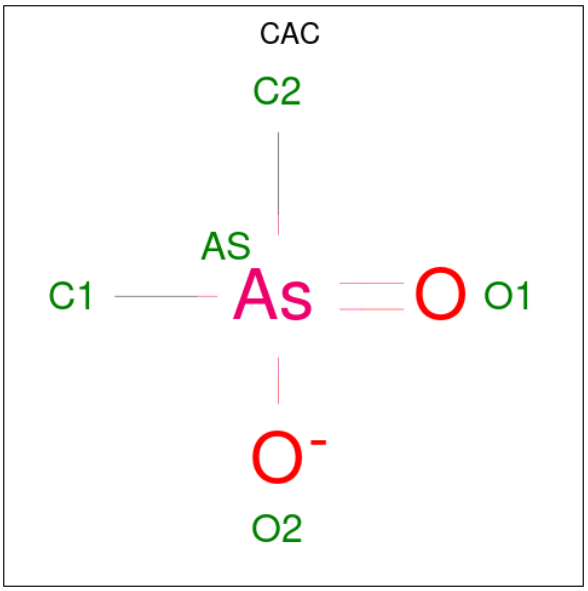
- Molecule 1 is a protein called TRANSDUCIN.

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

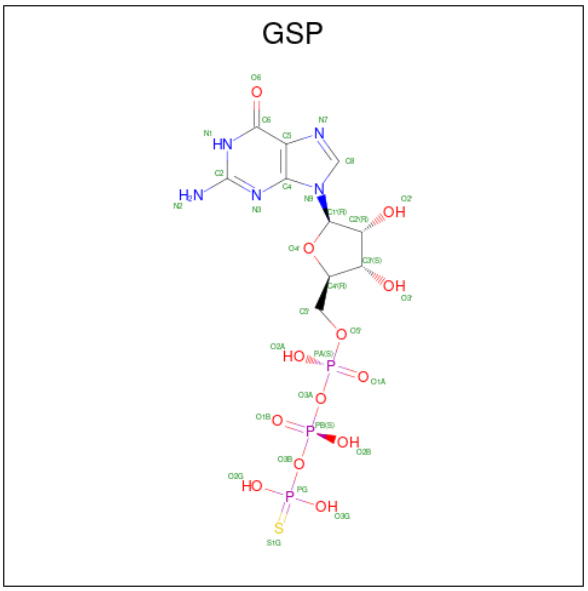
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



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

- Molecule 5 is water.

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

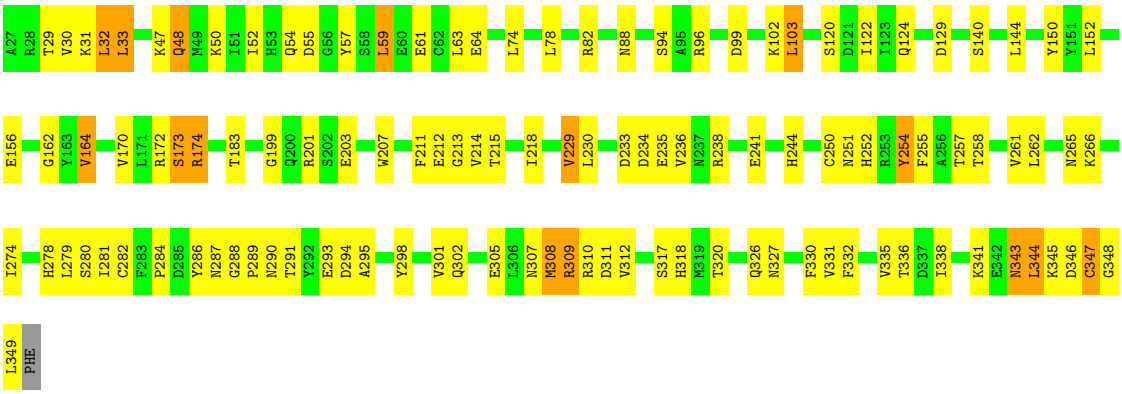
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

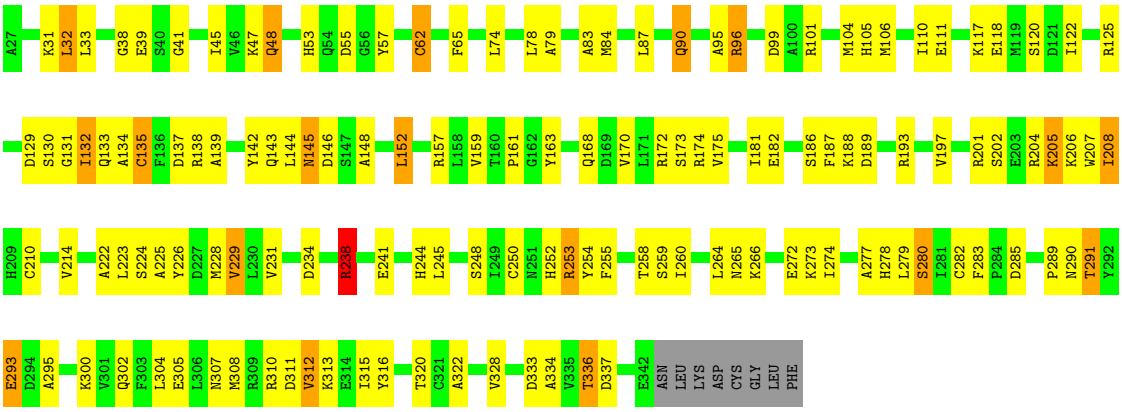
• Molecule 1: TRANSDUCIN

Chain A: 64% 31% 5%



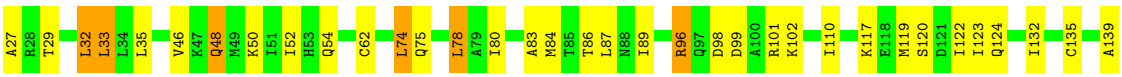
• Molecule 1: TRANSDUCIN

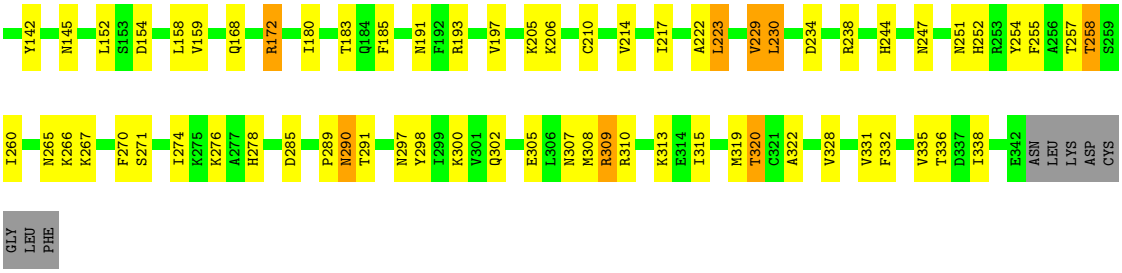
Chain B: 55% 37% 6%



• Molecule 1: TRANSDUCIN

Chain C: 66% 27%




Y142
N145
L152
S153
D154
L158
V159
Q168
R172
I180
T183
Q184
F185
N191
F192
R193
V197
K205
K206
C210
V214
I217
A222
L223
V229
L230
D234
R238
H244
N247
N251
H252
R253
Y254
F255
A256
T257
T258
S259
I260
N265
K266
K267
F270
S271
I274
K275
K276
A277
H278
D285
P289
N290
T291
N297
Y298
I299
K300
V301
Q302
E305
L306
N307
M308
R309
R310
K313
E314
I315
M319
T320
C321
A322
V328
V331
F332
V335
T336
D337
I338
E342
ASN
LEU
LYS
ASP
CYS
GLY
LEU
PHE

4 Data and refinement statistics (i)

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	74.50Å 108.30Å 79.00Å 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 (i)

5.1 Standard geometry (i)

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	0.71	1/2635 (0.0%)	0.87	2/3552 (0.1%)
1	B	0.67	1/2584 (0.0%)	0.84	2/3484 (0.1%)
1	C	0.67	0/2584	0.82	1/3484 (0.0%)
All	All	0.68	2/7803 (0.0%)	0.85	5/10520 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	CYS	CB-SG	-7.92	1.68	1.82
1	A	250	CYS	CB-SG	-6.99	1.70	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	32	LEU	CA-CB-CG	7.14	131.72	115.30
1	A	32	LEU	CA-CB-CG	6.75	130.83	115.30
1	B	238	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	33	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	245	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	84	0
1	B	2539	0	2518	116	0
1	C	2539	0	2520	92	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	1	0
3	C	2	0	0	2	0
4	A	32	0	12	1	0
4	B	32	0	12	3	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	290	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 19.

All (290) 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
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:A:307:ASN:OD1	1:A:309:ARG:HG2	1.84	0.77
1:B:84:MET:HE3	1:B:135:CYS:HB2	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:332:PHE:O	1:A:336:THR:HG23	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLY:HA3	1:A:348:GLY:CA	2.31	0.61
1:A:174:ARG:HD3	5:A:629:HOH:O	2.01	0.61
1:B:210:CYS:HG	3:B:354:CAC:AS	2.43	0.60
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:C:197:VAL:CG2	1:C:206:LYS:HZ2	2.23	0.51
1:B:96:ARG:HA	1:B:96:ARG:HH11	1.75	0.51
1:C:180:ILE:CG1	1:C:206:LYS:HZ3	2.24	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: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:C:223:LEU:HD21	1:C:319:MET:HE1	1.93	0.50
1:A:156:GLU:HG3	5:A:393:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:334:ALA:O	1:B:337:ASP:HB2	2.13	0.49
1:C:223:LEU:HD21	1:C:319:MET:HE3	1.93	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:197:VAL:HG23	1:B:206:LYS:HZ1	1.77	0.48
1:B:197:VAL:CG2	1:B:206:LYS:HZ2	2.26	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:SER:HA	1:B:205:LYS:HE2	1.96	0.46
1:C:197:VAL:HG23	1:C:206:LYS:HZ2	1.77	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:95:ALA:C	1:B:96:ARG:HH11	2.19	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:180:ILE:HG13	1:C:206:LYS:HZ3	1.80	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
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: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:A:310:ARG:HD3	1:A:310:ARG:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:HB3	5:B:573:HOH:O	2.18	0.44
1:C:75:GLN:CD	5:C:404:HOH:O	2.55	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:B:170:VAL:O	1:B:173:SER:OG	2.28	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:266:LYS:HG2	4:A:351:GSP:C6	2.54	0.42
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: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:A:215:THR:HG1	1:A:346:ASP:HA	1.84	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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%)	9 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	314/324 (97%)	292 (93%)	18 (6%)	4 (1%)	12	9
1	C	314/324 (97%)	301 (96%)	12 (4%)	1 (0%)	41	46
All	All	949/972 (98%)	887 (94%)	52 (6%)	10 (1%)	14	12

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
1	C	290	ASN
1	B	253	ARG
1	A	94	SER
1	A	288	GLY

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	287/288 (100%)	262 (91%)	25 (9%)	10	10
1	B	281/288 (98%)	253 (90%)	28 (10%)	7	7
1	C	281/288 (98%)	257 (92%)	24 (8%)	10	10
All	All	849/864 (98%)	772 (91%)	77 (9%)	9	9

All (77) 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

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Mol	Chain	Res	Type
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	254	TYR
1	A	257	THR
1	A	287	ASN
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	B	32	LEU
1	B	48	GLN
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	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	259	SER

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Mol	Chain	Res	Type
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	336	THR
1	C	32	LEU
1	C	33	LEU
1	C	48	GLN
1	C	74	LEU
1	C	78	LEU
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	247	ASN
1	C	258	THR
1	C	271	SER
1	C	309	ARG
1	C	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	145	ASN
1	A	184	GLN
1	A	251	ASN

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Mol	Chain	Res	Type
1	A	252	HIS
1	A	318	HIS
1	A	343	ASN
1	B	48	GLN
1	B	53	HIS
1	B	90	GLN
1	B	133	GLN
1	B	143	GLN
1	B	247	ASN
1	B	302	GLN
1	B	307	ASN
1	C	48	GLN
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 monosaccharides 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	26,34,34	1.52	5 (19%)	27,54,54	1.32	3 (11%)
4	GSP	A	351	2	26,34,34	1.62	7 (26%)	27,54,54	1.50	4 (14%)
4	GSP	B	351	2	26,34,34	1.76	5 (19%)	27,54,54	1.45	5 (18%)

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	-	3/17/38/38	0/3/3/3
4	GSP	A	351	2	-	3/17/38/38	0/3/3/3
4	GSP	B	351	2	-	5/17/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	351	GSP	O4'-C1'	4.39	1.47	1.41
4	C	351	GSP	C2'-C1'	-3.34	1.48	1.53
4	B	351	GSP	C6-N1	3.22	1.42	1.37
4	A	351	GSP	PG-O2G	-3.07	1.45	1.54
4	A	351	GSP	C2'-C1'	-3.06	1.49	1.53
4	A	351	GSP	C8-N7	-2.72	1.30	1.35
4	B	351	GSP	C8-N7	-2.67	1.30	1.35
4	B	351	GSP	C5'-C4'	2.66	1.59	1.51
4	C	351	GSP	C8-N7	-2.63	1.30	1.35
4	C	351	GSP	PG-O2G	-2.60	1.46	1.54
4	A	351	GSP	C6-N1	2.43	1.41	1.37
4	C	351	GSP	PG-O3G	-2.40	1.47	1.54
4	A	351	GSP	O4'-C4'	-2.22	1.40	1.45
4	A	351	GSP	C5'-C4'	2.18	1.58	1.51
4	B	351	GSP	PA-O5'	2.15	1.68	1.59
4	A	351	GSP	PB-O2B	-2.04	1.45	1.55
4	C	351	GSP	C5-C4	-2.02	1.37	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	351	GSP	C2'-C3'-C4'	3.66	109.76	102.64
4	A	351	GSP	O4'-C1'-C2'	-3.46	101.87	106.93
4	C	351	GSP	O6-C6-C5	3.20	130.62	124.37
4	C	351	GSP	O4'-C1'-C2'	3.13	111.50	106.93
4	B	351	GSP	O2'-C2'-C1'	2.90	121.57	110.85
4	A	351	GSP	O6-C6-C5	2.68	129.60	124.37
4	B	351	GSP	O4'-C1'-C2'	2.46	110.53	106.93
4	B	351	GSP	O2A-PA-O1A	2.45	124.34	112.24
4	A	351	GSP	C3'-C2'-C1'	2.30	104.45	100.98
4	A	351	GSP	O2'-C2'-C3'	2.29	119.22	111.82
4	B	351	GSP	C5-C6-N1	-2.14	110.17	113.95
4	C	351	GSP	O6-C6-N1	-2.07	118.20	120.65

There are no chirality outliers.

All (11) 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	A	351	GSP	C5'-O5'-PA-O3A
4	B	351	GSP	C5'-O5'-PA-O3A
4	B	351	GSP	PA-O3A-PB-O2B
4	A	351	GSP	C4'-C5'-O5'-PA
4	A	351	GSP	C5'-O5'-PA-O2A
4	B	351	GSP	C5'-O5'-PA-O1A
4	C	351	GSP	C5'-O5'-PA-O1A

There are no ring outliers.

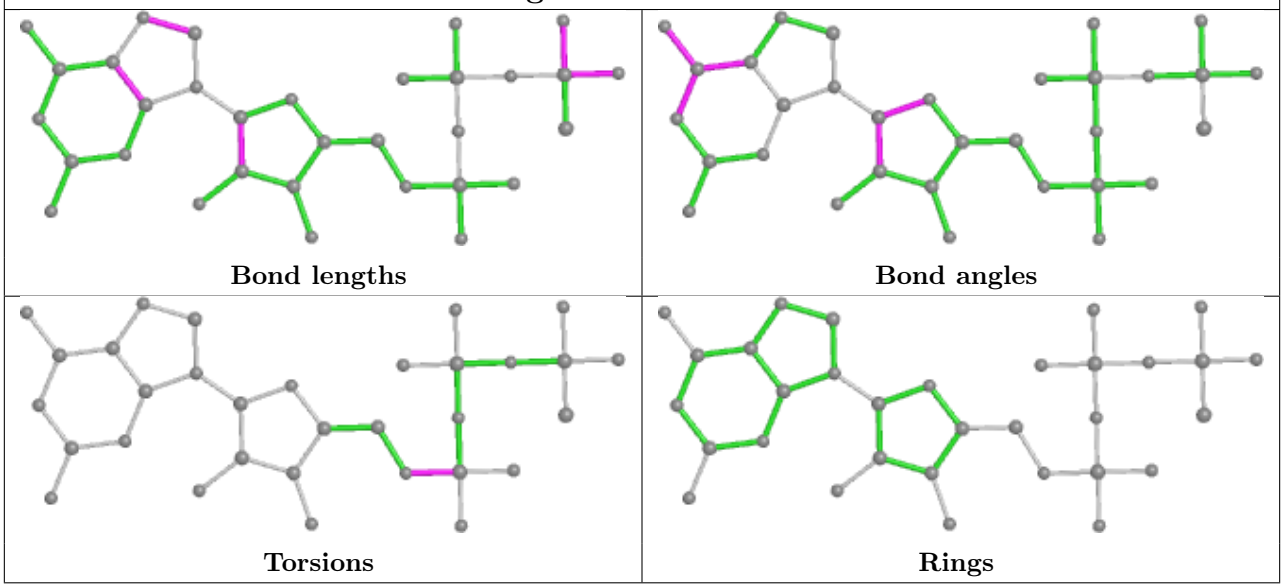
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	351	GSP	1	0
4	B	351	GSP	3	0

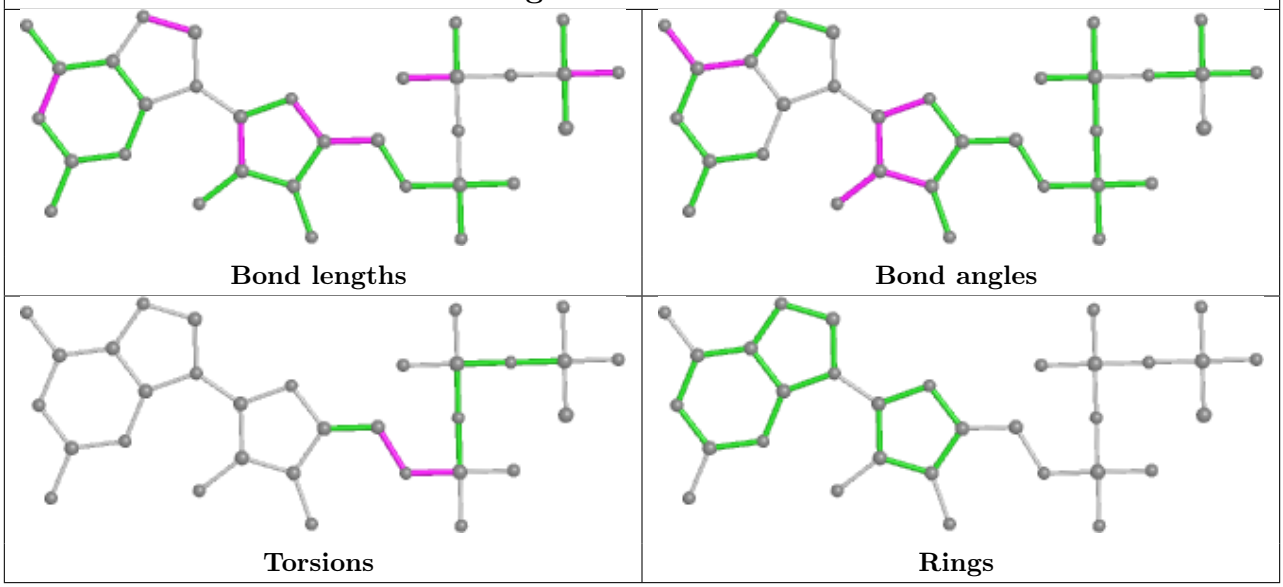
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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

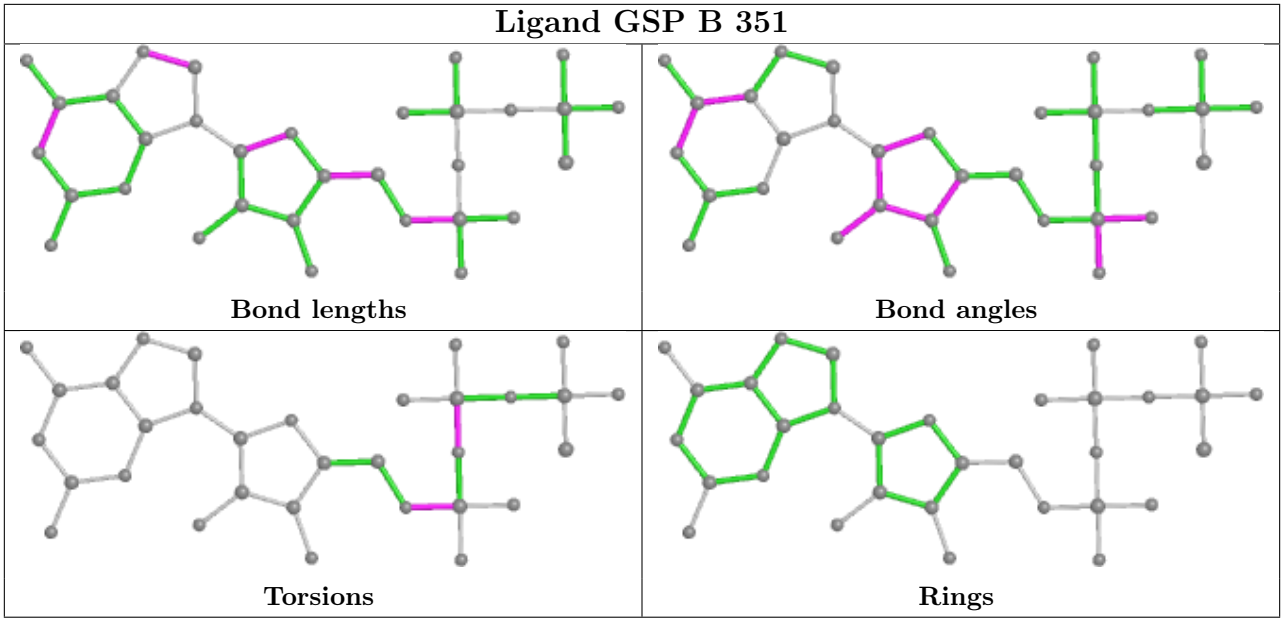
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

Ligand GSP C 351



Ligand GSP A 351





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.