



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 04:17 PM EST

PDB ID : 3DZY  
Title : Intact PPAR gamma - RXR alpha Nuclear Receptor Complex on DNA bound with Rosiglitazone, 9-cis Retinoic Acid and NCOA2 Peptide  
Authors : Chandra, V.; Huang, P.; Hamuro, Y.; Raghuram, S.; Wang, Y.; Burris, T.P.; Rastinejad, F.  
Deposited on : 2008-07-30  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

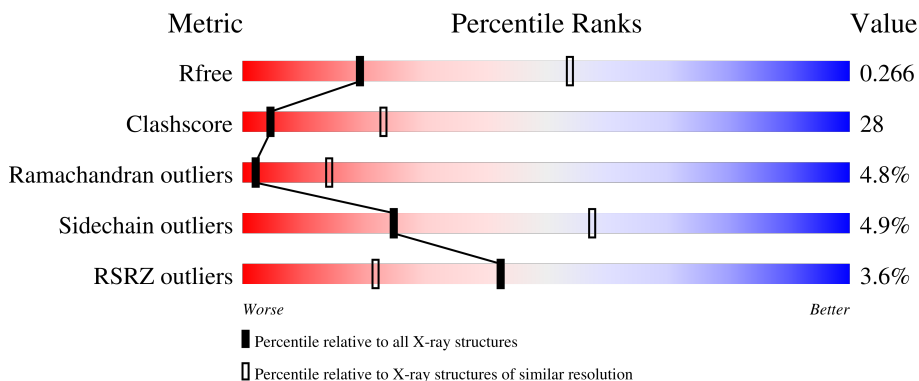
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	467	 3% 33% 28% 35%
2	D	419	 2% 45% 34% 5% 16%
3	C	20	 10% 75% 15%
4	F	20	 5% 90% 5%

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Mol	Chain	Length	Quality of chain
5	E	13	 38% 38% 23%
5	G	13	 46% 23% 31%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 6271 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	302	2407	1512	436	438	21	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP P19793
A	-3	ALA	-	expression tag	UNP P19793
A	-2	HIS	-	expression tag	UNP P19793
A	-1	HIS	-	expression tag	UNP P19793
A	0	HIS	-	expression tag	UNP P19793
A	1	HIS	-	expression tag	UNP P19793
A	2	HIS	-	expression tag	UNP P19793
A	3	HIS	-	expression tag	UNP P19793
A	4	VAL	-	expression tag	UNP P19793
A	5	ASP	-	expression tag	UNP P19793
A	6	ASP	-	expression tag	UNP P19793
A	7	ASP	-	expression tag	UNP P19793
A	8	ASP	-	expression tag	UNP P19793
A	9	LYS	-	expression tag	UNP P19793
A	10	MET	-	expression tag	UNP P19793

- Molecule 2 is a protein called Peroxisome proliferator-activated receptor gamma.

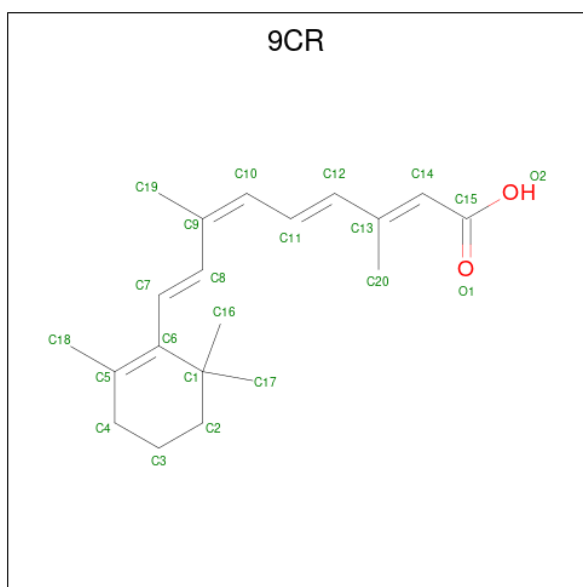
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	354	2834	1809	485	519	21	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	59	MET	-	expression tag	UNP P37231

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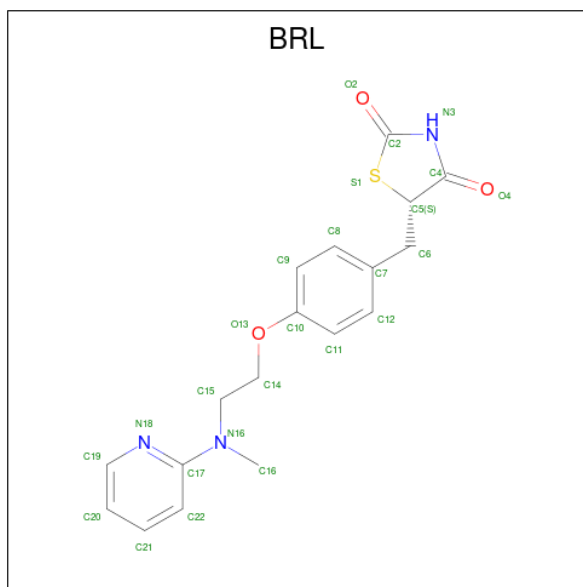


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			22	20 2		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

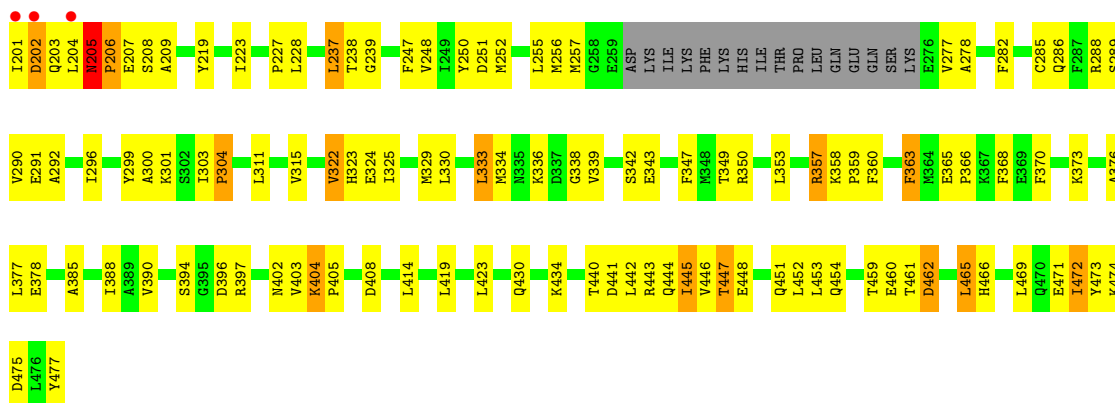
- Molecule 8 is 2,4-THIAZOLIDINEDIONE, 5-[[4-[2-(METHYL-2-PYRIDINYLAMINO)ETHOXY]PHENYL]METHYL]-(9CL) (three-letter code: BRL) (formula: C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S).



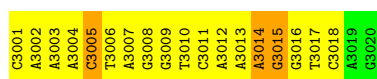
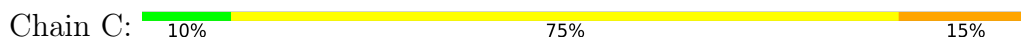
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	D	1	25	18	3	3	1	0	0



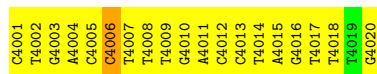




- Molecule 3: DNA (5'-D(\*DCP\*DAP\*DAP\*DAP\*DCP\*DTP\*DAP\*DGP\*DGP\*DTP\*DCP\*DAP\*DAP\*DAP\*DGP\*DGP\*DTP\*DCP\*DAP\*DG)-3')



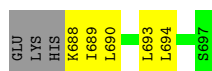
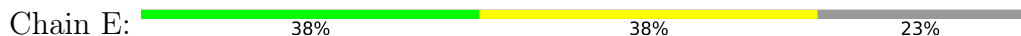
- Molecule 4: DNA (5'-D(\*DCP\*DTP\*DGP\*DAP\*DCP\*DCP\*DTP\*DTP\*DTP\*DGP\*DAP\*DCP\*DCP\*DTP\*DAP\*DGP\*DTP\*DTP\*DTP\*DG)-3')



- Molecule 5: NCOA2 Peptide



- Molecule 5: NCOA2 Peptide



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.80Å 146.51Å 67.22Å 90.00° 115.59° 90.00°	Depositor
Resolution (Å)	46.71 – 3.10 46.71 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.3 (46.71-3.10) 94.0 (46.71-2.99)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 3.01Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.213 , 0.268 0.208 , 0.266	Depositor DCC
$R_{free}$ test set	4034 reflections (9.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtrriage
Anisotropy	0.454	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 74.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6271	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BRL, ZN, 9CR

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	0.38	0/2448	0.66	0/3287
2	D	0.40	0/2882	0.64	0/3871
3	C	0.49	0/463	0.80	0/713
4	F	0.45	0/449	0.87	0/691
5	E	0.38	0/86	0.80	0/112
5	G	0.31	0/79	0.57	0/104
All	All	0.41	0/6407	0.68	0/8778

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3
4	F	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	3005	DC	Sidechain
3	C	3014	DA	Sidechain
3	C	3015	DG	Sidechain
4	F	4006	DC	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2407	0	2427	156	0
2	D	2834	0	2885	154	0
3	C	411	0	225	35	0
4	F	403	0	230	19	0
5	E	86	0	93	5	0
5	G	79	0	88	8	0
6	A	22	0	27	2	0
7	A	2	0	0	0	0
7	D	2	0	0	0	0
8	D	25	0	19	2	0
All	All	6271	0	5994	347	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 28.

All (347) 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:454:MET:HE1	5:G:690:LEU:HD12	1.42	1.01
2:D:193:LEU:HB2	2:D:197:ILE:HG12	1.44	1.00
2:D:357:ARG:HG2	2:D:357:ARG:HH11	1.24	0.98
2:D:125:VAL:HG11	2:D:175:MET:HG2	1.47	0.95
2:D:185:MET:HB3	2:D:188:ALA:HB2	1.51	0.93
2:D:200:ASP:O	2:D:204:LEU:HB3	1.77	0.85
1:A:320:VAL:HG21	1:A:325:LEU:HD11	1.57	0.85
2:D:325:ILE:HD12	2:D:388:ILE:HG23	1.59	0.85
4:F:4004:DA:H1'	4:F:4005:DC:H5'	1.59	0.83
2:D:205:ASN:HB2	2:D:206:PRO:HA	1.59	0.82
3:C:3007:DA:H2''	3:C:3008:DG:H5'	1.60	0.82
1:A:312:SER:HB3	1:A:371:ARG:NH1	1.98	0.78
1:A:294:LEU:O	1:A:294:LEU:HD23	1.83	0.78
2:D:125:VAL:CG1	2:D:175:MET:HG2	2.14	0.76
2:D:125:VAL:HG11	2:D:175:MET:CG	2.14	0.76
3:C:3007:DA:H2''	3:C:3008:DG:C5'	2.16	0.76
1:A:186:ARG:HA	1:A:186:ARG:HH11	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:CG	1:A:174:ASN:H	1.90	0.74
2:D:474:LYS:O	2:D:475:ASP:HB2	1.87	0.74
1:A:230:MET:HG2	1:A:396:VAL:HG22	1.69	0.74
1:A:289:PHE:CD1	1:A:375:LEU:HD21	2.22	0.74
3:C:3006:DT:H2''	3:C:3007:DA:C8	2.23	0.73
2:D:109:ILE:HD12	2:D:109:ILE:H	1.52	0.73
1:A:238:ALA:HA	1:A:285:ARG:HD2	1.71	0.73
4:F:4007:DT:H1'	4:F:4008:DT:H5''	1.71	0.73
3:C:3005:DC:H2'	3:C:3006:DT:H72	1.71	0.72
1:A:209:ARG:NE	3:C:3015:DG:H4'	2.05	0.72
1:A:315:HIS:O	1:A:318:ILE:HG12	1.90	0.71
2:D:206:PRO:HG2	2:D:207:GLU:H	1.53	0.71
2:D:252:MET:O	2:D:256:MET:HG2	1.89	0.71
2:D:300:ALA:O	2:D:303:ILE:HG12	1.92	0.70
1:A:140:ASP:OD1	1:A:141:ARG:N	2.24	0.70
2:D:443:ARG:O	2:D:447:THR:HG23	1.92	0.69
2:D:322:VAL:HG23	2:D:323:HIS:N	2.07	0.69
4:F:4008:DT:H2''	4:F:4009:DT:H5'	1.74	0.68
1:A:182:ARG:HG3	1:A:183:GLN:HG2	1.75	0.67
1:A:285:ARG:NH1	1:A:285:ARG:HB2	2.08	0.67
1:A:421:ARG:NH1	1:A:421:ARG:HA	2.09	0.67
1:A:442:ILE:HG22	1:A:442:ILE:O	1.94	0.66
2:D:349:THR:O	2:D:353:LEU:HD12	1.96	0.66
2:D:357:ARG:HG2	2:D:357:ARG:NH1	2.01	0.66
1:A:226:ALA:C	1:A:228:GLU:H	2.00	0.65
2:D:322:VAL:HG23	2:D:323:HIS:H	1.62	0.64
3:C:3002:DA:H1'	3:C:3003:DA:H5'	1.78	0.64
1:A:197:ALA:HA	2:D:248:VAL:HG11	1.77	0.64
2:D:405:PRO:O	2:D:408:ASP:HB3	1.97	0.64
2:D:473:TYR:HE2	8:D:478:BRL:HN3	1.45	0.64
2:D:394:SER:O	2:D:397:ARG:HG2	1.98	0.64
1:A:268:ILE:HA	1:A:326:LEU:HD13	1.79	0.64
1:A:363:ASP:HB3	1:A:366:GLU:HG3	1.79	0.64
3:C:3003:DA:H1'	3:C:3004:DA:H5'	1.79	0.63
4:F:4006:DC:H2''	4:F:4007:DT:OP2	1.98	0.62
2:D:109:ILE:HD12	2:D:109:ILE:N	2.14	0.62
2:D:465:LEU:HD13	2:D:465:LEU:O	1.98	0.62
1:A:165:LYS:O	1:A:167:LEU:HD23	1.99	0.62
2:D:204:LEU:O	2:D:209:ALA:HB2	1.99	0.62
1:A:280:VAL:O	1:A:284:LYS:HB2	2.00	0.62
4:F:4008:DT:H5'	4:F:4008:DT:H6	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:NH2	3:C:3016:DG:OP2	2.33	0.61
2:D:441:ASP:O	2:D:444:GLN:HB3	1.99	0.61
3:C:3009:DG:H1'	3:C:3010:DT:H5'	1.82	0.61
1:A:225:SER:C	1:A:227:ASN:H	2.03	0.61
1:A:232:VAL:HG11	1:A:403:TYR:CD2	2.36	0.61
1:A:312:SER:CB	1:A:371:ARG:NH1	2.62	0.61
1:A:352:GLU:HG3	1:A:428:ILE:HD11	1.82	0.61
2:D:193:LEU:HB2	2:D:197:ILE:CG1	2.27	0.61
4:F:4008:DT:H2'	4:F:4009:DT:H71	1.83	0.61
1:A:305:TRP:HE3	1:A:309:LEU:HD12	1.66	0.61
2:D:228:LEU:HD23	2:D:333:LEU:HD22	1.82	0.61
1:A:436:LEU:HD11	6:A:463:9CR:H23	1.84	0.60
2:D:289:SER:OG	8:D:478:BRL:H5	2.01	0.60
3:C:3006:DT:H5'	3:C:3006:DT:H6	1.66	0.60
1:A:349:VAL:HG13	1:A:353:LEU:HD12	1.83	0.60
1:A:182:ARG:HG3	1:A:183:GLN:H	1.65	0.60
2:D:140:ARG:O	2:D:141:LEU:HD23	2.02	0.60
1:A:298:VAL:HG13	5:G:690:LEU:HD13	1.84	0.59
1:A:345:ILE:HG23	1:A:346:PHE:N	2.16	0.59
2:D:182:PHE:HB2	4:F:4018:DT:H5'	1.84	0.59
2:D:434:LYS:NZ	2:D:434:LYS:HB3	2.17	0.59
1:A:233:GLU:H	1:A:233:GLU:CD	2.07	0.59
1:A:345:ILE:HG23	1:A:346:PHE:H	1.67	0.59
1:A:173:ASP:CG	1:A:174:ASN:N	2.56	0.58
1:A:268:ILE:HA	1:A:326:LEU:CD1	2.33	0.58
1:A:298:VAL:HG13	5:G:690:LEU:HD22	1.85	0.58
1:A:319:ALA:O	1:A:320:VAL:C	2.42	0.58
2:D:402:ASN:HB3	2:D:405:PRO:HG2	1.85	0.58
1:A:451:LEU:O	1:A:455:LEU:HD13	2.03	0.58
1:A:345:ILE:HD13	1:A:431:LYS:HD3	1.85	0.58
2:D:116:ASP:OD1	2:D:116:ASP:N	2.37	0.58
1:A:206:GLN:HE21	3:C:3014:DA:H4'	1.69	0.57
1:A:264:PRO:HG2	1:A:265:VAL:H	1.69	0.57
3:C:3011:DC:H2''	3:C:3012:DA:OP2	2.03	0.57
1:A:186:ARG:HH11	1:A:186:ARG:CA	2.17	0.57
2:D:154:ILE:HD12	2:D:154:ILE:N	2.20	0.57
3:C:3006:DT:H2''	3:C:3007:DA:N7	2.20	0.57
1:A:264:PRO:N	1:A:267:ASN:ND2	2.52	0.57
1:A:289:PHE:HD1	1:A:375:LEU:HD21	1.66	0.57
2:D:219:TYR:O	2:D:223:ILE:HG12	2.05	0.57
2:D:228:LEU:CD2	2:D:333:LEU:HD22	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HG3	1:A:183:GLN:N	2.20	0.57
1:A:203:GLU:CD	1:A:203:GLU:H	2.07	0.57
1:A:221:GLU:O	1:A:222:SER:CB	2.53	0.57
1:A:226:ALA:O	1:A:228:GLU:N	2.33	0.56
1:A:154:GLY:HA2	4:F:4003:DG:H2'	1.87	0.56
3:C:3006:DT:H5'	3:C:3006:DT:C6	2.40	0.56
1:A:312:SER:HB3	1:A:371:ARG:HH12	1.67	0.56
1:A:318:ILE:HD12	1:A:358:ARG:HA	1.86	0.56
1:A:407:LYS:HB3	1:A:408:TYR:CD2	2.40	0.56
2:D:159:ARG:O	2:D:166:ARG:HD2	2.05	0.56
1:A:320:VAL:HG11	1:A:325:LEU:CD1	2.35	0.56
2:D:282:PHE:CE2	2:D:286:GLN:NE2	2.73	0.56
2:D:193:LEU:HD22	2:D:197:ILE:HD11	1.88	0.56
1:A:288:HIS:HB3	1:A:392:LEU:HD21	1.88	0.55
5:E:693:LEU:HD12	5:E:693:LEU:H	1.71	0.55
1:A:405:LYS:O	1:A:409:PRO:HG3	2.05	0.55
3:C:3014:DA:H2''	3:C:3015:DG:H8	1.71	0.55
2:D:170:CYS:HA	2:D:173:VAL:HG22	1.88	0.55
1:A:408:TYR:N	1:A:409:PRO:HD3	2.21	0.55
1:A:209:ARG:N	3:C:3016:DG:OP1	2.37	0.55
1:A:230:MET:SD	1:A:287:PRO:HG2	2.47	0.55
1:A:285:ARG:HB2	1:A:285:ARG:HH11	1.70	0.54
1:A:443:GLY:O	1:A:445:THR:HG22	2.07	0.54
2:D:277:VAL:HG13	2:D:278:ALA:N	2.21	0.54
3:C:3016:DG:H5'	3:C:3016:DG:H8	1.72	0.54
1:A:454:MET:C	1:A:455:LEU:HD12	2.27	0.54
1:A:318:ILE:O	1:A:319:ALA:HB3	2.07	0.54
2:D:204:LEU:O	2:D:205:ASN:HB3	2.07	0.54
1:A:312:SER:CB	1:A:371:ARG:HH12	2.18	0.54
2:D:139:ILE:C	2:D:141:LEU:H	2.09	0.54
1:A:221:GLU:O	1:A:222:SER:HB2	2.06	0.54
2:D:204:LEU:O	2:D:204:LEU:HG	2.09	0.53
1:A:420:LEU:O	1:A:423:PRO:HD2	2.08	0.53
2:D:109:ILE:HG22	2:D:110:GLU:N	2.23	0.53
2:D:404:LYS:O	2:D:404:LYS:HD3	2.09	0.53
2:D:451:GLN:O	2:D:454:GLN:HB2	2.09	0.53
2:D:461:THR:O	2:D:461:THR:HG22	2.09	0.53
2:D:338:GLY:HA3	2:D:347:PHE:CZ	2.44	0.53
1:A:423:PRO:HG3	2:D:440:THR:HG22	1.91	0.52
2:D:205:ASN:HD22	2:D:205:ASN:C	2.11	0.52
2:D:441:ASP:HA	2:D:444:GLN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:NH2	4:F:4003:DG:OP1	2.43	0.52
1:A:333:HIS:O	1:A:336:SER:HB3	2.09	0.52
1:A:288:HIS:O	1:A:291:GLU:HG2	2.10	0.52
2:D:255:LEU:HD23	2:D:255:LEU:C	2.29	0.52
2:D:315:VAL:HG22	5:E:694:LEU:CD1	2.40	0.52
2:D:147:ARG:HG2	2:D:148:CYS:N	2.25	0.52
2:D:199:SER:O	2:D:203:GLN:HB2	2.10	0.52
1:A:207:GLU:OE1	1:A:207:GLU:N	2.41	0.52
3:C:3007:DA:C2'	3:C:3008:DG:H5''	2.40	0.52
2:D:282:PHE:HE2	2:D:286:GLN:NE2	2.07	0.51
2:D:357:ARG:NH1	2:D:357:ARG:CG	2.69	0.51
1:A:276:LEU:HD23	1:A:279:LEU:HD12	1.90	0.51
2:D:138:THR:HG21	2:D:167:PHE:CZ	2.45	0.51
2:D:453:LEU:O	2:D:453:LEU:HD23	2.09	0.51
1:A:136:ALA:O	1:A:198:MET:HG3	2.10	0.51
1:A:360:MET:O	1:A:361:GLN:HB2	2.11	0.51
2:D:139:ILE:O	2:D:141:LEU:N	2.43	0.51
3:C:3007:DA:C2'	3:C:3008:DG:C5'	2.87	0.51
1:A:279:LEU:HD11	1:A:309:LEU:HG	1.93	0.51
3:C:3005:DC:C2'	3:C:3006:DT:H72	2.39	0.51
2:D:324:GLU:HG2	2:D:442:LEU:HB3	1.92	0.51
1:A:354:VAL:O	1:A:358:ARG:HB2	2.11	0.50
2:D:394:SER:HB3	2:D:396:ASP:OD1	2.11	0.50
1:A:358:ARG:NH1	1:A:358:ARG:HG2	2.26	0.50
2:D:139:ILE:C	2:D:141:LEU:N	2.63	0.50
2:D:277:VAL:CG1	2:D:278:ALA:N	2.74	0.50
1:A:320:VAL:HG11	1:A:325:LEU:HD12	1.93	0.50
1:A:450:PHE:HA	5:G:689:ILE:CD1	2.41	0.50
1:A:311:ALA:HB2	1:A:425:LEU:HD11	1.94	0.50
2:D:350:ARG:HG3	2:D:368:PHE:CD2	2.47	0.50
1:A:220:VAL:HG21	1:A:223:THR:HA	1.93	0.50
2:D:330:LEU:HG	2:D:334:MET:HE2	1.93	0.50
1:A:228:GLU:OE1	1:A:231:PRO:HA	2.12	0.49
3:C:3015:DG:H2''	3:C:3016:DG:H5'	1.94	0.49
3:C:3014:DA:H5'	3:C:3014:DA:H8	1.77	0.49
1:A:201:LYS:NZ	2:D:239:GLY:HA3	2.27	0.49
1:A:311:ALA:HB2	1:A:425:LEU:CD1	2.42	0.49
1:A:395:LYS:O	1:A:398:ALA:HB3	2.13	0.49
3:C:3004:DA:H2''	3:C:3005:DC:O5'	2.11	0.49
1:A:425:LEU:O	1:A:425:LEU:HG	2.11	0.49
3:C:3017:DT:H2''	3:C:3018:DC:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:ARG:HG3	2:D:160:ASN:HD22	1.76	0.49
2:D:122:HIS:CE1	2:D:132:LYS:HD2	2.48	0.49
1:A:192:TYR:O	1:A:195:CYS:HB2	2.12	0.49
2:D:159:ARG:HG3	2:D:160:ASN:N	2.27	0.49
2:D:194:LEU:O	2:D:196:GLU:N	2.46	0.48
2:D:206:PRO:C	2:D:208:SER:H	2.17	0.48
2:D:402:ASN:C	2:D:405:PRO:HD2	2.33	0.48
1:A:426:ARG:HD3	2:D:444:GLN:HB2	1.95	0.48
2:D:201:ILE:HG13	2:D:202:ASP:OD1	2.13	0.48
1:A:334:ARG:O	1:A:336:SER:N	2.46	0.48
2:D:434:LYS:HB3	2:D:434:LYS:HZ3	1.77	0.48
2:D:365:GLU:HB2	2:D:366:PRO:HD3	1.95	0.48
1:A:305:TRP:CG	1:A:306:ASN:N	2.81	0.48
1:A:397:TYR:O	1:A:401:GLU:HB2	2.14	0.48
2:D:247:PHE:HZ	2:D:257:MET:HE3	1.78	0.48
2:D:330:LEU:HG	2:D:334:MET:CE	2.44	0.48
5:E:690:LEU:HA	5:E:693:LEU:HD13	1.96	0.48
1:A:266:THR:HG23	1:A:446:PRO:HB2	1.96	0.48
2:D:430:GLN:O	2:D:434:LYS:HG3	2.14	0.48
1:A:392:LEU:O	1:A:396:VAL:HG23	2.13	0.48
2:D:359:PRO:HG2	2:D:360:PHE:CD2	2.49	0.48
4:F:4001:DC:H2''	4:F:4002:DT:H5'	1.96	0.48
2:D:448:GLU:O	2:D:452:LEU:HD13	2.14	0.47
2:D:193:LEU:O	2:D:197:ILE:HG23	2.14	0.47
2:D:286:GLN:OE1	2:D:465:LEU:HA	2.13	0.47
2:D:342:SER:O	2:D:343:GLU:HB2	2.14	0.47
2:D:419:LEU:O	2:D:423:LEU:HG	2.14	0.47
1:A:360:MET:CE	1:A:417:LYS:HG2	2.44	0.47
2:D:111:CYS:SG	2:D:127:ALA:HA	2.54	0.47
2:D:292:ALA:O	2:D:296:ILE:HG13	2.14	0.47
3:C:3016:DG:H2'	3:C:3017:DT:H72	1.95	0.47
4:F:4008:DT:H5'	4:F:4008:DT:C6	2.46	0.47
1:A:349:VAL:O	1:A:353:LEU:HB2	2.14	0.47
2:D:121:PHE:CE2	2:D:124:GLY:HA2	2.49	0.47
1:A:209:ARG:CD	3:C:3015:DG:H4'	2.45	0.47
2:D:219:TYR:CE1	2:D:223:ILE:HD11	2.50	0.47
2:D:469:LEU:O	2:D:473:TYR:HB2	2.14	0.47
4:F:4008:DT:C2'	4:F:4009:DT:H71	2.44	0.47
1:A:264:PRO:N	1:A:267:ASN:HD21	2.13	0.47
1:A:426:ARG:CD	2:D:444:GLN:HB2	2.45	0.47
2:D:193:LEU:HD12	2:D:195:ALA:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:PRO:HG2	2:D:228:LEU:H	1.78	0.47
3:C:3007:DA:H1'	3:C:3008:DG:H5''	1.97	0.46
2:D:322:VAL:CG2	2:D:323:HIS:N	2.78	0.46
1:A:324:ILE:HD11	1:A:346:PHE:CE2	2.50	0.46
1:A:403:TYR:O	1:A:403:TYR:CD1	2.68	0.46
2:D:109:ILE:H	2:D:109:ILE:CD1	2.25	0.46
1:A:442:ILE:O	1:A:444:ASP:N	2.49	0.46
2:D:130:GLY:HA2	4:F:4010:DG:H2'	1.97	0.46
1:A:316:ARG:NH2	6:A:463:9CR:O1	2.49	0.46
2:D:330:LEU:O	2:D:334:MET:HE2	2.16	0.46
1:A:226:ALA:C	1:A:228:GLU:N	2.67	0.46
1:A:163:VAL:HG13	1:A:202:ARG:NH1	2.31	0.46
1:A:203:GLU:HB2	2:D:238:THR:HG22	1.97	0.46
1:A:288:HIS:HA	1:A:291:GLU:HG2	1.98	0.46
2:D:197:ILE:HA	2:D:200:ASP:HB2	1.97	0.46
1:A:145:LYS:HB2	3:C:3013:DA:OP2	2.16	0.46
2:D:376:ALA:O	2:D:378:GLU:HG3	2.16	0.45
1:A:146:HIS:HB2	1:A:151:SER:OG	2.16	0.45
2:D:459:THR:O	2:D:460:GLU:HB2	2.16	0.45
1:A:236:LEU:HD13	1:A:236:LEU:C	2.37	0.45
1:A:320:VAL:HG11	1:A:325:LEU:HD11	1.99	0.45
1:A:276:LEU:HB3	1:A:450:PHE:CD1	2.52	0.45
1:A:430:LEU:HD11	2:D:444:GLN:OE1	2.16	0.45
2:D:204:LEU:C	2:D:209:ALA:HB2	2.37	0.45
2:D:444:GLN:O	2:D:448:GLU:HG3	2.17	0.45
2:D:116:ASP:HB3	2:D:156:LYS:NZ	2.32	0.45
2:D:343:GLU:OE2	2:D:343:GLU:HA	2.16	0.45
2:D:333:LEU:H	2:D:333:LEU:HG	1.66	0.45
2:D:390:VAL:HG21	2:D:414:LEU:HD23	1.99	0.45
3:C:3016:DG:H5'	3:C:3016:DG:C8	2.52	0.45
2:D:138:THR:HG21	2:D:167:PHE:CE1	2.51	0.44
2:D:171:LEU:HD23	2:D:171:LEU:HA	1.82	0.44
1:A:426:ARG:HD2	2:D:440:THR:O	2.17	0.44
2:D:202:ASP:O	2:D:205:ASN:ND2	2.50	0.44
2:D:285:CYS:O	2:D:288:ARG:N	2.50	0.44
1:A:436:LEU:C	1:A:438:PHE:H	2.20	0.44
2:D:434:LYS:NZ	2:D:434:LYS:CB	2.80	0.44
1:A:236:LEU:O	1:A:240:LEU:HG	2.17	0.44
2:D:181:ARG:HH12	2:D:185:MET:HE1	1.82	0.44
1:A:355:SER:O	1:A:358:ARG:N	2.51	0.44
4:F:4011:DA:H1'	4:F:4012:DC:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HH11	1:A:285:ARG:CB	2.31	0.44
1:A:337:ALA:O	1:A:340:ALA:N	2.51	0.44
4:F:4008:DT:H2''	4:F:4009:DT:C5'	2.43	0.44
1:A:313:PHE:C	1:A:313:PHE:CD2	2.91	0.44
2:D:196:GLU:OE1	2:D:199:SER:HB2	2.17	0.44
3:C:3008:DG:H2''	3:C:3009:DG:C8	2.53	0.44
2:D:198:SER:O	2:D:201:ILE:HG12	2.18	0.44
3:C:3014:DA:H5'	3:C:3014:DA:C8	2.53	0.44
1:A:325:LEU:HD12	1:A:325:LEU:N	2.33	0.43
2:D:205:ASN:HA	2:D:209:ALA:HB2	1.99	0.43
2:D:250:TYR:O	2:D:251:ASP:HB3	2.18	0.43
2:D:445:ILE:O	2:D:448:GLU:N	2.52	0.43
3:C:3005:DC:H2''	3:C:3006:DT:H5'	1.99	0.43
4:F:4016:DG:H2''	4:F:4017:DT:OP2	2.18	0.43
1:A:208:GLU:C	1:A:210:GLN:H	2.22	0.43
2:D:114:CYS:SG	2:D:116:ASP:OD1	2.76	0.43
1:A:206:GLN:NE2	3:C:3014:DA:H4'	2.32	0.43
1:A:348:ARG:O	1:A:352:GLU:HG2	2.17	0.43
2:D:323:HIS:HE1	2:D:472:ILE:HG21	1.84	0.43
1:A:447:ILE:C	1:A:447:ILE:HD12	2.38	0.43
1:A:455:LEU:HD12	1:A:455:LEU:N	2.33	0.43
2:D:187:GLN:O	2:D:190:LYS:HB3	2.18	0.43
2:D:205:ASN:CA	2:D:209:ALA:HB2	2.48	0.43
2:D:206:PRO:CG	2:D:207:GLU:H	2.28	0.43
2:D:116:ASP:OD2	2:D:159:ARG:NH2	2.51	0.43
2:D:334:MET:HG2	2:D:339:VAL:HB	2.00	0.43
1:A:444:ASP:C	1:A:446:PRO:HD3	2.40	0.42
1:A:444:ASP:O	1:A:446:PRO:HD3	2.19	0.42
2:D:299:TYR:OH	2:D:385:ALA:O	2.34	0.42
5:G:690:LEU:O	5:G:694:LEU:HB2	2.20	0.42
1:A:272:ALA:O	1:A:276:LEU:N	2.51	0.42
3:C:3014:DA:H1'	3:C:3015:DG:H5'	2.01	0.42
2:D:404:LYS:N	2:D:405:PRO:CD	2.83	0.42
5:E:693:LEU:HD12	5:E:693:LEU:N	2.34	0.42
2:D:111:CYS:HB3	2:D:115:GLY:H	1.84	0.42
2:D:336:LYS:HB2	2:D:336:LYS:HE3	1.77	0.42
1:A:224:SER:C	1:A:226:ALA:H	2.23	0.42
1:A:369:CYS:O	1:A:373:ILE:HG13	2.19	0.42
2:D:147:ARG:CG	2:D:148:CYS:N	2.83	0.42
2:D:205:ASN:C	2:D:205:ASN:ND2	2.73	0.42
1:A:222:SER:O	1:A:223:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:288:ARG:O	2:D:291:GLU:N	2.52	0.42
2:D:462:ASP:OD1	2:D:462:ASP:N	2.53	0.42
1:A:360:MET:CE	1:A:421:ARG:HD2	2.50	0.41
2:D:202:ASP:C	2:D:205:ASN:HD21	2.23	0.41
2:D:402:ASN:O	2:D:405:PRO:HD2	2.20	0.41
1:A:227:ASN:N	1:A:227:ASN:HD22	2.18	0.41
1:A:398:ALA:HA	2:D:430:GLN:NE2	2.36	0.41
4:F:4015:DA:H2''	4:F:4016:DG:OP2	2.20	0.41
5:E:688:LYS:C	5:E:689:ILE:HD12	2.41	0.41
1:A:176:ASP:O	1:A:176:ASP:OD2	2.38	0.41
1:A:203:GLU:HG2	2:D:237:LEU:O	2.20	0.41
1:A:219:GLU:HG2	1:A:220:VAL:HG13	2.01	0.41
1:A:317:SER:CB	1:A:324:ILE:HG22	2.50	0.41
1:A:271:ALA:O	1:A:275:GLN:HB2	2.19	0.41
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.84	0.41
1:A:450:PHE:HA	5:G:689:ILE:HD13	2.02	0.41
2:D:182:PHE:CD2	2:D:182:PHE:N	2.88	0.41
2:D:188:ALA:O	2:D:192:LYS:N	2.53	0.41
1:A:297:GLN:OE1	5:G:694:LEU:HD22	2.20	0.41
2:D:141:LEU:O	2:D:143:LEU:N	2.54	0.41
1:A:275:GLN:O	1:A:278:THR:HB	2.20	0.41
1:A:288:HIS:HA	1:A:291:GLU:CD	2.41	0.41
1:A:346:PHE:CE1	1:A:350:LEU:HD21	2.56	0.41
3:C:3001:DC:H2''	3:C:3002:DA:C8	2.55	0.41
2:D:114:CYS:HA	2:D:154:ILE:HG22	2.02	0.41
2:D:184:ARG:O	2:D:186:PRO:HD3	2.21	0.41
2:D:441:ASP:C	2:D:444:GLN:HB3	2.40	0.41
4:F:4013:DC:H2''	4:F:4014:DT:OP2	2.20	0.41
1:A:289:PHE:CE1	1:A:375:LEU:HD21	2.54	0.41
1:A:298:VAL:CG1	5:G:690:LEU:HD13	2.51	0.41
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.84	0.41
1:A:450:PHE:O	1:A:454:MET:HG2	2.21	0.41
2:D:157:LYS:HD2	2:D:158:SER:N	2.36	0.41
2:D:184:ARG:HH11	4:F:4020:DG:H5'	1.86	0.41
2:D:290:VAL:HG21	2:D:466:HIS:CD2	2.56	0.41
1:A:225:SER:O	1:A:226:ALA:HB3	2.21	0.41
1:A:407:LYS:C	1:A:409:PRO:HD3	2.42	0.41
1:A:383:LEU:C	1:A:385:ASN:N	2.73	0.40
1:A:445:THR:HG23	1:A:445:THR:O	2.20	0.40
1:A:197:ALA:C	1:A:199:GLY:H	2.24	0.40
1:A:225:SER:C	1:A:227:ASN:N	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:377:LEU:HD21	2:D:434:LYS:HZ2	1.85	0.40
2:D:370:PHE:CZ	2:D:442:LEU:HD21	2.56	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	298/467 (64%)	234 (78%)	48 (16%)	16 (5%)	2	12
2	D	350/419 (84%)	280 (80%)	54 (15%)	16 (5%)	2	15
5	E	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
5	G	7/13 (54%)	5 (71%)	2 (29%)	0	100	100
All	All	663/912 (73%)	526 (79%)	105 (16%)	32 (5%)	2	14

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	SER
1	A	223	THR
2	D	195	ALA
1	A	181	LYS
1	A	208	GLU
1	A	213	LYS
1	A	334	ARG
1	A	335	ASN
1	A	355	SER
1	A	443	GLY
2	D	206	PRO
2	D	304	PRO
2	D	311	LEU

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Mol	Chain	Res	Type
2	D	322	VAL
1	A	219	GLU
1	A	320	VAL
2	D	140	ARG
2	D	147	ARG
2	D	358	LYS
2	D	363	PHE
2	D	471	GLU
1	A	294	LEU
1	A	447	ILE
2	D	142	LYS
2	D	205	ASN
2	D	301	LYS
1	A	332	VAL
1	A	362	MET
1	A	445	THR
2	D	472	ILE
2	D	446	VAL
2	D	445	ILE

### 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	262/405 (65%)	254 (97%)	8 (3%)	40	70
2	D	313/375 (84%)	292 (93%)	21 (7%)	16	46
5	E	10/13 (77%)	10 (100%)	0	100	100
5	G	9/13 (69%)	9 (100%)	0	100	100
All	All	594/806 (74%)	565 (95%)	29 (5%)	25	57

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	ARG
1	A	187	CYS

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Mol	Chain	Res	Type
1	A	203	GLU
1	A	207	GLU
1	A	213	LYS
1	A	395	LYS
1	A	421	ARG
1	A	450	PHE
2	D	157	LYS
2	D	159	ARG
2	D	165	CYS
2	D	185	MET
2	D	193	LEU
2	D	200	ASP
2	D	202	ASP
2	D	205	ASN
2	D	237	LEU
2	D	304	PRO
2	D	329	MET
2	D	333	LEU
2	D	357	ARG
2	D	363	PHE
2	D	373	LYS
2	D	403	VAL
2	D	404	LYS
2	D	447	THR
2	D	462	ASP
2	D	465	LEU
2	D	477	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	227	ASN
1	A	267	ASN
2	D	160	ASN
2	D	205	ASN
2	D	437	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	9CR	A	463	-	22,22,22	4.15	10 (45%)	30,30,30	2.23	9 (30%)
8	BRL	D	478	-	27,27,27	2.87	16 (59%)	36,36,36	2.73	11 (30%)

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	9CR	A	463	-	-	7/15/32/32	0/1/1/1
8	BRL	D	478	-	-	0/14/26/26	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	463	9CR	C1-C6	12.38	1.70	1.53
6	A	463	9CR	C5-C6	9.37	1.50	1.34
8	D	478	BRL	C17-N16	7.03	1.56	1.37
6	A	463	9CR	C10-C9	5.33	1.42	1.35
8	D	478	BRL	C9-C10	5.07	1.48	1.38
6	A	463	9CR	C2-C1	4.46	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	478	BRL	C17-N18	4.23	1.43	1.34
6	A	463	9CR	C20-C13	4.05	1.59	1.50
6	A	463	9CR	C16-C1	3.95	1.61	1.53
8	D	478	BRL	C22-C17	3.74	1.48	1.39
6	A	463	9CR	C4-C5	3.52	1.57	1.51
6	A	463	9CR	C2-C3	3.41	1.61	1.52
8	D	478	BRL	C8-C7	3.34	1.46	1.38
8	D	478	BRL	C16-N16	3.29	1.51	1.46
8	D	478	BRL	C11-C10	3.28	1.45	1.38
8	D	478	BRL	C5-C4	3.16	1.54	1.52
8	D	478	BRL	C2-N3	-3.09	1.32	1.36
6	A	463	9CR	C14-C13	2.75	1.39	1.35
8	D	478	BRL	C12-C7	2.72	1.44	1.38
8	D	478	BRL	C12-C11	2.64	1.43	1.38
8	D	478	BRL	C19-N18	2.42	1.39	1.34
8	D	478	BRL	O13-C10	2.41	1.43	1.37
8	D	478	BRL	C21-C22	2.34	1.43	1.38
6	A	463	9CR	C14-C15	2.31	1.54	1.47
8	D	478	BRL	C21-C20	2.26	1.44	1.38
8	D	478	BRL	C9-C8	2.18	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	478	BRL	S1-C2-N3	8.51	116.36	110.40
8	D	478	BRL	C4-N3-C2	-8.06	112.79	118.24
6	A	463	9CR	C17-C1-C6	5.22	118.77	110.30
6	A	463	9CR	C7-C8-C9	4.82	133.51	126.23
6	A	463	9CR	C19-C9-C10	-4.75	116.28	122.92
8	D	478	BRL	O2-C2-N3	-4.29	121.34	125.76
8	D	478	BRL	C6-C5-S1	-4.21	108.67	113.04
8	D	478	BRL	C19-N18-C17	4.04	122.20	116.86
8	D	478	BRL	C5-C4-N3	3.76	115.28	112.01
8	D	478	BRL	C5-S1-C2	-3.72	90.86	92.86
6	A	463	9CR	C19-C9-C8	3.41	123.45	118.08
6	A	463	9CR	C20-C13-C12	3.33	123.33	118.08
8	D	478	BRL	C22-C17-N18	-3.28	117.39	123.41
6	A	463	9CR	C8-C7-C6	3.01	135.65	127.20
8	D	478	BRL	N18-C17-N16	2.86	120.02	116.39
6	A	463	9CR	C1-C6-C5	-2.75	118.74	122.61
8	D	478	BRL	O2-C2-S1	-2.47	122.30	124.62
8	D	478	BRL	O4-C4-N3	-2.38	122.06	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	463	9CR	C18-C5-C6	2.26	127.07	124.53
6	A	463	9CR	O2-C15-C14	2.01	119.75	113.50

There are no chirality outliers.

All (7) torsion outliers are listed below:

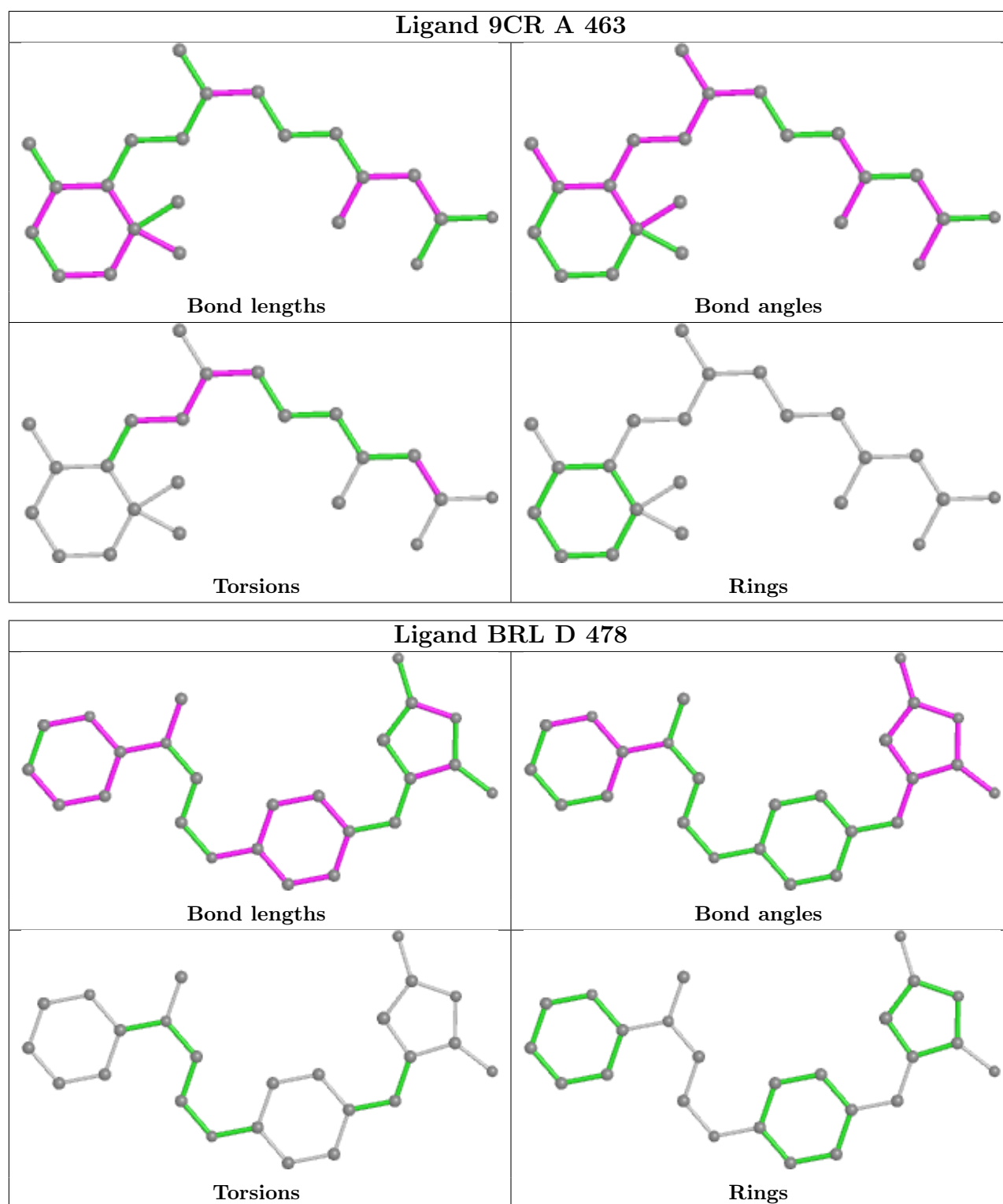
Mol	Chain	Res	Type	Atoms
6	A	463	9CR	C6-C7-C8-C9
6	A	463	9CR	C7-C8-C9-C10
6	A	463	9CR	C7-C8-C9-C19
6	A	463	9CR	C13-C14-C15-O1
6	A	463	9CR	C13-C14-C15-O2
6	A	463	9CR	C11-C10-C9-C19
6	A	463	9CR	C11-C10-C9-C8

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	463	9CR	2	0
8	D	478	BRL	2	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/467 (64%)	0.09	16 (5%) 26 12	29, 76, 167, 200	0
2	D	354/419 (84%)	-0.01	10 (2%) 53 30	22, 65, 138, 196	0
3	C	20/20 (100%)	-0.22	0 100 100	42, 69, 89, 90	0
4	F	20/20 (100%)	-0.18	0 100 100	41, 71, 86, 87	0
5	E	10/13 (76%)	-0.12	0 100 100	48, 70, 123, 133	0
5	G	9/13 (69%)	0.41	0 100 100	90, 113, 148, 152	0
All	All	715/952 (75%)	0.02	26 (3%) 42 22	22, 71, 149, 200	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ASN	7.5
1	A	219	GLU	6.1
1	A	215	ARG	5.5
1	A	217	GLU	4.8
1	A	221	GLU	4.1
1	A	218	ASN	4.1
1	A	214	ASP	4.0
1	A	441	LEU	3.9
1	A	445	THR	3.2
2	D	198	SER	3.2
1	A	446	PRO	3.1
2	D	200	ASP	3.1
2	D	199	SER	3.0
1	A	444	ASP	3.0
1	A	224	SER	2.8
2	D	204	LEU	2.7
2	D	201	ILE	2.7
2	D	195	ALA	2.7
1	A	220	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	442	ILE	2.4
1	A	448	ASP	2.2
1	A	222	SER	2.1
2	D	185	MET	2.1
2	D	112	ARG	2.1
2	D	124	GLY	2.0
2	D	202	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

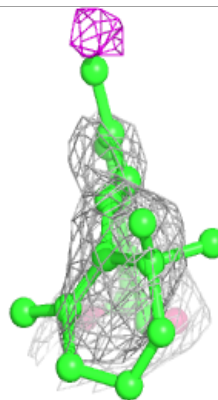
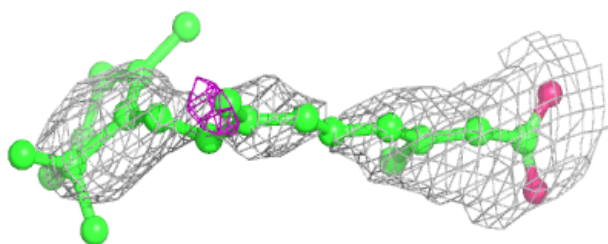
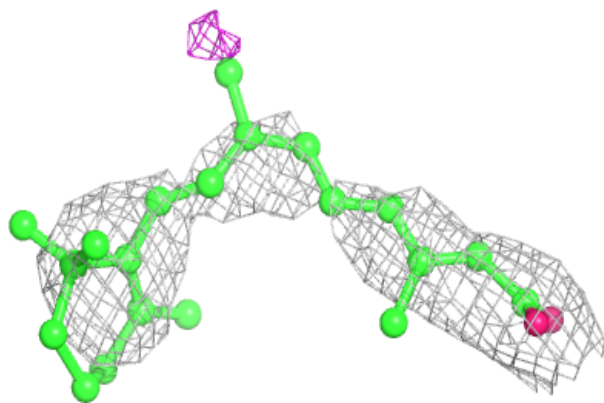
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	9CR	A	463	22/22	0.91	0.58	75,92,102,103	0
8	BRL	D	478	25/25	0.93	0.25	58,62,64,66	0
7	ZN	A	7221	1/1	0.95	0.15	60,60,60,60	0
7	ZN	D	7122	1/1	0.97	0.14	65,65,65,65	0
7	ZN	A	7222	1/1	0.98	0.11	52,52,52,52	0
7	ZN	D	7121	1/1	0.99	0.13	63,63,63,63	0

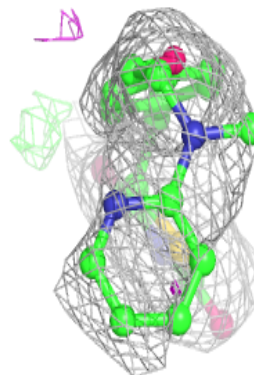
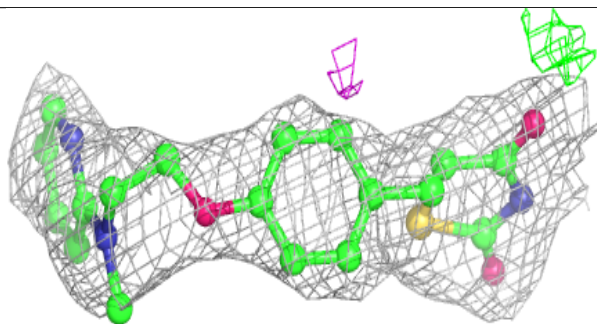
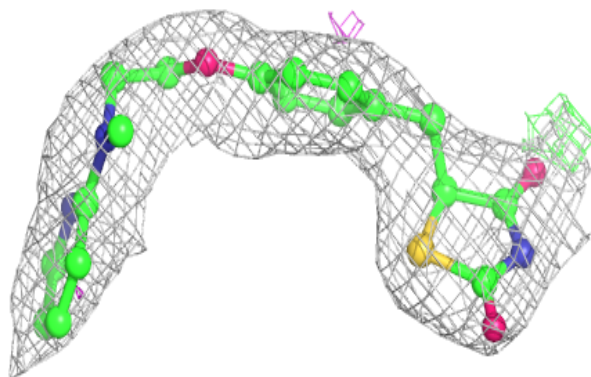
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 9CR A 463:**

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

**Electron density around BRL D 478:**

$2mF_o-DF_c$  (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.