



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 08:41 AM EST

PDB ID : 1FM9  
Title : THE 2.1 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE HETERODIMER OF THE HUMAN RXRALPHA AND PPARGAMMA LIGAND BINDING DOMAINS RESPECTIVELY BOUND WITH 9-CIS RETINOIC ACID AND GI262570 AND CO-ACTIVATOR PEPTIDES.  
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Deposited on : 2000-08-16  
Resolution : 2.10 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)

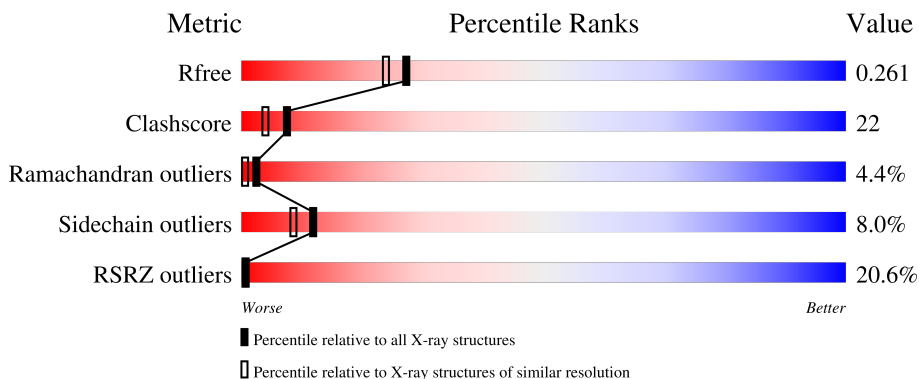
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)


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	238	
2	D	272	
3	B	25	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
3	E	25	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into five segments: a green segment (24%), a red segment (32%), a yellow segment (8%), an orange segment (36%), and a grey segment (48%). The percentages are labeled below the segments.</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4342 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	232	1754	1117	306	321	10	0	0	0

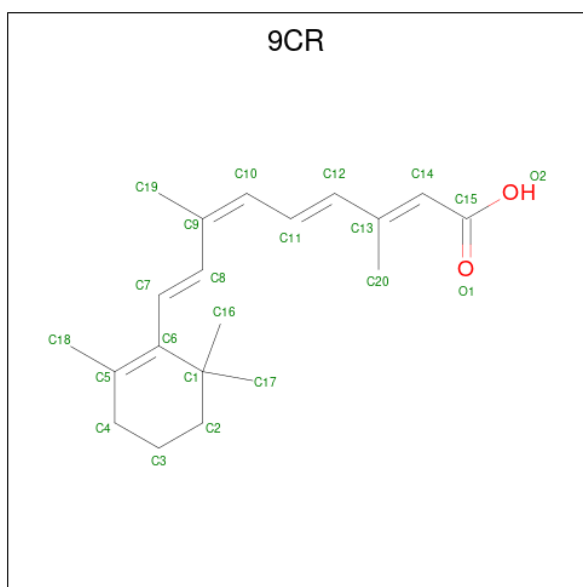
- Molecule 2 is a protein called PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	272	2179	1407	355	407	10	0	0	0

- Molecule 3 is a protein called STEROID RECEPTOR COACTIVATOR.

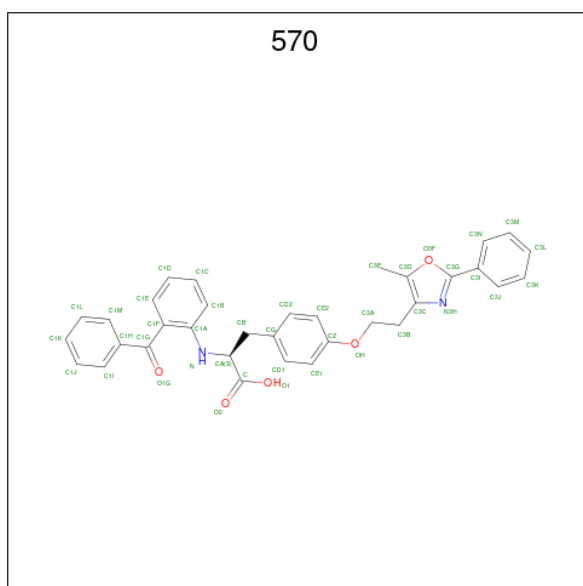
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	10	86	55	18	13	0	0	0
3	E	16	129	79	27	23	0	0	0

- Molecule 4 is (9cis)-retinoic acid (three-letter code: 9CR) (formula: C<sub>20</sub>H<sub>28</sub>O<sub>2</sub>).



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

- Molecule 5 is 2-(2-BENZOYL-PHENYLAMINO)-3-{4-[2-(5-METHYL-2-PHENYL-OXAZOL-4-YL)-ETHOXY]-PHENYL}-PROPIONIC ACID (three-letter code: 570) (formula:  $C_{34}H_{30}N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			41	34	2	5		

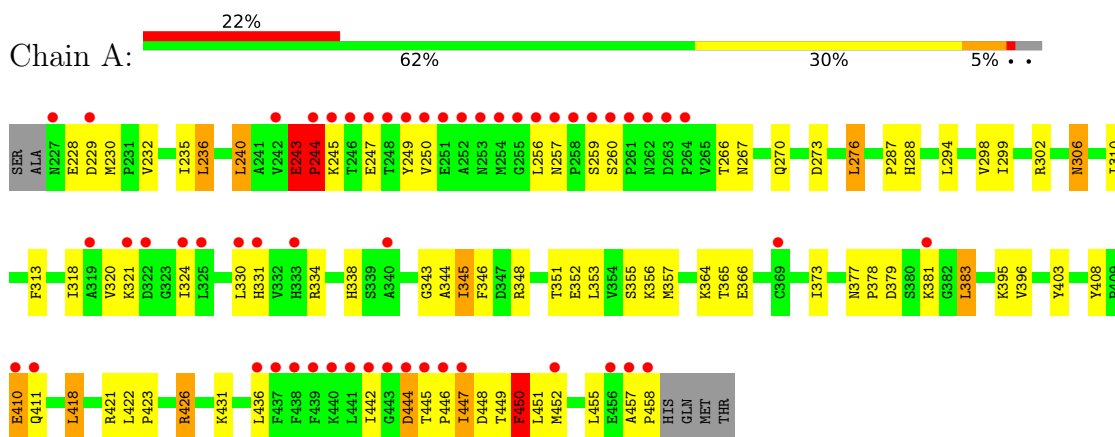
- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	36	Total 36	O 36	0	0
6	D	89	Total 89	O 89	0	0
6	E	6	Total 6	O 6	0	0

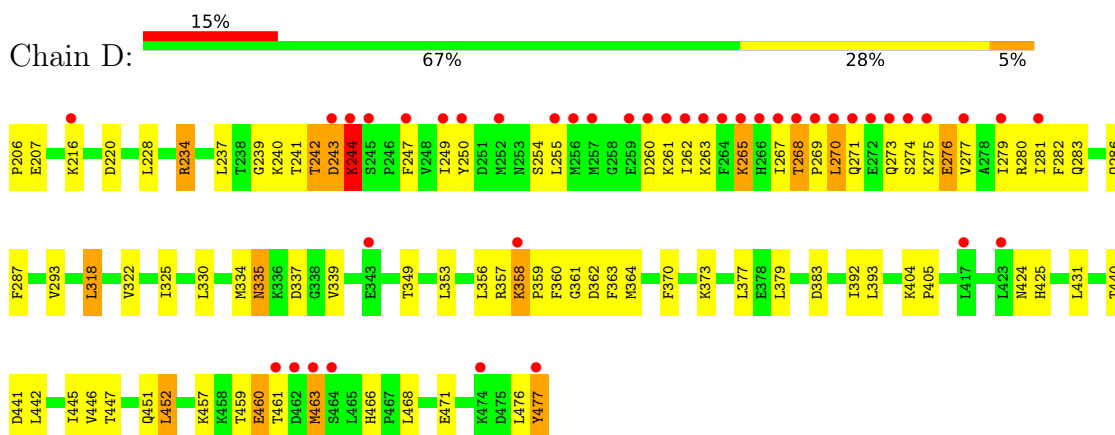
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

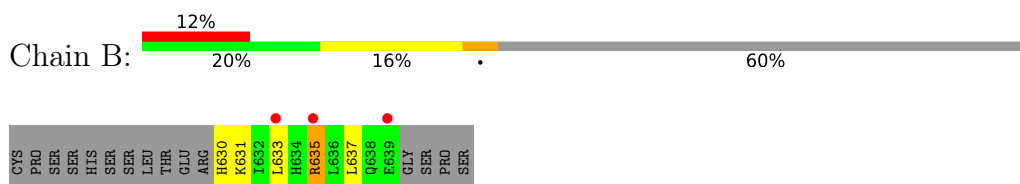
- Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA



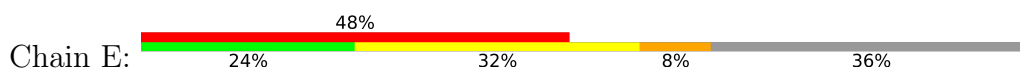
- Molecule 2: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA



- Molecule 3: STEROID RECEPTOR COACTIVATOR



- Molecule 3: STEROID RECEPTOR COACTIVATOR



CYS	
PRO	
SER	
SER	
HIS	
SER	
SER	
LEU	
THR	
E685	●
R686	●
H687	
K688	
I689	
L690	●
H691	
R692	●
L693	●
L694	●
Q695	●
E696	●
G697	●
S698	●
P699	●
S700	●



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.14Å 54.05Å 211.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-2.10) 91.9 (19.69-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.11Å)	Xtrriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.239 , 0.268 0.233 , 0.261	Depositor DCC
$R_{free}$ test set	2895 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtrriage
Anisotropy	0.254	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9CR, 570

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	0.37	0/1789	0.64	2/2414 (0.1%)
2	D	0.42	0/2217	0.71	1/2987 (0.0%)
3	B	0.38	0/87	0.72	0/116
3	E	0.28	0/131	0.52	0/175
All	All	0.40	0/4224	0.68	3/5692 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	GLU	C-N-CD	-10.66	97.14	120.60
1	A	243	GLU	C-N-CA	6.33	148.58	122.00
2	D	206	PRO	N-CA-CB	5.39	109.77	103.30

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	1754	0	1733	80	0
2	D	2179	0	2237	99	0
3	B	86	0	86	7	0
3	E	129	0	125	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	27	4	0
5	D	41	0	29	5	0
6	A	36	0	0	3	0
6	D	89	0	0	2	0
6	E	6	0	0	1	0
All	All	4342	0	4237	187	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 22.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:268:THR:H	2:D:269:PRO:HD2	1.25	0.99
2:D:293:VAL:HG22	2:D:322:VAL:HG11	1.57	0.86
1:A:306:ASN:H	1:A:306:ASN:HD22	1.24	0.85
1:A:230:MET:CE	1:A:235:ILE:HD11	2.07	0.84
1:A:236:LEU:HD22	1:A:240:LEU:HD22	1.58	0.83
1:A:230:MET:HE3	1:A:235:ILE:HD11	1.60	0.83
1:A:338:HIS:HD2	1:A:343:GLY:HA3	1.46	0.81
2:D:242:THR:O	2:D:243:ASP:HB3	1.80	0.81
1:A:426:ARG:HB2	1:A:426:ARG:HH11	1.46	0.79
2:D:243:ASP:O	2:D:244:LYS:O	2.01	0.78
2:D:276:GLU:HG2	2:D:277:VAL:H	1.51	0.76
2:D:358:LYS:HB2	2:D:359:PRO:HD2	1.67	0.75
2:D:471:GLU:OE1	3:E:689:ILE:HG22	1.88	0.74
2:D:279:ILE:O	2:D:283:GLN:HG2	1.86	0.74
2:D:457:LYS:HA	2:D:463:MET:HG3	1.70	0.74
2:D:268:THR:N	2:D:269:PRO:HD2	2.00	0.73
2:D:268:THR:H	2:D:269:PRO:CD	2.00	0.73
2:D:357:ARG:HH11	2:D:357:ARG:HG3	1.54	0.72
2:D:357:ARG:NH1	2:D:358:LYS:CG	2.53	0.72
2:D:357:ARG:HH12	2:D:358:LYS:HB2	1.56	0.70
2:D:357:ARG:NH1	2:D:358:LYS:HB2	2.07	0.70
2:D:358:LYS:HB2	2:D:359:PRO:CD	2.22	0.69
2:D:466:HIS:HD2	2:D:468:LEU:H	1.40	0.69
2:D:335:ASN:C	2:D:335:ASN:HD22	1.96	0.68
1:A:306:ASN:H	1:A:306:ASN:ND2	1.92	0.66
1:A:426:ARG:HB2	1:A:426:ARG:NH1	2.09	0.66
2:D:383:ASP:OD2	2:D:425:HIS:HE1	1.77	0.66
2:D:358:LYS:CB	2:D:359:PRO:CD	2.73	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:ILE:HD11	2:D:392:ILE:HG13	1.79	0.65
1:A:338:HIS:CD2	1:A:343:GLY:HA3	2.29	0.65
2:D:243:ASP:O	2:D:243:ASP:OD1	2.15	0.65
2:D:286:GLN:OE1	5:D:200:570:H1C	1.98	0.64
2:D:273:GLN:HA	2:D:280:ARG:HD3	1.78	0.64
2:D:275:LYS:O	2:D:276:GLU:O	2.15	0.64
2:D:293:VAL:HG22	2:D:322:VAL:CG1	2.28	0.64
2:D:466:HIS:CD2	2:D:468:LEU:H	2.16	0.63
1:A:366:GLU:HG2	1:A:418:LEU:HD21	1.79	0.62
2:D:262:ILE:HA	2:D:265:LYS:HD2	1.80	0.62
3:E:685:GLU:HB2	3:E:687:HIS:CE1	2.33	0.62
1:A:320:VAL:HG21	1:A:331:HIS:CE1	2.34	0.62
1:A:343:GLY:O	1:A:344:ALA:HB3	2.00	0.60
2:D:377:LEU:HD22	2:D:431:LEU:HD12	1.82	0.60
2:D:357:ARG:HG3	2:D:357:ARG:NH1	2.16	0.60
2:D:357:ARG:NH1	2:D:358:LYS:HG2	2.16	0.59
1:A:447:ILE:HG12	1:A:452:MET:CE	2.33	0.59
2:D:446:VAL:HG11	2:D:477:TYR:HE1	1.68	0.59
2:D:262:ILE:HA	2:D:265:LYS:CD	2.32	0.59
2:D:247:PHE:HE2	2:D:254:SER:O	1.86	0.58
3:E:686:ARG:HH12	3:E:691:HIS:CD2	2.22	0.58
1:A:243:GLU:HB2	1:A:244:PRO:O	2.02	0.58
2:D:357:ARG:NH1	2:D:358:LYS:CB	2.67	0.57
1:A:320:VAL:HG21	1:A:331:HIS:NE2	2.20	0.57
1:A:423:PRO:HG3	2:D:440:THR:HG22	1.87	0.57
2:D:276:GLU:HG2	2:D:277:VAL:N	2.20	0.57
1:A:228:GLU:O	1:A:229:ASP:HB2	2.05	0.56
2:D:239:GLY:O	2:D:240:LYS:HD3	2.04	0.56
3:E:685:GLU:HG2	3:E:686:ARG:H	1.68	0.56
1:A:320:VAL:HG22	1:A:321:LYS:N	2.21	0.56
4:A:201:9CR:H8	4:A:201:9CR:H19	1.88	0.56
1:A:298:VAL:HG13	3:B:633:LEU:HD12	1.88	0.56
1:A:436:LEU:HD22	4:A:201:9CR:H16	1.88	0.55
2:D:270:LEU:O	2:D:270:LEU:HD22	2.06	0.55
1:A:306:ASN:ND2	6:A:10:HOH:O	2.40	0.54
2:D:281:ILE:HD12	2:D:356:LEU:HD11	1.88	0.54
2:D:377:LEU:HD22	2:D:431:LEU:CD1	2.38	0.54
1:A:298:VAL:HA	3:B:633:LEU:HD11	1.89	0.54
2:D:325:ILE:HD11	2:D:392:ILE:CG1	2.38	0.54
1:A:451:LEU:O	1:A:455:LEU:HD13	2.08	0.53
1:A:447:ILE:HD11	1:A:452:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:HA	1:A:410:GLU:OE2	2.08	0.52
2:D:270:LEU:HD21	6:D:90:HOH:O	2.09	0.52
1:A:243:GLU:OE1	1:A:364:LYS:NZ	2.43	0.51
2:D:335:ASN:ND2	2:D:337:ASP:H	2.08	0.51
2:D:260:ASP:HA	2:D:263:LYS:HG3	1.93	0.51
1:A:345:ILE:HG12	1:A:431:LYS:CD	2.40	0.51
1:A:423:PRO:CG	2:D:440:THR:HG22	2.41	0.51
2:D:275:LYS:O	2:D:279:ILE:HG22	2.11	0.51
2:D:357:ARG:HH11	2:D:358:LYS:HG2	1.74	0.51
1:A:313:PHE:CE1	1:A:324:ILE:HD13	2.46	0.51
2:D:249:ILE:HD13	2:D:255:LEU:HD12	1.92	0.51
1:A:273:ASP:OD1	1:A:449:THR:O	2.29	0.51
1:A:318:ILE:HD11	1:A:357:MET:HB3	1.93	0.50
1:A:351:THR:HA	1:A:355:SER:OG	2.10	0.50
1:A:267:ASN:HB3	1:A:330:LEU:HD13	1.93	0.50
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.46	0.50
2:D:261:LYS:O	2:D:265:LYS:HG3	2.12	0.50
1:A:423:PRO:CD	2:D:440:THR:HG22	2.42	0.49
1:A:266:THR:O	1:A:270:GLN:HG3	2.12	0.49
2:D:334:MET:HG2	2:D:339:VAL:HB	1.94	0.49
1:A:423:PRO:N	2:D:440:THR:HG22	2.27	0.49
3:E:685:GLU:N	3:E:685:GLU:OE1	2.45	0.49
1:A:298:VAL:HG22	3:B:633:LEU:CD1	2.43	0.49
1:A:267:ASN:HD22	1:A:330:LEU:HD11	1.78	0.49
2:D:477:TYR:C	2:D:477:TYR:CD1	2.83	0.49
2:D:356:LEU:HB2	2:D:361:GLY:HA2	1.93	0.49
1:A:365:THR:HG21	1:A:403:TYR:CE2	2.48	0.48
1:A:228:GLU:O	1:A:228:GLU:HG3	2.12	0.48
2:D:370:PHE:HB2	2:D:445:ILE:HD11	1.95	0.48
2:D:447:THR:HG22	2:D:477:TYR:OXT	2.12	0.48
1:A:243:GLU:HB3	1:A:244:PRO:C	2.34	0.48
1:A:449:THR:O	1:A:450:PHE:CB	2.59	0.48
2:D:377:LEU:HB2	2:D:379:LEU:HD12	1.95	0.48
1:A:426:ARG:HH11	1:A:426:ARG:CB	2.19	0.48
2:D:275:LYS:O	2:D:279:ILE:CG2	2.61	0.48
2:D:260:ASP:O	2:D:263:LYS:HB2	2.13	0.48
2:D:262:ILE:HA	2:D:265:LYS:CG	2.44	0.48
2:D:270:LEU:HD22	2:D:270:LEU:C	2.35	0.47
1:A:230:MET:CE	1:A:396:VAL:HG22	2.44	0.47
2:D:468:LEU:HD13	3:E:689:ILE:CG2	2.44	0.47
2:D:468:LEU:CD1	3:E:689:ILE:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:ASP:O	2:D:243:ASP:CG	2.52	0.47
2:D:273:GLN:HA	2:D:280:ARG:CD	2.45	0.47
3:E:695:GLN:HE21	3:E:695:GLN:CA	2.28	0.47
1:A:306:ASN:ND2	1:A:306:ASN:N	2.63	0.47
1:A:444:ASP:O	1:A:445:THR:OG1	2.33	0.47
2:D:404:LYS:HB3	2:D:405:PRO:HD3	1.97	0.47
2:D:466:HIS:HD2	2:D:468:LEU:N	2.10	0.47
2:D:255:LEU:HD23	2:D:277:VAL:HG23	1.95	0.47
3:E:686:ARG:NE	3:E:686:ARG:HA	2.29	0.47
1:A:273:ASP:CG	1:A:448:ASP:HB2	2.36	0.46
1:A:381:LYS:H	1:A:381:LYS:HG3	1.45	0.46
2:D:447:THR:O	2:D:451:GLN:HG3	2.16	0.46
2:D:234:ARG:NH2	2:D:334:MET:O	2.46	0.46
1:A:299:ILE:HG21	1:A:383:LEU:HD13	1.98	0.46
6:A:23:HOH:O	2:D:440:THR:HG23	2.16	0.46
2:D:282:PHE:CZ	5:D:200:570:H1D	2.51	0.46
1:A:330:LEU:HD23	1:A:331:HIS:N	2.31	0.45
1:A:436:LEU:CD2	4:A:201:9CR:H16	2.46	0.45
1:A:373:ILE:HG13	1:A:396:VAL:HG11	1.99	0.45
2:D:287:PHE:CD1	2:D:287:PHE:C	2.90	0.45
4:A:201:9CR:H8	4:A:201:9CR:H10	1.80	0.45
1:A:243:GLU:CB	1:A:244:PRO:C	2.85	0.45
3:B:633:LEU:C	3:B:633:LEU:HD13	2.37	0.45
1:A:421:ARG:NH2	6:A:25:HOH:O	2.50	0.45
1:A:228:GLU:O	1:A:229:ASP:CB	2.65	0.44
1:A:230:MET:SD	1:A:287:PRO:HG2	2.56	0.44
2:D:250:TYR:CD1	2:D:250:TYR:N	2.85	0.44
2:D:335:ASN:C	2:D:335:ASN:ND2	2.68	0.44
1:A:422:LEU:CB	2:D:440:THR:HG21	2.47	0.44
3:B:631:LYS:O	3:B:635:ARG:HB2	2.18	0.44
1:A:229:ASP:O	1:A:288:HIS:NE2	2.51	0.44
3:B:633:LEU:HD13	3:B:637:LEU:HD12	1.99	0.44
2:D:216:LYS:NZ	2:D:220:ASP:OD1	2.50	0.44
2:D:273:GLN:HG2	2:D:274:SER:H	1.83	0.44
1:A:353:LEU:O	1:A:357:MET:HG3	2.18	0.43
2:D:353:LEU:HD13	2:D:364:MET:HG3	2.01	0.43
1:A:230:MET:HE2	1:A:396:VAL:HG22	1.99	0.43
2:D:277:VAL:O	2:D:277:VAL:HG22	2.18	0.43
3:E:688:LYS:O	3:E:691:HIS:HB2	2.18	0.43
2:D:468:LEU:HD13	3:E:689:ILE:HG23	2.01	0.43
1:A:294:LEU:C	1:A:294:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:O	1:A:352:GLU:HB2	2.19	0.43
1:A:344:ALA:O	1:A:348:ARG:HG3	2.19	0.42
1:A:356:LYS:HG3	1:A:421:ARG:NH1	2.34	0.42
2:D:273:GLN:HG2	2:D:274:SER:N	2.33	0.42
2:D:286:GLN:HB2	5:D:200:570:C1C	2.49	0.42
2:D:249:ILE:HD13	2:D:255:LEU:CD1	2.49	0.42
2:D:360:PHE:HD1	5:D:200:570:H1L	1.84	0.42
2:D:459:THR:C	2:D:460:GLU:HG2	2.39	0.42
2:D:476:LEU:CG	2:D:477:TYR:H	2.32	0.42
3:E:698:SER:HA	3:E:699:PRO:HD3	1.92	0.42
1:A:276:LEU:HB3	1:A:450:PHE:CE1	2.54	0.42
1:A:320:VAL:CG2	1:A:321:LYS:N	2.83	0.42
1:A:267:ASN:HD22	1:A:330:LEU:CD1	2.32	0.42
2:D:468:LEU:CD1	3:E:689:ILE:CG2	2.98	0.42
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.85	0.41
1:A:379:ASP:OD1	2:D:373:LYS:HE2	2.20	0.41
1:A:229:ASP:HB3	1:A:395:LYS:HD3	2.01	0.41
1:A:313:PHE:C	1:A:313:PHE:CD1	2.93	0.41
3:E:695:GLN:OE1	6:E:65:HOH:O	2.22	0.41
2:D:318:LEU:HD21	3:E:694:LEU:HD21	2.02	0.41
1:A:302:ARG:HD2	3:B:630:HIS:CD2	2.55	0.41
1:A:348:ARG:NH1	1:A:431:LYS:HE3	2.35	0.41
1:A:345:ILE:CG2	1:A:346:PHE:N	2.84	0.41
2:D:330:LEU:O	2:D:334:MET:HG3	2.20	0.41
1:A:247:GLU:C	1:A:249:TYR:H	2.23	0.41
1:A:447:ILE:HG12	1:A:452:MET:HE1	2.01	0.41
2:D:377:LEU:HB2	2:D:379:LEU:CD1	2.51	0.41
2:D:392:ILE:HG22	2:D:393:LEU:HD22	2.03	0.41
2:D:441:ASP:OD2	6:D:66:HOH:O	2.21	0.41
2:D:476:LEU:HG	2:D:477:TYR:H	1.86	0.41
1:A:366:GLU:CG	1:A:418:LEU:HD21	2.49	0.41
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.89	0.40
1:A:447:ILE:HD12	1:A:451:LEU:HG	2.02	0.40
2:D:360:PHE:CD1	5:D:200:570:H1L	2.57	0.40
2:D:363:PHE:CZ	2:D:452:LEU:HB3	2.56	0.40
2:D:446:VAL:HG11	2:D:477:TYR:CE1	2.52	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	230/238 (97%)	196 (85%)	20 (9%)	14 (6%)	1	0
2	D	270/272 (99%)	255 (94%)	7 (3%)	8 (3%)	4	1
3	B	8/25 (32%)	7 (88%)	1 (12%)	0	100	100
3	E	14/25 (56%)	10 (71%)	3 (21%)	1 (7%)	1	0
All	All	522/560 (93%)	468 (90%)	31 (6%)	23 (4%)	2	0

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	244	PRO
1	A	257	ASN
1	A	259	SER
1	A	260	SER
1	A	446	PRO
2	D	243	ASP
2	D	244	LYS
2	D	276	GLU
2	D	358	LYS
1	A	245	LYS
1	A	256	LEU
1	A	442	ILE
1	A	450	PHE
2	D	267	ILE
1	A	250	VAL
2	D	265	LYS
2	D	271	GLN
1	A	457	ALA
2	D	268	THR
1	A	444	ASP
3	E	699	PRO
1	A	447	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	182/205 (89%)	167 (92%)	15 (8%)	11	8
2	D	243/245 (99%)	224 (92%)	19 (8%)	12	9
3	B	9/24 (38%)	8 (89%)	1 (11%)	6	3
3	E	14/24 (58%)	13 (93%)	1 (7%)	14	11
All	All	448/498 (90%)	412 (92%)	36 (8%)	12	8

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	236	LEU
1	A	240	LEU
1	A	244	PRO
1	A	276	LEU
1	A	306	ASN
1	A	334	ARG
1	A	345	ILE
1	A	383	LEU
1	A	410	GLU
1	A	411	GLN
1	A	418	LEU
1	A	426	ARG
1	A	450	PHE
1	A	458	PRO
2	D	207	GLU
2	D	228	LEU
2	D	234	ARG
2	D	237	LEU
2	D	241	THR
2	D	242	THR
2	D	244	LYS
2	D	270	LEU
2	D	318	LEU

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Mol	Chain	Res	Type
2	D	335	ASN
2	D	349	THR
2	D	362	ASP
2	D	424	ASN
2	D	442	LEU
2	D	452	LEU
2	D	460	GLU
2	D	461	THR
2	D	463	MET
2	D	477	TYR
3	B	635	ARG
3	E	695	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	270	GLN
1	A	306	ASN
1	A	338	HIS
2	D	273	GLN
2	D	308	ASN
2	D	335	ASN
2	D	375	ASN
2	D	424	ASN
2	D	425	HIS
2	D	454	GLN
2	D	466	HIS
3	B	634	HIS
3	B	638	GLN
3	E	691	HIS
3	E	695	GLN

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	570	D	200	-	40,45,45	2.39	17 (42%)	47,61,61	1.85	4 (8%)
4	9CR	A	201	-	22,22,22	3.59	11 (50%)	30,30,30	2.44	12 (40%)

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
5	570	D	200	-	-	1/25/30/30	0/5/5/5
4	9CR	A	201	-	-	6/15/32/32	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	9CR	C1-C6	9.49	1.66	1.53
4	A	201	9CR	C5-C6	9.07	1.50	1.34
5	D	200	570	CA-N	5.27	1.51	1.45
4	A	201	9CR	C16-C1	4.73	1.63	1.53
5	D	200	570	C1F-C1G	4.53	1.59	1.50
5	D	200	570	CE2-CZ	4.29	1.47	1.38
5	D	200	570	C3E-C3D	4.01	1.53	1.48
4	A	201	9CR	C10-C9	3.98	1.41	1.35
5	D	200	570	C1A-N	3.88	1.46	1.37
5	D	200	570	C1F-C1A	3.88	1.47	1.41
4	A	201	9CR	C20-C13	3.41	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	200	570	C1I-C1H	3.36	1.45	1.39
4	A	201	9CR	C2-C1	3.25	1.61	1.54
4	A	201	9CR	C4-C5	3.14	1.57	1.51
5	D	200	570	C1E-C1F	3.11	1.44	1.39
5	D	200	570	C1B-C1A	2.90	1.44	1.39
4	A	201	9CR	C2-C3	2.89	1.59	1.52
4	A	201	9CR	C14-C13	2.57	1.39	1.35
5	D	200	570	C3M-C3N	2.49	1.42	1.36
5	D	200	570	CE1-CZ	2.47	1.43	1.38
5	D	200	570	C1M-C1H	2.44	1.43	1.39
5	D	200	570	OH-CZ	2.41	1.43	1.37
5	D	200	570	C3K-C3J	2.41	1.42	1.36
4	A	201	9CR	C14-C15	2.40	1.54	1.47
5	D	200	570	CD2-CG	2.32	1.43	1.38
5	D	200	570	CD1-CG	2.30	1.43	1.38
5	D	200	570	C3B-C3C	2.14	1.57	1.51
4	A	201	9CR	C8-C9	-2.04	1.41	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	200	570	C1A-C1F-C1G	6.91	126.47	121.96
5	D	200	570	C1F-C1G-C1H	6.58	130.39	119.53
4	A	201	9CR	C17-C1-C6	5.05	118.49	110.30
4	A	201	9CR	C16-C1-C6	-4.74	102.61	110.30
5	D	200	570	O1G-C1G-C1H	-4.62	112.75	120.12
5	D	200	570	C1A-N-CA	4.40	133.24	124.51
4	A	201	9CR	C19-C9-C10	-4.38	116.79	122.92
4	A	201	9CR	C19-C9-C8	4.22	124.73	118.08
4	A	201	9CR	C7-C8-C9	3.92	132.16	126.23
4	A	201	9CR	C11-C10-C9	-3.63	122.12	127.31
4	A	201	9CR	C20-C13-C12	3.58	123.72	118.08
4	A	201	9CR	C2-C1-C6	3.34	115.62	110.48
4	A	201	9CR	C1-C6-C5	-2.91	118.51	122.61
4	A	201	9CR	C8-C7-C6	2.82	135.13	127.20
4	A	201	9CR	C7-C6-C5	2.15	126.66	121.46
4	A	201	9CR	O2-C15-C14	2.13	120.11	113.50

There are no chirality outliers.

All (7) torsion outliers are listed below:

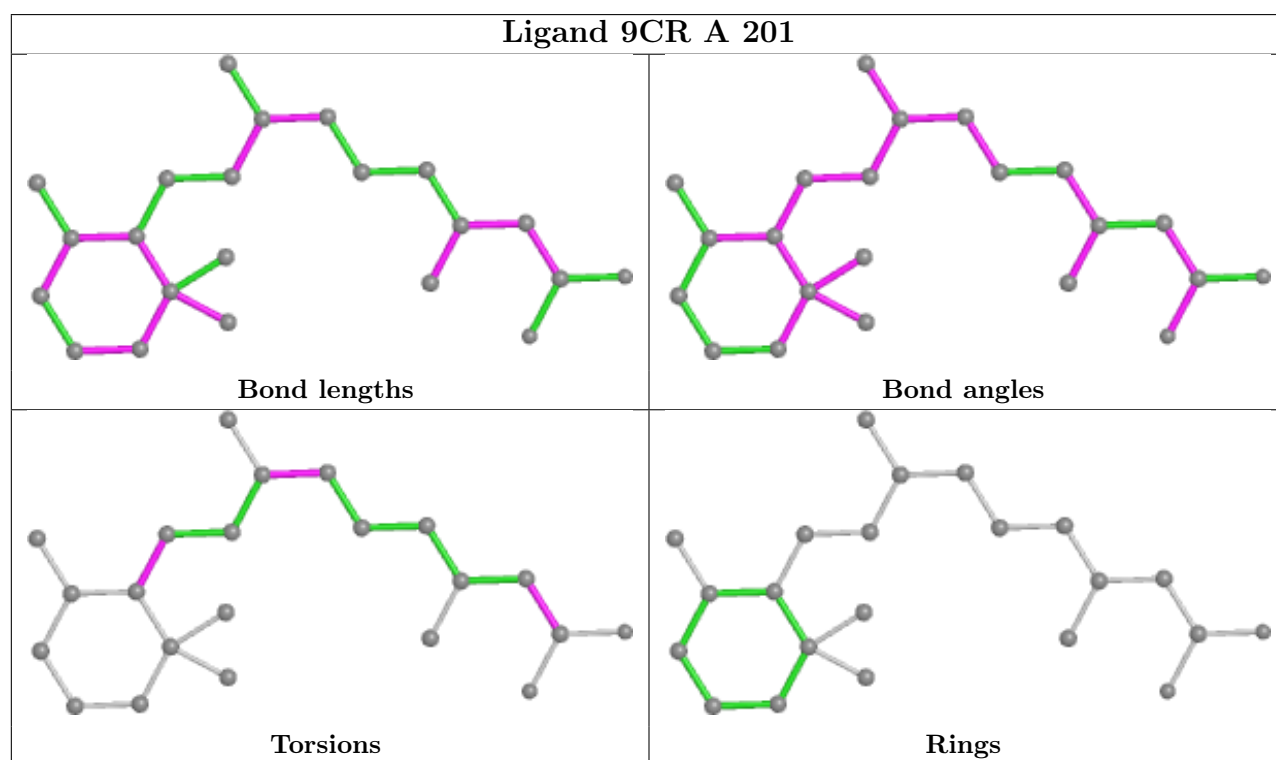
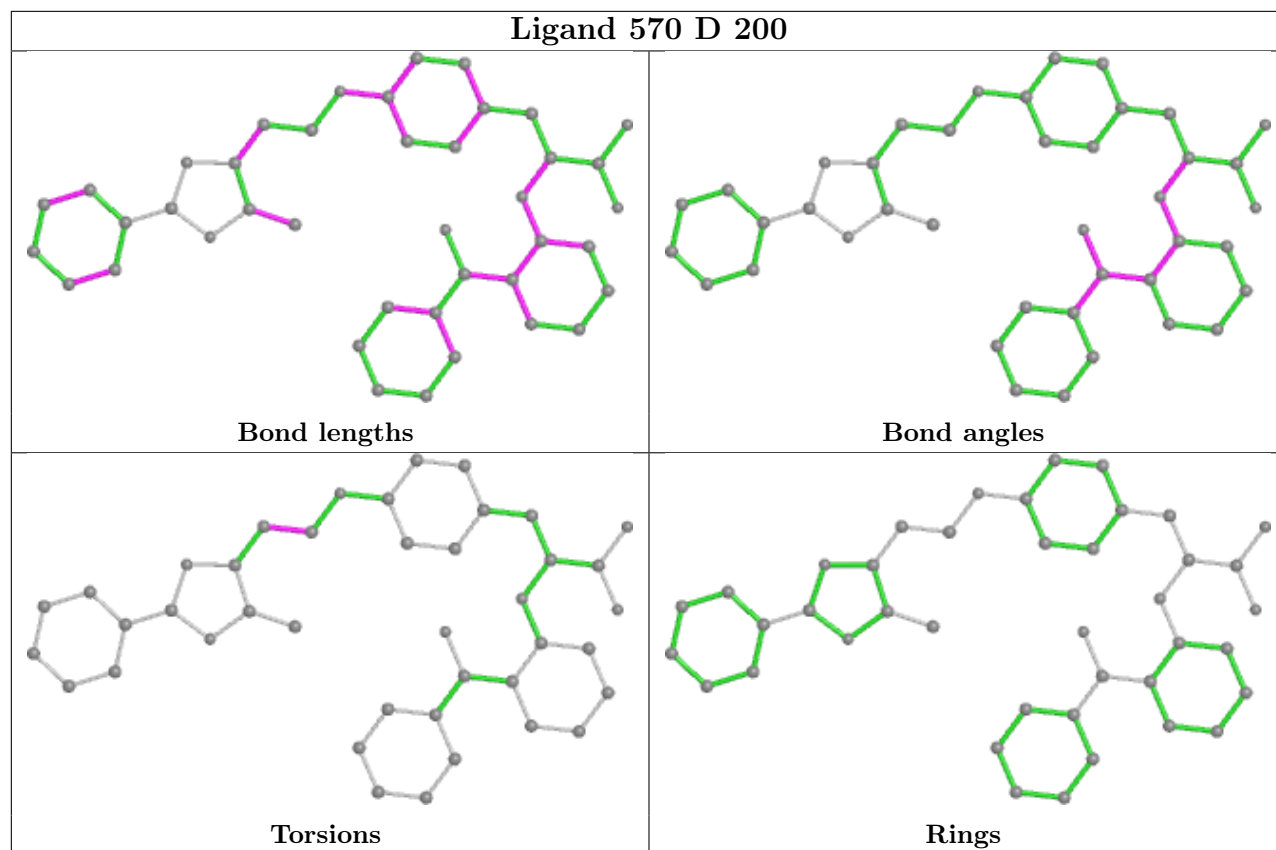
Mol	Chain	Res	Type	Atoms
4	A	201	9CR	C5-C6-C7-C8
4	A	201	9CR	C1-C6-C7-C8
4	A	201	9CR	C13-C14-C15-O1
4	A	201	9CR	C13-C14-C15-O2
4	A	201	9CR	C11-C10-C9-C19
4	A	201	9CR	C11-C10-C9-C8
5	D	200	570	OH-C3A-C3B-C3C

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	200	570	5	0
4	A	201	9CR	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

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	232/238 (97%)	1.91	53 (22%) 0 0	23, 42, 109, 124	0
2	D	272/272 (100%)	1.33	41 (15%) 2 3	26, 39, 115, 131	0
3	B	10/25 (40%)	1.62	3 (30%) 0 0	50, 57, 69, 76	0
3	E	16/25 (64%)	3.69	12 (75%) 0 0	60, 68, 96, 98	0
All	All	530/560 (94%)	1.66	109 (20%) 1 1	23, 41, 110, 131	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	267	ILE	31.8
1	A	256	LEU	18.2
1	A	252	ALA	18.0
2	D	274	SER	18.0
2	D	266	HIS	16.9
1	A	249	TYR	14.1
2	D	264	PHE	13.7
2	D	270	LEU	13.7
1	A	441	LEU	13.1
2	D	265	LYS	13.1
1	A	259	SER	12.8
1	A	442	ILE	12.6
1	A	444	ASP	12.5
2	D	268	THR	12.4
2	D	262	ILE	12.2
1	A	258	PRO	11.9
1	A	445	THR	11.9
1	A	253	ASN	11.5
2	D	272	GLU	11.2
1	A	257	ASN	11.1
3	E	700	SER	11.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	260	SER	11.0
1	A	250	VAL	11.0
2	D	269	PRO	10.8
1	A	446	PRO	10.7
1	A	227	ASN	10.6
1	A	262	ASN	10.4
1	A	248	THR	9.6
1	A	245	LYS	9.4
1	A	443	GLY	9.4
1	A	261	PRO	9.3
2	D	271	GLN	9.1
2	D	263	LYS	9.0
3	E	699	PRO	8.9
1	A	458	PRO	8.8
1	A	255	GLY	8.7
1	A	247	GLU	8.1
1	A	457	ALA	8.1
3	E	698	SER	8.0
1	A	254	MET	7.4
2	D	260	ASP	7.2
2	D	275	LYS	6.9
2	D	244	LYS	6.9
2	D	257	MET	6.7
3	E	685	GLU	6.1
1	A	251	GLU	5.9
2	D	273	GLN	5.7
1	A	244	PRO	5.6
2	D	477	TYR	5.2
2	D	461	THR	5.2
1	A	246	THR	4.9
2	D	261	LYS	4.8
1	A	456	GLU	4.4
1	A	447	ILE	4.1
2	D	259	GLU	3.9
3	E	696	GLU	3.7
2	D	463	MET	3.6
2	D	358	LYS	3.6
3	E	686	ARG	3.6
2	D	462	ASP	3.4
3	E	697	GLY	3.4
1	A	229	ASP	3.2
1	A	437	PHE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	319	ALA	3.2
2	D	256	MET	3.2
2	D	252	MET	3.2
1	A	452	MET	3.1
2	D	250	TYR	3.1
3	E	690	LEU	3.1
3	B	633	LEU	3.0
1	A	264	PRO	3.0
1	A	340	ALA	3.0
1	A	438	PHE	3.0
1	A	322	ASP	2.9
2	D	343	GLU	2.9
2	D	243	ASP	2.9
2	D	281	ILE	2.8
2	D	277	VAL	2.8
1	A	321	LYS	2.7
2	D	255	LEU	2.7
1	A	440	LYS	2.7
2	D	245	SER	2.7
3	B	635	ARG	2.6
1	A	436	LEU	2.6
1	A	324	ILE	2.6
3	B	639	GLU	2.6
2	D	464	SER	2.5
1	A	381	LYS	2.5
1	A	439	PHE	2.5
2	D	247	PHE	2.5
1	A	410	GLU	2.4
3	E	695	GLN	2.4
1	A	325	LEU	2.3
1	A	242	VAL	2.3
1	A	331	HIS	2.3
2	D	279	ILE	2.3
3	E	694	LEU	2.2
1	A	263	ASP	2.2
1	A	333	HIS	2.2
1	A	411	GLN	2.1
3	E	692	ARG	2.1
3	E	693	LEU	2.1
2	D	423	LEU	2.1
2	D	249	ILE	2.1
1	A	369	CYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	417	LEU	2.0
2	D	216	LYS	2.0
1	A	330	LEU	2.0
2	D	474	LYS	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](#)

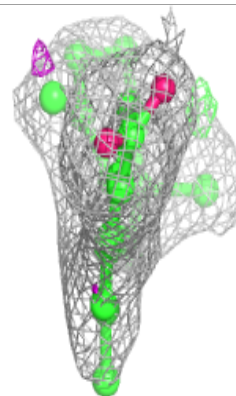
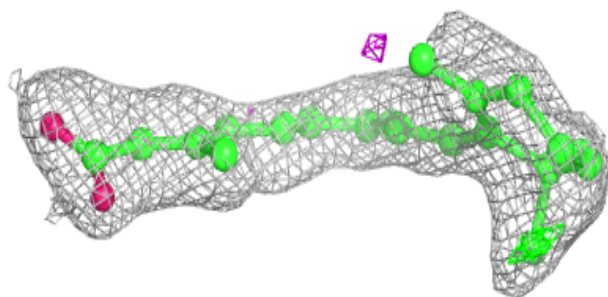
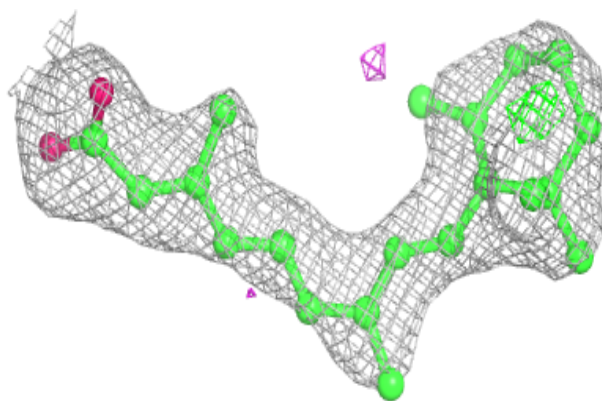
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	9CR	A	201	22/22	0.88	0.25	43,48,50,50	0
5	570	D	200	41/41	0.93	0.17	33,38,44,44	0

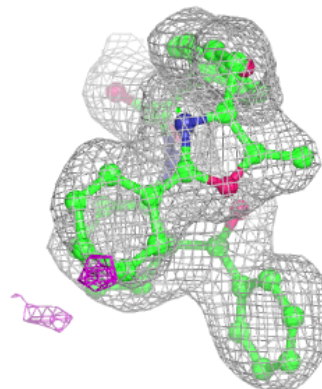
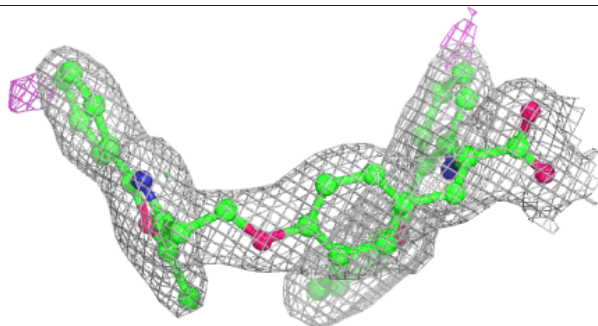
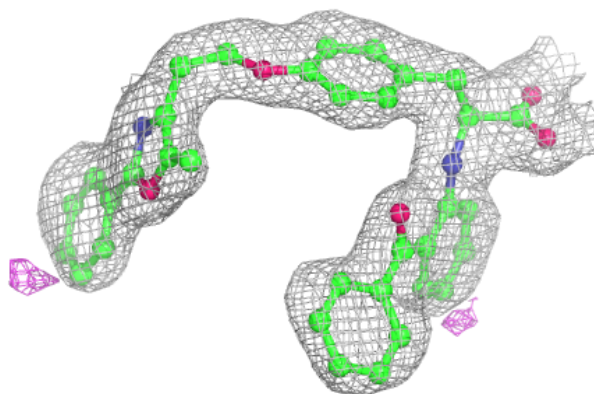
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 9CR A 201:**

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

**Electron density around 570 D 200:**

$2mF_o-DF_c$  (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.