



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:45 PM UTC

PDB ID : 1FM9 / pdb_00001fm9
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

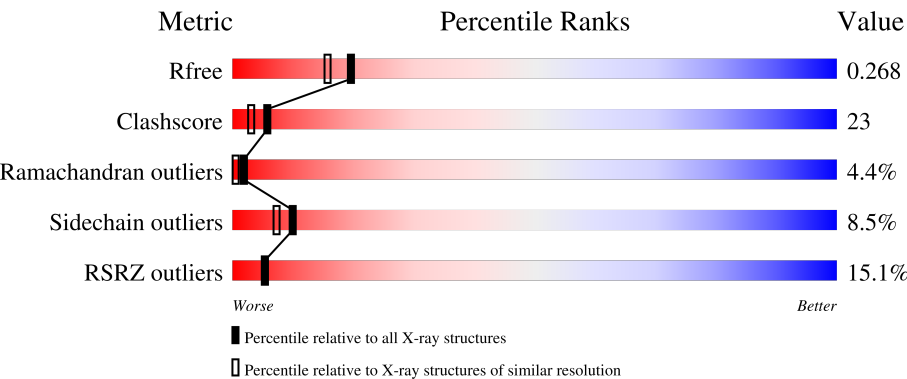
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 ≥ 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	18% 61% 28% 7%
2	D	272	11% 64% 28% 7%
3	B	25	8% 16% 24% 60%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
3	E	25	16% 24% 32% 8% 36%

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
1	A	232	Total	C	N	O	S	0	0	0
			1754	1117	306	321	10			

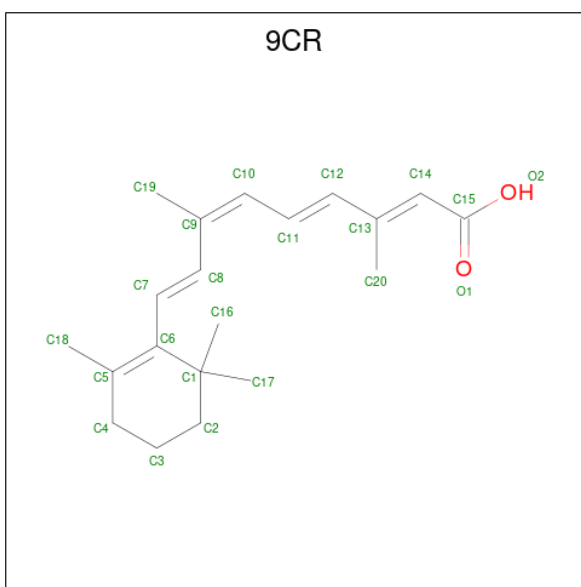
- Molecule 2 is a protein called PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA.

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

- Molecule 3 is a protein called STEROID RECEPTOR COACTIVATOR.

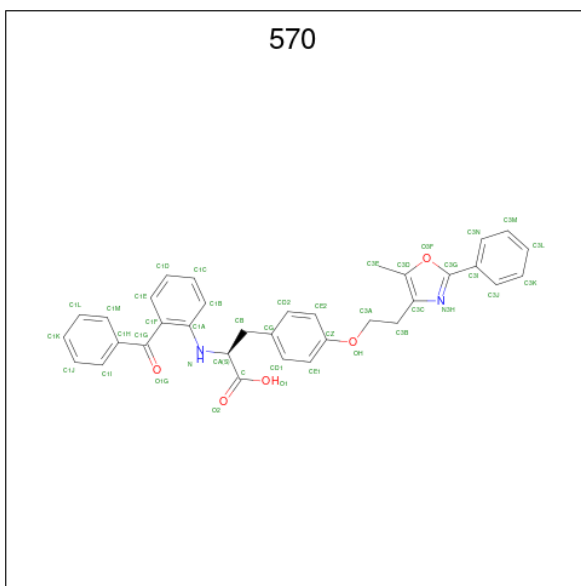
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	10	Total	C	N	O	0	0	0
			86	55	18	13			
3	E	16	Total	C	N	O	0	0	0
			129	79	27	23			

- Molecule 4 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: C₂₀H₂₈O₂).



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-OXAZO L-4-YL)-ETHOXY]-PHENYL}-PROPIONIC ACID (CCD ID: 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		

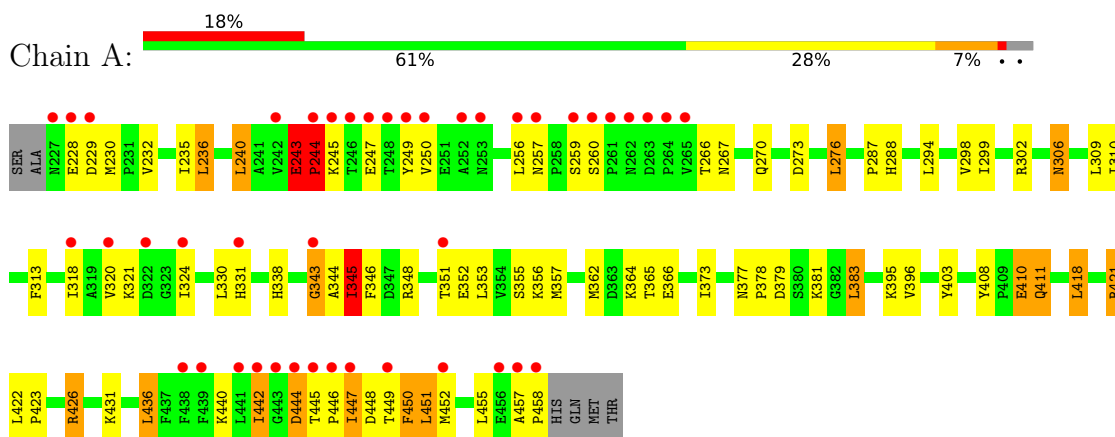
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

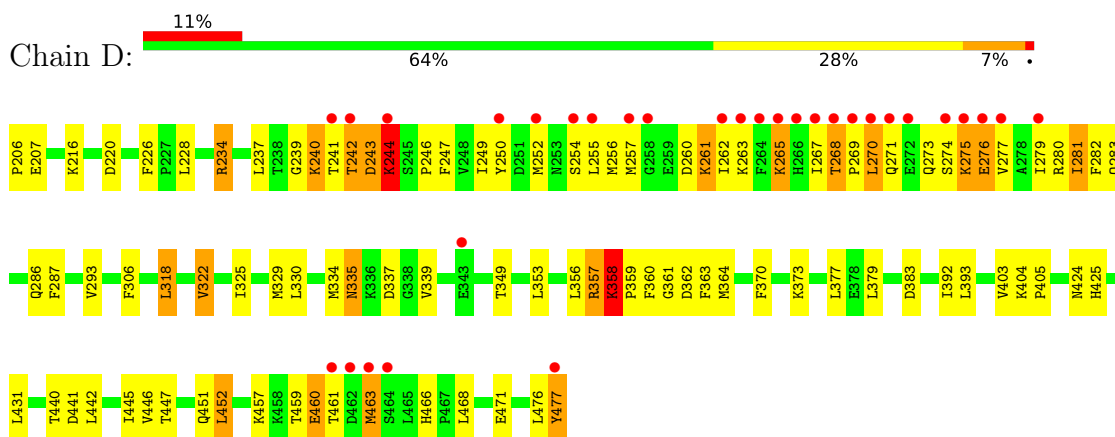
3 Residue-property plots

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.

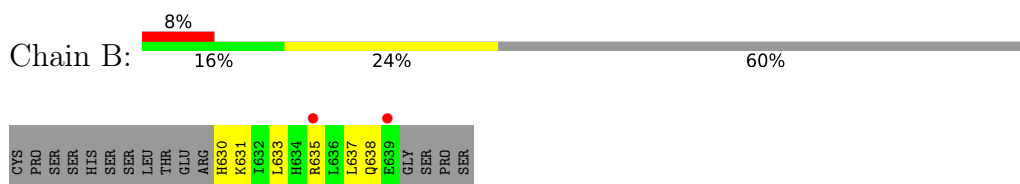
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA



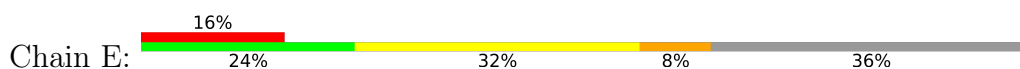
• Molecule 2: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA



• 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	S698	P699	S700

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.14Å 54.05Å 211.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-2.10) 91.7 (20.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.11Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.239 , 0.268 0.239 , 0.268	Depositor DCC
R_{free} test set	2895 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4342	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 570, 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	0.46	0/1789	0.99	9/2414 (0.4%)
2	D	0.55	0/2217	0.99	9/2987 (0.3%)
3	B	0.48	0/87	0.99	1/116 (0.9%)
3	E	0.33	0/131	0.94	0/175
All	All	0.51	0/4224	0.99	19/5692 (0.3%)

There are no bond length outliers.

All (19) 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	CA-C-N	8.99	148.58	127.00
1	A	243	GLU	C-N-CA	8.99	148.58	127.00
2	D	322	VAL	N-CA-C	7.91	118.67	110.36
2	D	403	VAL	N-CA-C	7.76	118.56	110.72
1	A	451	LEU	N-CA-C	-7.70	102.88	111.28
2	D	240	LYS	N-CA-C	6.67	119.41	110.88
2	D	358	LYS	CA-C-N	-6.57	112.95	120.04
2	D	358	LYS	C-N-CA	-6.57	112.95	120.04
2	D	246	PRO	N-CA-C	6.56	121.37	111.14
2	D	206	PRO	N-CA-CB	6.15	109.77	103.00
3	B	638	GLN	N-CA-C	6.15	119.82	112.93
2	D	306	PHE	N-CA-C	6.06	117.55	111.07
1	A	411	GLN	CA-C-N	5.95	126.37	119.47
1	A	411	GLN	C-N-CA	5.95	126.37	119.47
1	A	421	ARG	N-CA-C	-5.84	106.16	113.28
1	A	345	ILE	N-CA-C	-5.70	104.96	110.72
2	D	261	LYS	N-CA-C	-5.19	106.21	112.54
1	A	343	GLY	N-CA-C	-5.11	103.65	111.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1754	0	1733	82	0
2	D	2179	0	2237	106	0
3	B	86	0	86	7	0
3	E	129	0	125	15	0
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	196	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 23.

All (196) 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
1:A:230:MET:HE2	1:A:396:VAL:HG22	1.49	0.92
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: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
1:A:230:MET:HE3	1:A:235:ILE:HD11	1.64	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:335:ASN:C	2:D:335:ASN:HD22	1.96	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
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
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:CE1	2:D:257:MET:HE2	2.38	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:ILE:HG12	1:A:452:MET:HE2	1.88	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
1:A:320:VAL:HG22	1:A:321:LYS:N	2.21	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
2:D:477:TYR:C	2:D:477:TYR:CD1	2.83	0.53
1:A:243:GLU:HB3	1:A:244:PRO:C	2.34	0.53
1:A:451:LEU:O	1:A:455:LEU:HD13	2.08	0.53
2:D:270:LEU:HD22	2:D:270:LEU:C	2.35	0.52
1:A:447:ILE:HD11	1:A:452:MET:SD	2.50	0.52
2:D:243:ASP:O	2:D:243:ASP:CG	2.52	0.52
2:D:226:PHE:CG	2:D:329:MET:HE1	2.45	0.52
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:247:PHE:HE1	2:D:257:MET:HE2	1.73	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:273:ASP:CG	1:A:448:ASP:HB2	2.36	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:PHE:CD1	2:D:287:PHE:C	2.90	0.50
1:A:243:GLU:CB	1:A:244:PRO:C	2.85	0.50
3:B:633:LEU:C	3:B:633:LEU:HD13	2.37	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: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:357:MET:HG2	1:A:362:MET:HE3	1.94	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
1:A:294:LEU:C	1:A:294:LEU:HD23	2.38	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
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
2:D:275:LYS:HZ2	2:D:275:LYS:HB2	1.80	0.47
3:E:686:ARG:NE	3:E:686:ARG:HA	2.29	0.47
2:D:459:THR:C	2:D:460:GLU:HG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:C	1:A:249:TYR:H	2.23	0.45
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:313:PHE:C	1:A:313:PHE:CD1	2.93	0.45
1:A:373:ILE:HG13	1:A:396:VAL:HG11	1.99	0.45
4:A:201:9CR:H8	4:A:201:9CR:H10	1.80	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
1:A:422:LEU:CB	2:D:440:THR:HG21	2.47	0.44
2:D:335:ASN:C	2:D:335:ASN:ND2	2.68	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
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
2:D:273:GLN:C	2:D:275:LYS:H	2.26	0.43
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: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
2:D:252:MET:HE3	2:D:256:MET:SD	2.60	0.41
1:A:229:ASP:HB3	1:A:395:LYS:HD3	2.01	0.41
3:E:695:GLN:OE1	6:E:65:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:C	1:A:442:ILE:H	2.29	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
2:D:357:ARG:O	2:D:358:LYS:C	2.63	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
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:247:GLU:C	1:A:249:TYR:N	2.79	0.40
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/238 (97%)	196 (85%)	20 (9%)	14 (6%)	1	0
2	D	270/272 (99%)	255 (94%)	7 (3%)	8 (3%)	3	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 ⓘ

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%)	10	8
2	D	243/245 (99%)	221 (91%)	22 (9%)	9	6
3	B	9/24 (38%)	9 (100%)	0	100	100
3	E	14/24 (58%)	13 (93%)	1 (7%)	13	11
All	All	448/498 (90%)	410 (92%)	38 (8%)	10	7

All (38) 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	309	LEU
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	436	LEU
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	275	LYS
2	D	281	ILE
2	D	318	LEU
2	D	335	ASN
2	D	349	THR
2	D	357	ARG
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	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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	44,45,45	2.69	23 (52%)	57,61,61	3.05	9 (15%)
4	9CR	A	201	-	22,22,22	3.67	11 (50%)	30,30,30	2.48	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	-	-	1/30/30/30	0/5/5/5
4	9CR	A	201	-	-	6/15/32/32	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	9CR	C1-C6	10.16	1.66	1.53
4	A	201	9CR	C5-C6	9.33	1.50	1.34
5	D	200	570	C3G-N3H	8.34	1.41	1.30
4	A	201	9CR	C16-C1	4.93	1.63	1.53
5	D	200	570	C1F-C1G	4.69	1.59	1.49
5	D	200	570	CE2-CZ	4.54	1.47	1.38
5	D	200	570	C1A-N	4.07	1.46	1.37
5	D	200	570	C1F-C1A	3.91	1.47	1.41
5	D	200	570	C3I-C3G	-3.75	1.39	1.47
5	D	200	570	C1I-C1H	3.72	1.45	1.39
5	D	200	570	C3N-C3I	3.56	1.44	1.39
4	A	201	9CR	C20-C13	3.50	1.57	1.50
4	A	201	9CR	C4-C5	3.33	1.57	1.51
4	A	201	9CR	C2-C1	3.29	1.61	1.54
5	D	200	570	C1E-C1F	3.23	1.44	1.39
5	D	200	570	C1B-C1A	3.01	1.44	1.39
4	A	201	9CR	C2-C3	3.00	1.59	1.52
5	D	200	570	C3J-C3I	2.98	1.43	1.39
5	D	200	570	C1M-C1H	2.68	1.43	1.39
4	A	201	9CR	C14-C13	2.62	1.39	1.35
5	D	200	570	CE1-CZ	2.58	1.43	1.38
4	A	201	9CR	C14-C15	2.57	1.54	1.47
5	D	200	570	C3B-C3C	2.52	1.57	1.50
5	D	200	570	CD2-CG	2.50	1.43	1.38
5	D	200	570	CD1-CG	2.48	1.43	1.38
5	D	200	570	OH-CZ	2.45	1.43	1.37
5	D	200	570	C1J-C1I	2.35	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	9CR	C10-C9	2.27	1.41	1.35
5	D	200	570	C1K-C1J	2.19	1.43	1.38
5	D	200	570	CA-N	2.15	1.51	1.46
5	D	200	570	C3E-C3D	2.15	1.53	1.49
5	D	200	570	C1L-C1K	2.10	1.42	1.38
4	A	201	9CR	C8-C9	-2.06	1.41	1.46
5	D	200	570	C3M-C3N	2.02	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	200	570	O3F-C3D-C3C	-10.26	101.72	108.03
5	D	200	570	O3F-C3D-C3E	9.86	128.78	115.88
5	D	200	570	O3F-C3G-N3H	-8.45	105.14	114.37
5	D	200	570	C3E-C3D-C3C	-6.99	129.50	135.22
5	D	200	570	C1A-C1F-C1G	6.91	126.47	121.96
5	D	200	570	C1F-C1G-C1H	6.77	130.39	119.56
5	D	200	570	O3F-C3G-C3I	5.70	128.67	118.73
5	D	200	570	C3G-O3F-C3D	5.26	114.35	105.20
4	A	201	9CR	C17-C1-C6	5.26	118.49	110.24
4	A	201	9CR	C16-C1-C6	-4.87	102.61	110.24
5	D	200	570	O1G-C1G-C1H	-4.62	112.75	120.15
4	A	201	9CR	C19-C9-C8	4.35	124.73	118.09
4	A	201	9CR	C7-C8-C9	4.01	132.16	126.23
4	A	201	9CR	C19-C9-C10	-3.72	116.79	122.82
4	A	201	9CR	C20-C13-C12	3.69	123.72	118.09
4	A	201	9CR	C11-C10-C9	-3.68	122.12	127.28
4	A	201	9CR	C2-C1-C6	3.57	115.62	110.44
4	A	201	9CR	C8-C7-C6	3.04	135.13	127.00
4	A	201	9CR	C1-C6-C5	-3.02	118.51	122.64
4	A	201	9CR	O2-C15-C14	2.26	120.11	113.40
4	A	201	9CR	C7-C6-C5	2.22	126.66	121.56

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

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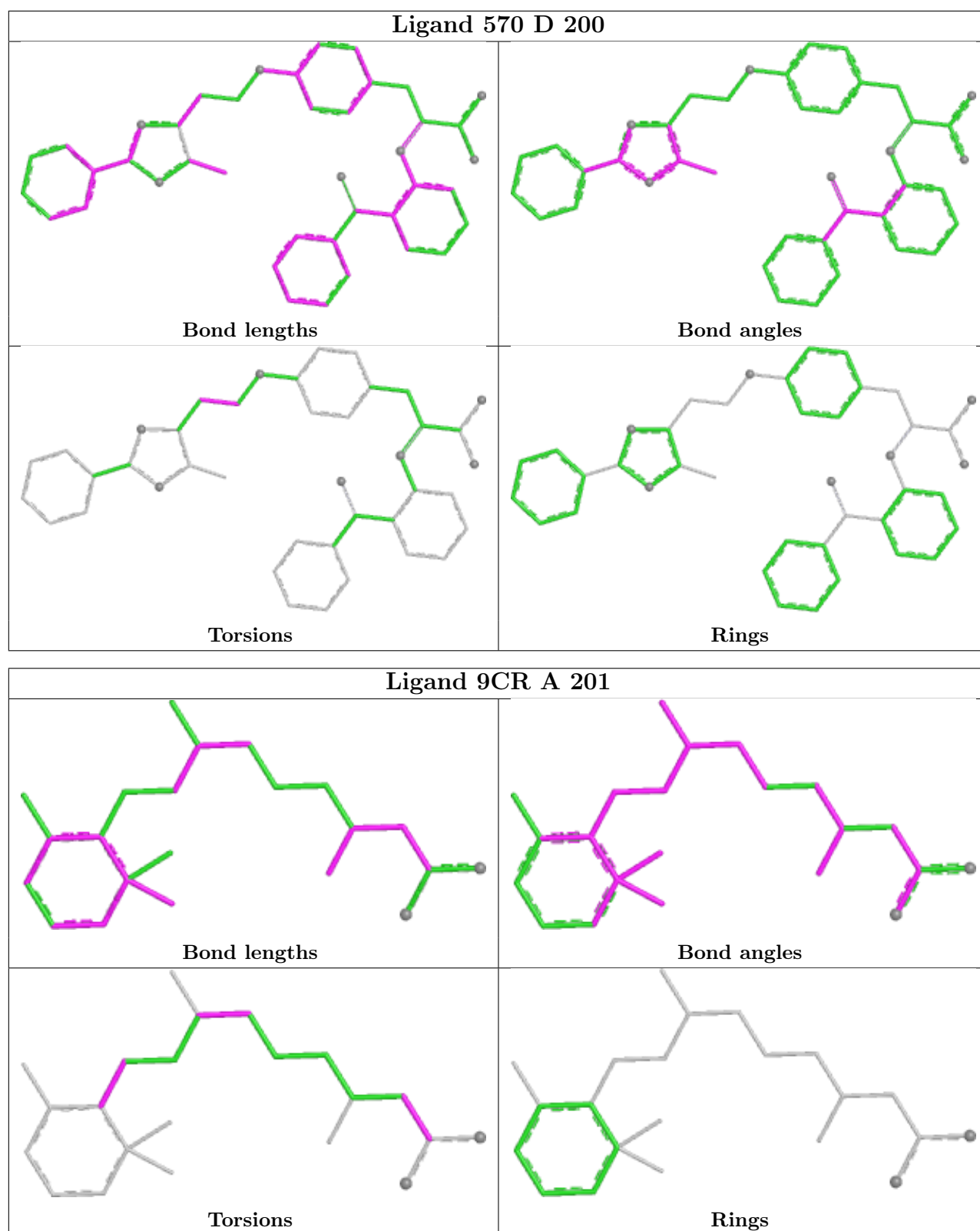
Mol	Chain	Res	Type	Atoms
4	A	201	9CR	C11-C10-C9-C8
5	D	200	570	OH-C3A-C3B-C3C

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	232/238 (97%)	0.83	43 (18%)	3 3	23, 42, 109, 124	0
2	D	272/272 (100%)	0.59	31 (11%)	10 10	26, 39, 115, 131	0
3	B	10/25 (40%)	1.48	2 (20%)	3 3	50, 57, 69, 76	0
3	E	16/25 (64%)	1.62	4 (25%)	2 2	60, 68, 96, 98	0
All	All	530/560 (94%)	0.74	80 (15%)	5 5	23, 41, 110, 131	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	267	ILE	8.9
1	A	446	PRO	7.0
1	A	441	LEU	6.7
2	D	274	SER	6.7
2	D	262	ILE	6.0
2	D	477	TYR	5.1
1	A	457	ALA	4.9
2	D	270	LEU	4.9
2	D	269	PRO	4.8
1	A	445	THR	4.6
1	A	227	ASN	4.6
1	A	447	ILE	4.3
1	A	443	GLY	4.3
1	A	244	PRO	4.3
1	A	442	ILE	4.2
1	A	264	PRO	4.0
1	A	444	ASP	3.9
1	A	250	VAL	3.9
2	D	271	GLN	3.8
1	A	259	SER	3.7
2	D	264	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	245	LYS	3.7
1	A	252	ALA	3.7
1	A	260	SER	3.6
3	E	698	SER	3.5
2	D	252	MET	3.4
2	D	275	LYS	3.4
2	D	463	MET	3.3
2	D	268	THR	3.2
2	D	265	LYS	3.2
1	A	263	ASP	3.2
1	A	261	PRO	3.1
2	D	266	HIS	3.1
2	D	263	LYS	2.9
3	B	639	GLU	2.8
2	D	258	GLY	2.8
1	A	242	VAL	2.8
1	A	439	PHE	2.8
1	A	256	LEU	2.8
2	D	255	LEU	2.8
1	A	248	THR	2.8
1	A	257	ASN	2.7
2	D	279	ILE	2.7
2	D	272	GLU	2.7
2	D	277	VAL	2.7
3	B	635	ARG	2.7
1	A	331	HIS	2.6
3	E	699	PRO	2.6
2	D	241	THR	2.6
1	A	249	TYR	2.5
1	A	262	ASN	2.5
1	A	458	PRO	2.5
3	E	694	LEU	2.5
1	A	322	ASP	2.5
1	A	228	GLU	2.4
1	A	438	PHE	2.4
1	A	265	VAL	2.4
2	D	257	MET	2.3
2	D	276	GLU	2.3
3	E	693	LEU	2.3
2	D	462	ASP	2.3
1	A	253	ASN	2.3
1	A	452	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	247	GLU	2.2
2	D	244	LYS	2.2
2	D	464	SER	2.2
2	D	254	SER	2.2
1	A	229	ASP	2.2
1	A	246	THR	2.2
1	A	449	THR	2.2
2	D	461	THR	2.2
2	D	343	GLU	2.1
2	D	250	TYR	2.1
1	A	324	ILE	2.1
1	A	343	GLY	2.1
1	A	320	VAL	2.1
1	A	456	GLU	2.0
1	A	351	THR	2.0
2	D	242	THR	2.0
1	A	318	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

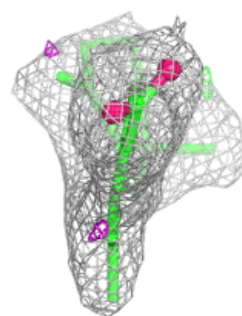
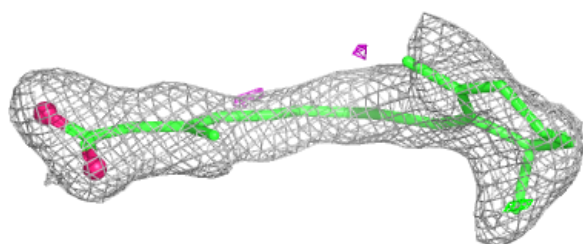
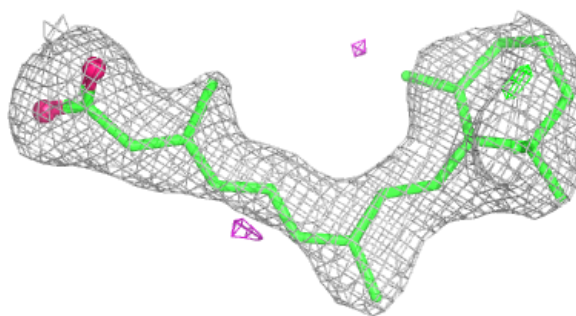
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	9CR	A	201	22/22	0.84	0.14	43,48,50,50	0
5	570	D	200	41/41	0.91	0.08	33,38,44,44	0

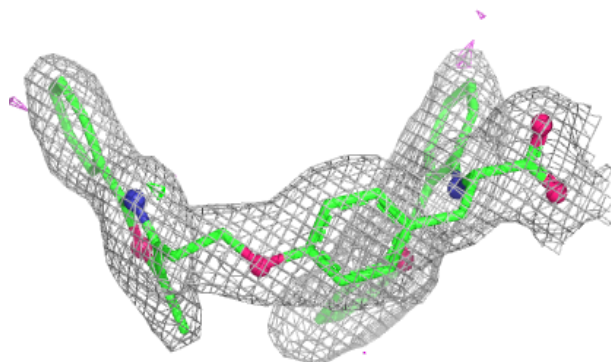
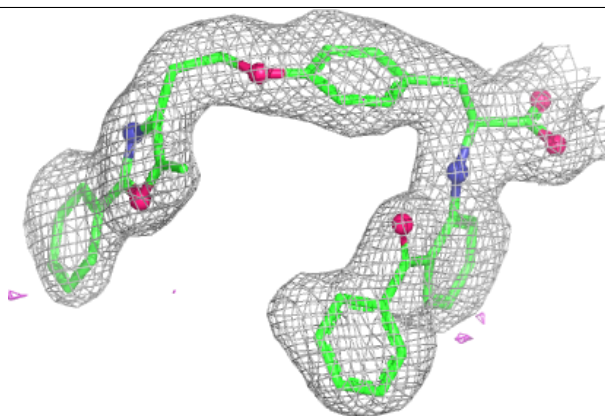
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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