



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2016 – 03:43 PM EDT

PDB ID : 1FBY
Title : CRYSTAL STRUCTURE OF THE HUMAN RXR ALPHA LIGAND BINDING DOMAIN BOUND TO 9-CIS RETINOIC ACID
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Deposited on : 2000-07-17
Resolution : 2.25 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

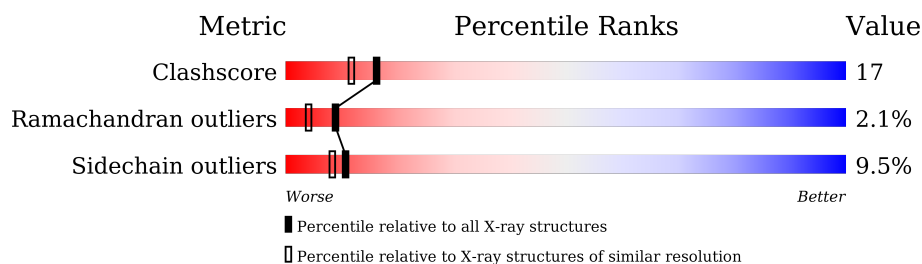
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	239	
1	B	239	

2 Entry composition [i](#)

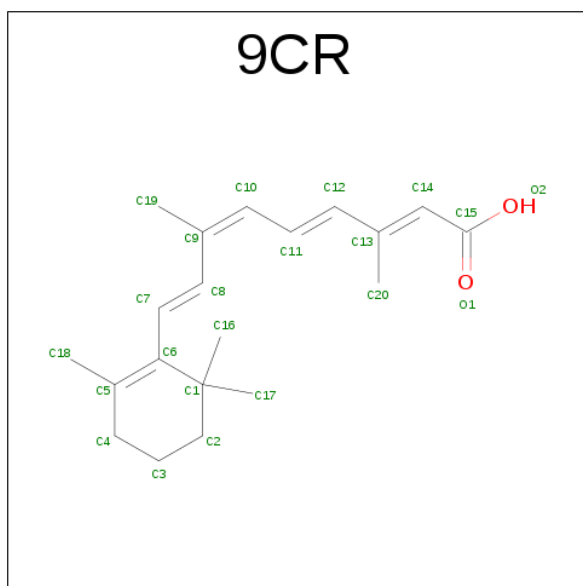
There are 3 unique types of molecules in this entry. The entry contains 3625 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	217	Total	C	N	O	S	0	0	0
			1706	1093	292	311	10			
1	B	212	Total	C	N	O	S	0	0	0
			1672	1075	286	301	10			

- Molecule 2 is (9CIS)-RETINOIC ACID (three-letter code: 9CR) (formula: C₂₀H₂₈O₂).



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

- Molecule 3 is water.

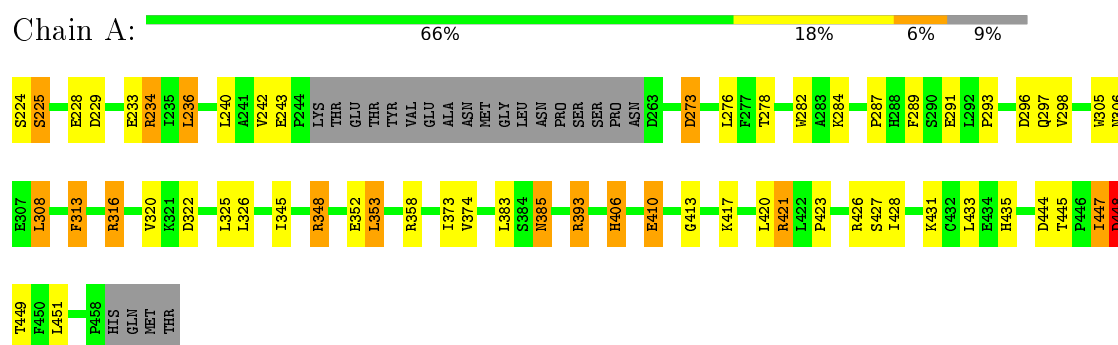
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total 125	O 125	0	0
3	B	78	Total 78	O 78	0	0

3 Residue-property plots [i](#)

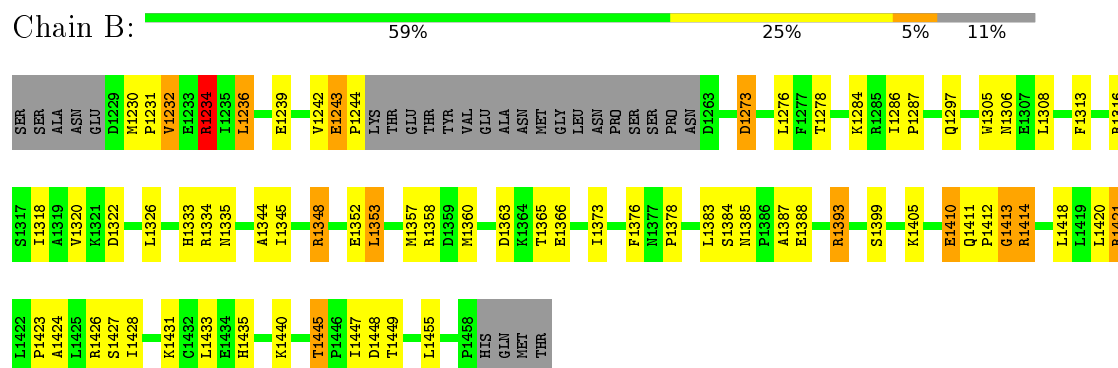
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA



• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.33 Å 86.36 Å 90.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 2.25	Depositor
% Data completeness (in resolution range)	80.2 (14.99-2.25)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3625	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.53	0/1740	0.72	2/2354 (0.1%)
1	B	0.49	0/1706	0.69	1/2308 (0.0%)
All	All	0.51	0/3446	0.71	3/4662 (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	B	1234	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	234	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	316	ARG	NE-CZ-NH2	-6.07	117.27	120.30

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	1706	0	1736	52	0
1	B	1672	0	1709	64	0
2	A	22	0	27	2	0
2	B	22	0	27	3	0
3	A	125	0	0	3	0
3	B	78	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3625	0	3499	116	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 17.

All (116) 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:B:1318:ILE:HG23	1:B:1358:ARG:HB2	1.56	0.88
1:B:1242:VAL:O	1:B:1243:GLU:HB3	1.77	0.82
1:B:1284:LYS:NZ	1:B:1297:GLN:HE22	1.80	0.79
1:A:421:ARG:HD3	3:A:1727:HOH:O	1.83	0.78
1:B:1366:GLU:OE1	1:B:1418:LEU:HD11	1.84	0.78
1:A:284:LYS:NZ	1:A:297:GLN:HE22	1.83	0.76
1:B:1239:GLU:OE1	3:B:1878:HOH:O	2.07	0.72
1:A:393:ARG:CB	1:A:393:ARG:HH11	2.04	0.70
1:B:1393:ARG:HH11	1:B:1393:ARG:CB	2.06	0.69
1:B:1318:ILE:HD11	1:B:1357:MET:HB3	1.76	0.68
1:B:1231:PRO:HD2	1:B:1399:SER:OG	1.93	0.67
1:B:1393:ARG:CG	1:B:1393:ARG:HH11	2.08	0.66
1:B:1243:GLU:HB2	1:B:1244:PRO:HD2	1.78	0.66
1:A:393:ARG:HH11	1:A:393:ARG:CG	2.07	0.64
1:A:447:ILE:HD13	1:A:447:ILE:H	1.63	0.64
1:B:1284:LYS:HZ1	1:B:1297:GLN:HE22	1.45	0.63
1:B:1393:ARG:HH11	1:B:1393:ARG:HB3	1.63	0.63
2:B:1500:9CR:O1	3:B:1801:HOH:O	2.16	0.63
1:A:410:GLU:H	1:A:410:GLU:CD	2.02	0.63
1:B:1440:LYS:HA	1:B:1445:THR:HB	1.82	0.62
1:A:393:ARG:HB3	1:A:393:ARG:HH11	1.63	0.62
1:B:1318:ILE:HD11	1:B:1357:MET:CB	2.30	0.62
1:A:348:ARG:NH2	1:A:427:SER:OG	2.33	0.61
1:B:1236:LEU:HD22	1:B:1236:LEU:O	2.02	0.60
1:A:234:ARG:HD3	1:A:287:PRO:HG3	1.82	0.60
1:A:224:SER:O	1:A:225:SER:HB3	2.00	0.59
1:B:1318:ILE:HG23	1:B:1358:ARG:CB	2.30	0.59
1:B:1242:VAL:O	1:B:1243:GLU:CB	2.50	0.58
1:A:308:LEU:HD13	1:A:374:VAL:CG1	2.35	0.57
1:B:1385:ASN:OD1	1:B:1388:GLU:HB2	2.05	0.57
1:B:1230:MET:HA	1:B:1399:SER:OG	2.05	0.56
1:B:1242:VAL:HG13	1:B:1278:THR:HB	1.87	0.56
1:B:1320:VAL:O	1:B:1358:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1373:ILE:HG23	1:B:1393:ARG:HD2	1.87	0.56
1:B:1316:ARG:HH22	2:B:1500:9CR:C15	2.19	0.56
1:A:316:ARG:HH22	2:A:500:9CR:C15	2.19	0.55
1:B:1230:MET:SD	3:B:1813:HOH:O	2.58	0.55
1:B:1385:ASN:HD21	1:B:1387:ALA:HB3	1.72	0.55
1:A:284:LYS:HZ3	1:A:297:GLN:HE22	1.53	0.53
1:B:1447:ILE:O	1:B:1447:ILE:HG22	2.07	0.53
1:A:345:ILE:HD13	1:A:431:LYS:HG2	1.92	0.53
1:A:431:LYS:O	1:A:435:HIS:HD2	1.91	0.53
1:B:1420:LEU:O	1:B:1423:PRO:HD2	2.09	0.52
1:B:1393:ARG:NH1	1:B:1393:ARG:CG	2.72	0.52
1:B:1410:GLU:H	1:B:1410:GLU:CD	2.14	0.51
1:A:236:LEU:O	1:A:236:LEU:HD22	2.11	0.51
1:B:1348:ARG:NH2	1:B:1427:SER:OG	2.42	0.51
1:B:1353:LEU:HD22	1:B:1428:ILE:HD12	1.93	0.51
1:B:1431:LYS:O	1:B:1435:HIS:HD2	1.94	0.51
1:A:284:LYS:HZ1	1:A:297:GLN:HE22	1.54	0.50
1:A:224:SER:HB3	1:A:229:ASP:OD2	2.12	0.50
1:A:320:VAL:HG11	1:A:325:LEU:HD21	1.93	0.50
1:B:1345:ILE:HD13	1:B:1431:LYS:HG2	1.94	0.50
1:B:1348:ARG:HG3	1:B:1352:GLU:OE2	2.12	0.50
1:A:420:LEU:O	1:A:423:PRO:HD2	2.12	0.49
1:A:353:LEU:HD22	1:A:428:ILE:HD12	1.93	0.49
1:B:1344:ALA:HB3	3:B:1819:HOH:O	2.12	0.49
1:A:242:VAL:HG13	1:A:278:THR:HB	1.93	0.48
1:A:393:ARG:HG2	1:A:393:ARG:NH1	2.28	0.48
1:B:1322:ASP:O	1:B:1334:ARG:HG2	2.13	0.48
1:B:1348:ARG:NH1	1:B:1352:GLU:OE2	2.41	0.48
1:B:1232:VAL:HG13	1:B:1365:THR:CG2	2.43	0.48
1:B:1333:HIS:CD2	1:B:1335:ASN:H	2.31	0.48
1:B:1414:ARG:NH1	1:B:1414:ARG:HG3	2.29	0.48
1:A:373:ILE:HG23	1:A:393:ARG:HD2	1.95	0.48
1:B:1333:HIS:HD2	1:B:1335:ASN:HB2	1.79	0.48
1:B:1414:ARG:HH11	1:B:1414:ARG:HG3	1.78	0.48
1:B:1273:ASP:OD2	1:B:1449:THR:HA	2.14	0.47
1:A:242:VAL:HG21	1:A:282:TRP:HB2	1.97	0.47
1:A:298:VAL:HG21	1:B:1440:LYS:HD3	1.96	0.47
1:A:293:PRO:O	1:A:296:ASP:N	2.45	0.47
1:B:1393:ARG:NH1	1:B:1393:ARG:HG2	2.28	0.47
1:A:385:ASN:HD22	1:A:385:ASN:C	2.17	0.47
1:A:273:ASP:OD2	1:A:449:THR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD13	1:A:374:VAL:HG11	1.96	0.46
1:A:413:GLY:O	1:A:417:LYS:HG3	2.14	0.46
1:B:1284:LYS:HZ3	1:B:1297:GLN:HE22	1.58	0.46
1:B:1421:ARG:HA	1:B:1421:ARG:HD3	1.63	0.45
1:A:313:PHE:C	1:A:313:PHE:CD1	2.89	0.45
1:B:1305:TRP:CG	1:B:1306:ASN:N	2.85	0.45
1:A:242:VAL:HG12	1:A:242:VAL:O	2.17	0.45
1:B:1348:ARG:HG2	1:B:1348:ARG:NH1	2.31	0.45
1:B:1411:GLN:C	1:B:1413:GLY:H	2.18	0.44
1:A:451:LEU:HA	1:A:451:LEU:HD23	1.72	0.44
1:A:320:VAL:O	1:A:358:ARG:NH1	2.50	0.44
1:A:421:ARG:HD3	1:A:421:ARG:HA	1.62	0.44
1:B:1411:GLN:O	1:B:1413:GLY:N	2.47	0.43
1:A:385:ASN:HD22	1:A:385:ASN:H	1.67	0.43
1:B:1348:ARG:CG	1:B:1352:GLU:OE2	2.67	0.43
1:B:1286:ILE:O	1:B:1287:PRO:C	2.57	0.43
1:A:326:LEU:HD22	2:A:500:9CR:H25	2.01	0.43
1:B:1424:ALA:O	1:B:1428:ILE:HG13	2.18	0.43
1:A:233:GLU:H	1:A:233:GLU:CD	2.23	0.43
1:B:1393:ARG:HH11	1:B:1393:ARG:HG2	1.78	0.42
1:B:1232:VAL:CG1	1:B:1365:THR:HG21	2.49	0.42
1:B:1242:VAL:HG13	1:B:1278:THR:CB	2.48	0.42
1:A:406:HIS:C	1:A:406:HIS:CD2	2.92	0.42
1:B:1231:PRO:O	1:B:1234:ARG:HB2	2.20	0.42
1:A:228:GLU:HA	1:A:228:GLU:OE2	2.19	0.42
1:B:1348:ARG:HH11	1:B:1348:ARG:CG	2.32	0.42
1:A:305:TRP:CG	1:A:306:ASN:N	2.88	0.41
1:A:308:LEU:HD13	1:A:374:VAL:HG12	2.03	0.41
1:A:348:ARG:HG3	1:A:352:GLU:OE2	2.20	0.41
1:A:348:ARG:NH1	1:A:348:ARG:HG2	2.35	0.41
1:B:1313:PHE:CD1	1:B:1313:PHE:C	2.94	0.41
1:B:1326:LEU:HD22	2:B:1500:9CR:H25	2.03	0.41
1:A:240:LEU:O	1:A:243:GLU:HG2	2.21	0.41
1:B:1363:ASP:OD2	1:B:1366:GLU:OE2	2.38	0.41
1:A:289:PHE:CZ	1:A:297:GLN:HB3	2.56	0.41
1:A:385:ASN:O	1:A:385:ASN:ND2	2.54	0.41
1:A:393:ARG:HH11	1:A:393:ARG:HG2	1.79	0.40
1:A:448:ASP:OD1	3:A:1638:HOH:O	2.22	0.40
1:A:421:ARG:CD	3:A:1727:HOH:O	2.57	0.40
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.81	0.40
1:B:1376:PHE:O	1:B:1378:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1433:LEU:HD22	1:B:1455:LEU:CD2	2.51	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	213/239 (89%)	207 (97%)	4 (2%)	2 (1%)	21	18
1	B	208/239 (87%)	190 (91%)	11 (5%)	7 (3%)	5	2
All	All	421/478 (88%)	397 (94%)	15 (4%)	9 (2%)	9	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1243	GLU
1	B	1448	ASP
1	A	448	ASP
1	B	1414	ARG
1	B	1360	MET
1	A	225	SER
1	B	1412	PRO
1	B	1232	VAL
1	B	1413	GLY

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/206 (90%)	166 (89%)	20 (11%)	8	6
1	B	182/206 (88%)	167 (92%)	15 (8%)	14	13
All	All	368/412 (89%)	333 (90%)	35 (10%)	11	8

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
1	A	273	ASP
1	A	276	LEU
1	A	291	GLU
1	A	308	LEU
1	A	313	PHE
1	A	322	ASP
1	A	348	ARG
1	A	353	LEU
1	A	383	LEU
1	A	385	ASN
1	A	393	ARG
1	A	406	HIS
1	A	410	GLU
1	A	421	ARG
1	A	426	ARG
1	A	444	ASP
1	A	445	THR
1	A	447	ILE
1	A	448	ASP
1	B	1234	ARG
1	B	1236	LEU
1	B	1273	ASP
1	B	1276	LEU
1	B	1308	LEU
1	B	1348	ARG
1	B	1353	LEU
1	B	1383	LEU
1	B	1384	SER
1	B	1393	ARG
1	B	1405	LYS
1	B	1410	GLU
1	B	1421	ARG
1	B	1426	ARG

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Mol	Chain	Res	Type
1	B	1445	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	333	HIS
1	A	385	ASN
1	A	406	HIS
1	A	411	GLN
1	A	435	HIS
1	B	1297	GLN
1	B	1333	HIS
1	B	1335	ASN
1	B	1385	ASN
1	B	1411	GLN
1	B	1435	HIS

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 carbohydrates 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	$\# Z > 2$
2	9CR	A	500	-	19,22,22	2.21	5 (26%)	26,30,30	2.27	7 (26%)
2	9CR	B	1500	-	19,22,22	2.35	6 (31%)	26,30,30	2.15	5 (19%)

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
2	9CR	A	500	-	-	0/13/32/32	0/1/1/1
2	9CR	B	1500	-	-	0/13/32/32	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1500	9CR	C8-C9	-2.23	1.41	1.45
2	A	500	9CR	C14-C13	-2.03	1.32	1.35
2	A	500	9CR	C4-C5	2.22	1.55	1.51
2	B	1500	9CR	C20-C13	2.40	1.55	1.50
2	B	1500	9CR	C18-C5	2.44	1.55	1.51
2	A	500	9CR	C12-C13	2.50	1.51	1.45
2	B	1500	9CR	C4-C5	2.80	1.56	1.51
2	B	1500	9CR	C5-C6	4.50	1.42	1.34
2	A	500	9CR	C5-C6	4.66	1.42	1.34
2	A	500	9CR	C1-C6	6.27	1.62	1.53
2	B	1500	9CR	C1-C6	6.73	1.63	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	9CR	C18-C5-C4	-3.72	106.27	113.47
2	B	1500	9CR	C18-C5-C4	-3.27	107.15	113.47
2	A	500	9CR	C3-C4-C5	2.11	117.36	113.87
2	A	500	9CR	C20-C13-C12	2.11	121.53	118.08
2	A	500	9CR	C11-C10-C9	3.01	131.59	127.22
2	B	1500	9CR	C11-C10-C9	3.30	132.03	127.22
2	A	500	9CR	C16-C1-C6	3.96	116.38	110.33
2	B	1500	9CR	C16-C1-C6	4.53	117.25	110.33
2	B	1500	9CR	C7-C8-C9	4.88	133.58	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	9CR	C7-C8-C9	5.51	134.53	126.21
2	B	1500	9CR	C18-C5-C6	6.02	131.03	124.62
2	A	500	9CR	C18-C5-C6	6.61	131.66	124.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	9CR	2	0
2	B	1500	9CR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.