Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 04:36 PM EST

PDB ID	:	2R40
Title	:	Crystal structure of 20E bound EcR/USP
Authors	:	Moras, D.; Billas, I.M.L.; Browning, C.
Deposited on	:	2007-08-30
Resolution	:	2.40 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	:	4.02b-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 2.40 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	Percentile Ranks	Value
Rfree		0.268
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		7.6%
RSRZ outliers		12.3%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
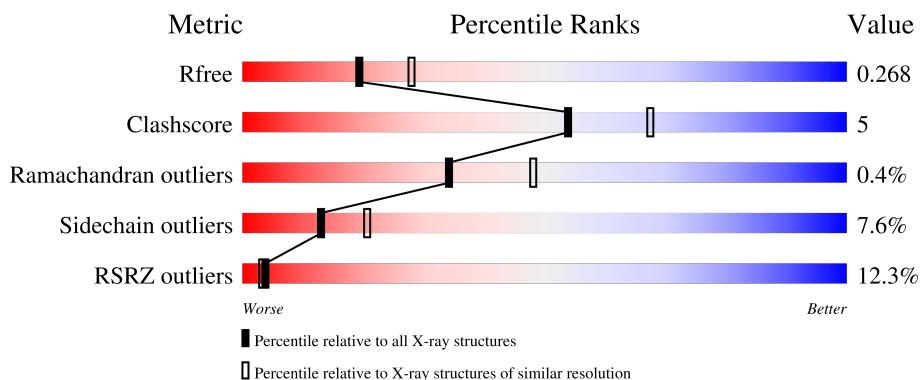
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	D	266	10% / 70% 15% · 12%
2	A	263	12% / 78% 11% · 10%
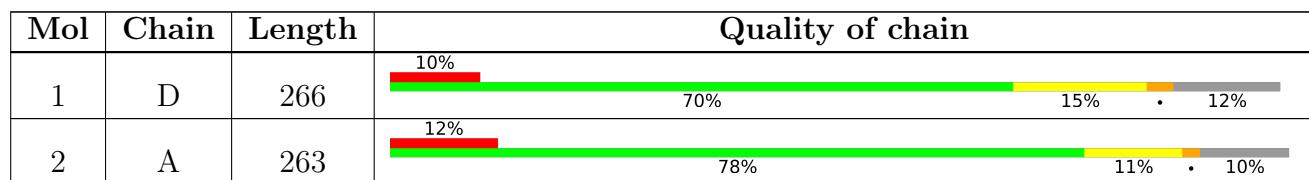
2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 3998 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 Ecdysone Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	233	1898	1212	322	346	18	0	2	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	267	GLY	-	expression tag	UNP O18473
D	268	SER	-	expression tag	UNP O18473
D	269	HIS	-	expression tag	UNP O18473
D	270	MET	-	expression tag	UNP O18473
D	271	ALA	-	expression tag	UNP O18473
D	272	SER	-	expression tag	UNP O18473
D	274	THR	-	expression tag	UNP O18473
D	275	GLY	-	expression tag	UNP O18473
D	276	GLY	-	expression tag	UNP O18473
D	277	GLN	-	expression tag	UNP O18473
D	279	MET	-	expression tag	UNP O18473
D	280	GLY	-	expression tag	UNP O18473
D	282	ASP	-	expression tag	UNP O18473
D	283	PRO	-	expression tag	UNP O18473
D	321	GLN	-	SEE REMARK 999	UNP O18473
D	322	THR	-	SEE REMARK 999	UNP O18473
D	323	TRP	-	SEE REMARK 999	UNP O18473
D	483	CYS	GLY	SEE REMARK 999	UNP O18473
D	489	LYS	GLU	SEE REMARK 999	UNP O18473

- Molecule 2 is a protein called Ultraspiracle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	238	1908	1222	332	342	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	MET	-	initiating methionine	UNP Q7SIF6

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).
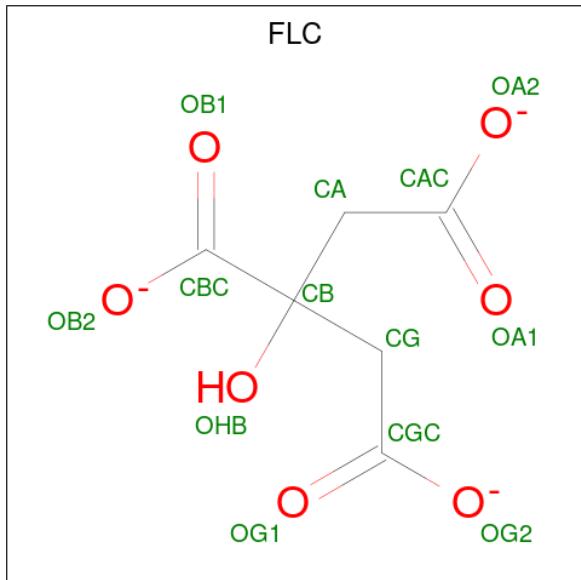
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 13	C 6	O 7	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
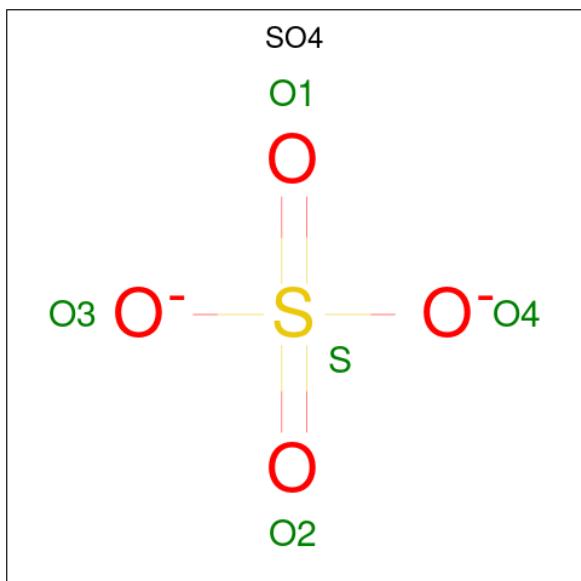
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 5	O 4	S 1	0	0

- Molecule 5 is (2beta,3beta,5beta,22R)-2,3,14,20,22,25-hexahydroxycholest-7-en-6-one (three-letter code: 20E) (formula: $C_{27}H_{44}O_7$).
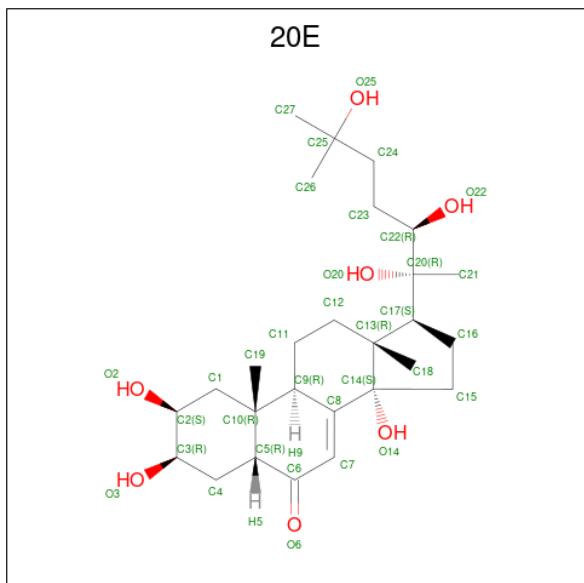

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 34	C 27	O 7	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
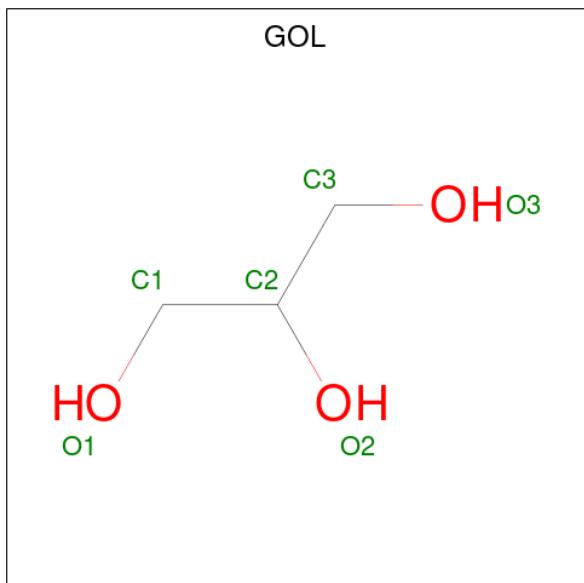
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).
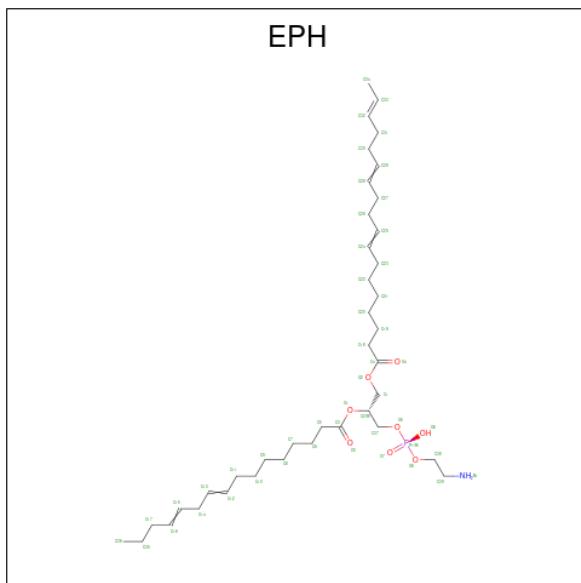
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	46	Total	O	0	0
			46	46		
8	A	39	Total	O	0	0
			39	39		

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: Ecdysone Receptor
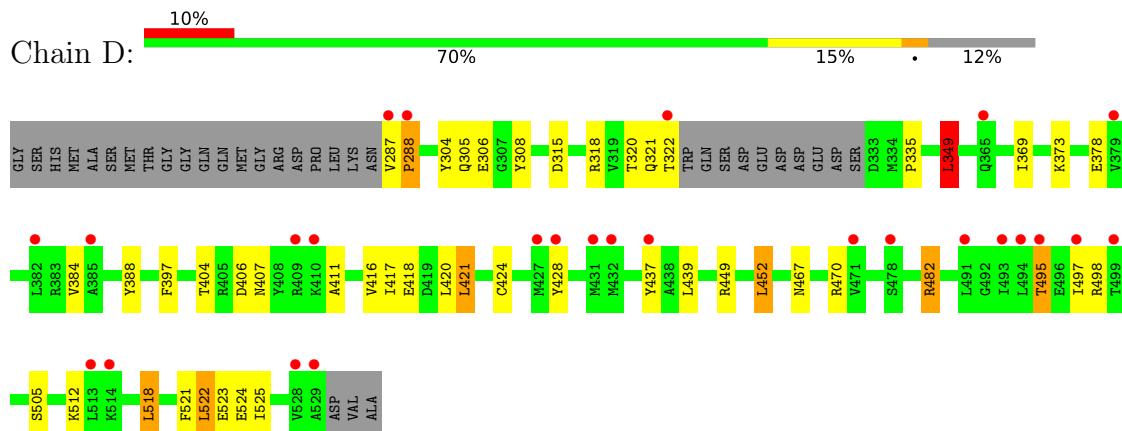
• Molecule 2: Ultraspiracle
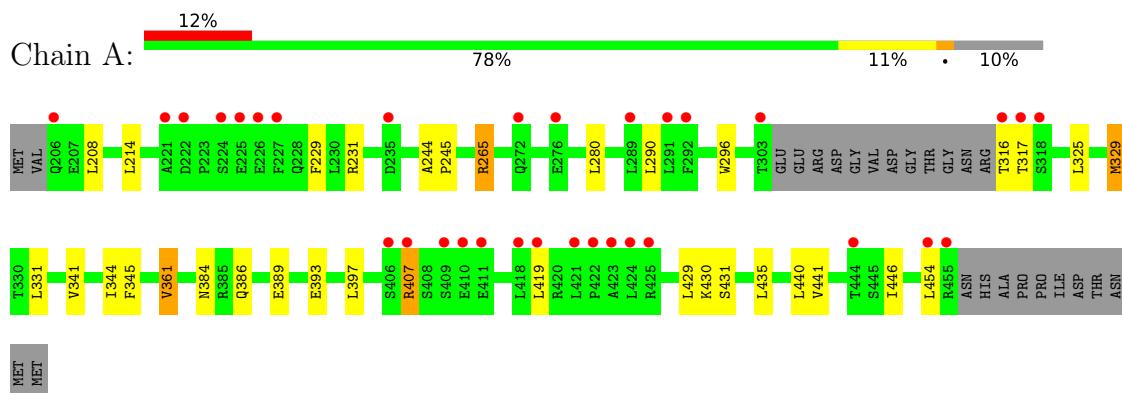
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	58.00Å 58.00Å 303.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.73 – 2.40 32.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.73-2.40) 99.2 (32.83-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.282 0.216 , 0.268	Depositor DCC
R_{free} test set	2391 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3998	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 20E, SO4, GOL, EPH, FLC

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	D	0.51	0/1931	0.66	3/2611 (0.1%)
2	A	0.47	0/1943	0.63	1/2622 (0.0%)
All	All	0.49	0/3874	0.65	4/5233 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	498	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	349	LEU	CA-CB-CG	6.27	129.72	115.30
2	A	290	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	498	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	D	1898	0	1935	24	0
2	A	1908	0	1957	18	0
3	D	13	0	5	0	0
4	D	5	0	0	0	0
5	D	34	0	44	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	6	0	8	0	0
7	A	49	0	67	3	0
8	A	39	0	0	0	0
8	D	46	0	0	2	0
All	All	3998	0	4016	42	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 5.

All (42) 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:A:407:ARG:HG2	2:A:407:ARG:HH11	1.23	1.02
1:D:404:THR:H	1:D:407:ASN:HD22	1.10	0.99
1:D:495:THR:HG21	8:D:9526:HOH:O	1.78	0.82
1:D:404:THR:H	1:D:407:ASN:ND2	1.82	0.77
2:A:407:ARG:HH11	2:A:407:ARG:CG	1.97	0.76
1:D:305:GLN:OE1	1:D:437:TYR:CD2	2.39	0.75
2:A:341:VAL:HG11	7:A:600:EPH:H101	1.74	0.68
1:D:404:THR:N	1:D:407:ASN:HD22	1.90	0.66
1:D:308:TYR:O	1:D:349:LEU:HG	1.95	0.66
2:A:344:ILE:HD12	2:A:430:LYS:HB3	1.78	0.65
1:D:418:GLU:HB2	8:D:9546:HOH:O	1.95	0.65
1:D:518:LEU:HD12	1:D:523:GLU:HG3	1.79	0.65
2:A:386:GLN:HE22	2:A:389:GLU:CD	2.00	0.65
1:D:335:PRO:HB2	1:D:411:ALA:HB2	1.80	0.64
2:A:244:ALA:HB3	2:A:245:PRO:HD3	1.79	0.63
1:D:320:THR:O	1:D:322:THR:N	2.31	0.62
2:A:431:SER:HB2	7:A:600:EPH:H141	1.82	0.62
2:A:389:GLU:O	2:A:393:GLU:HG3	2.00	0.62
2:A:407:ARG:HG2	2:A:407:ARG:NH1	2.03	0.61
1:D:482:ARG:HB3	1:D:482:ARG:HH11	1.67	0.59
1:D:384:VAL:HG11	1:D:420:LEU:HD11	1.86	0.56
2:A:435:LEU:HB3	2:A:441:VAL:HG23	1.89	0.54
2:A:296:TRP:HZ3	2:A:361:VAL:HG22	1.73	0.53
2:A:435:LEU:HB3	2:A:441:VAL:CG2	2.39	0.53
1:D:304:TYR:CD2	1:D:308:TYR:HE2	2.28	0.51
2:A:345:PHE:HB2	7:A:600:EPH:H361	1.95	0.49
1:D:315:ASP:OD1	1:D:318:ARG:NH2	2.44	0.48
1:D:521:PHE:HD2	1:D:522:LEU:HD13	1.80	0.46
1:D:373:LYS:HG2	1:D:525:ILE:HG13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ILE:HG13	1:D:421:LEU:HD22	1.98	0.46
2:A:296:TRP:HZ3	2:A:361:VAL:CG2	2.30	0.45
2:A:229:PHE:CD2	2:A:446:ILE:HG12	2.52	0.45
1:D:378:GLU:HB3	1:D:497:ILE:HD12	1.98	0.45
2:A:407:ARG:CG	2:A:407:ARG:NH1	2.66	0.44
1:D:304:TYR:HD2	1:D:308:TYR:HE2	1.64	0.44
2:A:265:ARG:HB2	2:A:454:LEU:CD2	2.48	0.44
1:D:397:PHE:CZ	5:D:9001:20E:H152	2.52	0.44
1:D:449:ARG:H	1:D:452:LEU:HD22	1.83	0.43
1:D:467:ASN:OD1	1:D:470:ARG:NH1	2.49	0.42
1:D:287:VAL:HA	1:D:288:PRO:HD2	1.81	0.41
2:A:325:LEU:HD22	2:A:329:MET:CE	2.51	0.40
1:D:388:TYR:CG	1:D:424:CYS:HB3	2.56	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	D	232/266 (87%)	226 (97%)	4 (2%)	2 (1%)	17	25
2	A	234/263 (89%)	227 (97%)	7 (3%)	0	100	100
All	All	466/529 (88%)	453 (97%)	11 (2%)	2 (0%)	34	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	321	GLN
1	D	288	PRO

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	D	211/235 (90%)	195 (92%)	16 (8%)	13	20
2	A	211/232 (91%)	195 (92%)	16 (8%)	13	20
All	All	422/467 (90%)	390 (92%)	32 (8%)	13	20

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	306	GLU
1	D	349	LEU
1	D	369	ILE
1	D	406	ASP
1	D	416	VAL
1	D	421	LEU
1	D	428	TYR
1	D	439	LEU
1	D	452	LEU
1	D	482	ARG
1	D	495	THR
1	D	505	SER
1	D	512	LYS
1	D	518	LEU
1	D	522	LEU
1	D	524	GLU
2	A	208	LEU
2	A	214	LEU
2	A	231	ARG
2	A	265	ARG
2	A	280	LEU
2	A	316	THR
2	A	317	THR
2	A	329	MET
2	A	331	LEU
2	A	361	VAL
2	A	384	ASN

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
2	A	397	LEU
2	A	407	ARG
2	A	419	LEU
2	A	429	LEU
2	A	440	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	310	GLN
1	D	407	ASN
1	D	515	ASN
2	A	287	ASN
2	A	334	ASN
2	A	363	GLN
2	A	384	ASN
2	A	386	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	$\#\|Z\| > 2$
7	EPH	A	600	-	48,48,48	1.32	5 (10%)	51,53,53	1.13	2 (3%)
4	SO4	D	1327	-	4,4,4	0.14	0	6,6,6	0.09	0
6	GOL	D	9500	-	5,5,5	0.37	0	5,5,5	0.42	0
5	20E	D	9001	-	37,37,37	1.65	9 (24%)	61,63,63	1.26	7 (11%)
3	FLC	D	9400	-	12,12,12	0.96	0	17,17,17	1.45	2 (11%)

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	20E	D	9001	-	-	0/18/88/88	0/4/4/4
7	EPH	A	600	-	-	19/52/52/52	-
3	FLC	D	9400	-	-	6/16/16/16	-
6	GOL	D	9500	-	-	4/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	9001	20E	C7-C8	4.80	1.40	1.34
7	A	600	EPH	C13-C12	3.82	1.53	1.31
7	A	600	EPH	C25-C24	3.74	1.53	1.31
7	A	600	EPH	C29-C28	3.69	1.53	1.31
7	A	600	EPH	C16-C15	3.66	1.53	1.31
7	A	600	EPH	C32-C33	3.17	1.53	1.29
5	D	9001	20E	C23-C22	2.97	1.56	1.52
5	D	9001	20E	C20-C17	2.95	1.60	1.55
5	D	9001	20E	C11-C9	2.53	1.58	1.53
5	D	9001	20E	C7-C6	-2.51	1.41	1.46
5	D	9001	20E	C20-C22	2.48	1.59	1.55
5	D	9001	20E	C14-C8	2.46	1.56	1.52
5	D	9001	20E	O22-C22	2.34	1.47	1.43
5	D	9001	20E	C9-C8	2.01	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	9400	FLC	OB2-CBC-CB	3.99	119.98	113.05
7	A	600	EPH	O1-C3-C5	3.58	119.21	111.50
5	D	9001	20E	C18-C13-C14	3.45	113.25	109.14
5	D	9001	20E	C4-C5-C6	-3.01	103.86	109.55
3	D	9400	FLC	OB1-CBC-CB	-2.75	118.36	122.25
5	D	9001	20E	C1-C10-C5	2.69	111.36	107.06
5	D	9001	20E	C14-C8-C9	2.69	118.03	114.42
7	A	600	EPH	C31-C32-C33	-2.53	110.99	131.07
5	D	9001	20E	C5-C6-C7	2.48	120.90	116.71
5	D	9001	20E	O6-C6-C5	-2.35	118.60	121.78
5	D	9001	20E	C4-C3-C2	2.10	112.88	110.27

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	9400	FLC	CA-CB-CG-CGC
3	D	9400	FLC	CBC-CB-CG-CGC
3	D	9400	FLC	OHB-CB-CG-CGC
7	A	600	EPH	C29-C30-C31-C32
7	A	600	EPH	C31-C32-C33-C34
7	A	600	EPH	C12-C13-C14-C15
7	A	600	EPH	C14-C15-C16-C17
7	A	600	EPH	C27-C28-C29-C30
6	D	9500	GOL	C1-C2-C3-O3
7	A	600	EPH	C5-C6-C7-C8
7	A	600	EPH	C20-C21-C22-C23
7	A	600	EPH	C9-C10-C11-C12
7	A	600	EPH	O2-C1-C2-C37
7	A	600	EPH	C18-C4-O2-C1
7	A	600	EPH	C23-C24-C25-C26
6	D	9500	GOL	O2-C2-C3-O3
3	D	9400	FLC	CAC-CA-CB-CBC
7	A	600	EPH	C25-C26-C27-C28
7	A	600	EPH	O4-C4-O2-C1
7	A	600	EPH	O2-C1-C2-O1
6	D	9500	GOL	O1-C1-C2-O2
7	A	600	EPH	C38-O8-P1-O5
3	D	9400	FLC	CAC-CA-CB-CG
7	A	600	EPH	C21-C22-C23-C24
7	A	600	EPH	C26-C27-C28-C29
3	D	9400	FLC	CG-CB-CBC-OB2
7	A	600	EPH	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	9500	GOL	O1-C1-C2-C3
7	A	600	EPH	C38-O8-P1-O7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	600	EPH	3	0
5	D	9001	20E	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand EPH A 600

Bond lengths   Bond angles

Torsions   Rings

Full wwPDB X-ray Structure Validation Report

Ligand 20E D 9001

Bond lengths

Bond angles

Torsions

Rings
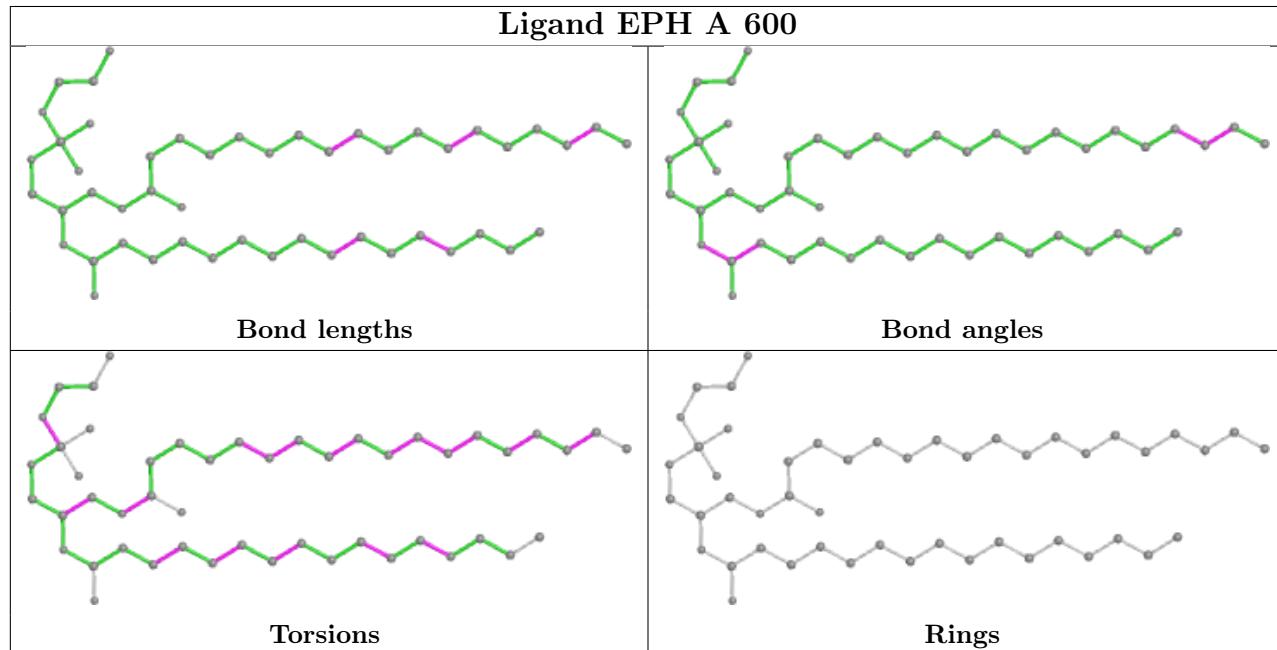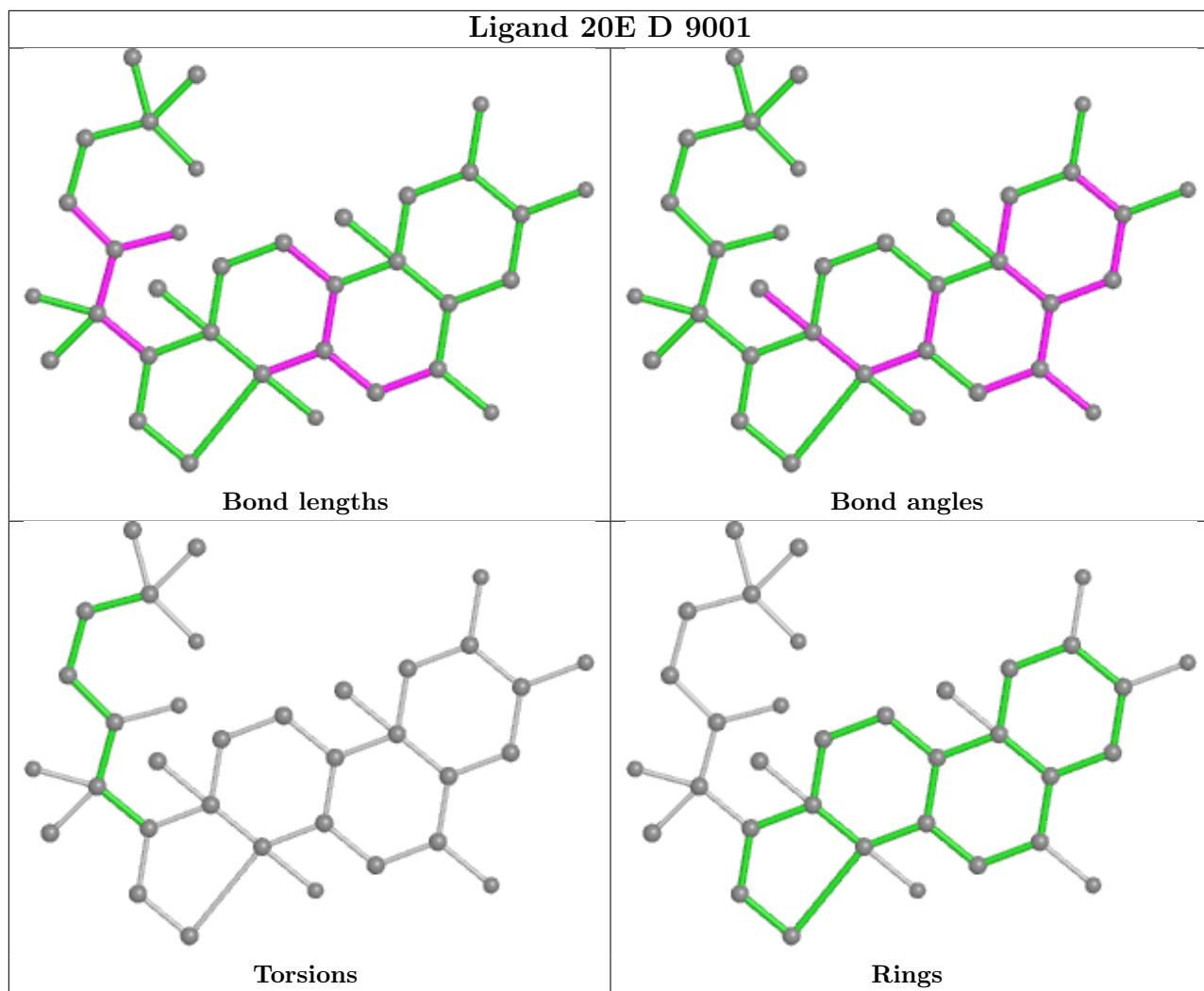
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	D	233/266 (87%)	0.68	26 (11%)	5	4	38, 49, 62, 72	0
2	A	238/263 (90%)	0.68	32 (13%)	3	2	44, 54, 67, 80	0
All	All	471/529 (89%)	0.68	58 (12%)	4	3	38, 52, 65, 80	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	317	THR	10.0
1	D	432[A]	MET	9.0
2	A	318	SER	6.7
2	A	226	GLU	6.6
1	D	431	MET	6.4
1	D	528	VAL	5.1
2	A	316	THR	4.8
1	D	529	ALA	4.7
1	D	494	LEU	4.2
2	A	272	GLN	4.1
2	A	303	THR	4.1
2	A	454	LEU	3.8
2	A	409	SER	3.5
1	D	428	TYR	3.4
1	D	495	THR	3.4
1	D	379	VAL	3.3
1	D	493	ILE	3.1
2	A	224	SER	3.1
1	D	497	ILE	3.0
1	D	409	ARG	3.0
2	A	422	PRO	2.9
2	A	206	GLN	2.9
2	A	225	GLU	2.8
2	A	411	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	276	GLU	2.7
2	A	421	LEU	2.7
1	D	288	PRO	2.6
2	A	222	ASP	2.6
2	A	410	GLU	2.6
2	A	419	LEU	2.6
2	A	424	LEU	2.6
1	D	514	LYS	2.6
2	A	289	LEU	2.6
2	A	406	SER	2.6
2	A	227	PHE	2.5
2	A	235	ASP	2.5
1	D	365	GLN	2.4
1	D	513	LEU	2.4
1	D	287	VAL	2.4
1	D	410	LYS	2.4
1	D	322	THR	2.4
2	A	291	LEU	2.3
1	D	491	LEU	2.3
1	D	499	THR	2.3
1	D	437	TYR	2.3
1	D	385	ALA	2.2
2	A	425	ARG	2.2
1	D	427	MET	2.2
2	A	455	ARG	2.2
2	A	221	ALA	2.2
2	A	292	PHE	2.2
2	A	407	ARG	2.2
1	D	478	SER	2.2
2	A	444	THR	2.2
1	D	471	VAL	2.1
1	D	382	LEU	2.1
2	A	418	LEU	2.1
2	A	423	ALA	2.0

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

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, 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($Å^2$)	Q<0.9
6	GOL	D	9500	6/6	0.79	0.14	74,75,75,75	0
7	EPH	A	600	49/49	0.85	0.27	63,70,79,82	0
3	FLC	D	9400	13/13	0.87	0.16	92,93,93,94	0
4	SO4	D	1327	5/5	0.90	0.31	92,92,92,93	0
5	20E	D	9001	34/34	0.95	0.11	24,34,36,37	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 EPH A 600:

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

Electron density around 20E D 9001:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.