Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:16 pm BST

PDB ID	:	1FEM
Title	:	CRYSTALLOGRAPHIC STUDIES ON COMPLEXES BETWEEN RETINOIDS AND PLASMA RETINOL-BINDING PROTEIN
Authors	:	Zanotti, G.; Marcello, M.; Malpeli, G.; Sartori, G.; Berni, R.
Deposited on	:	1994-08-29
Resolution	:	1.90 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 following versions of software and data (see references ①) were used in the production of this report:

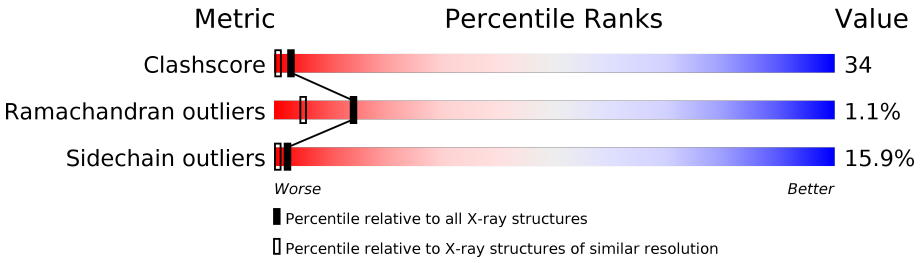
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	183	38% 40% 16%

2 Entry composition

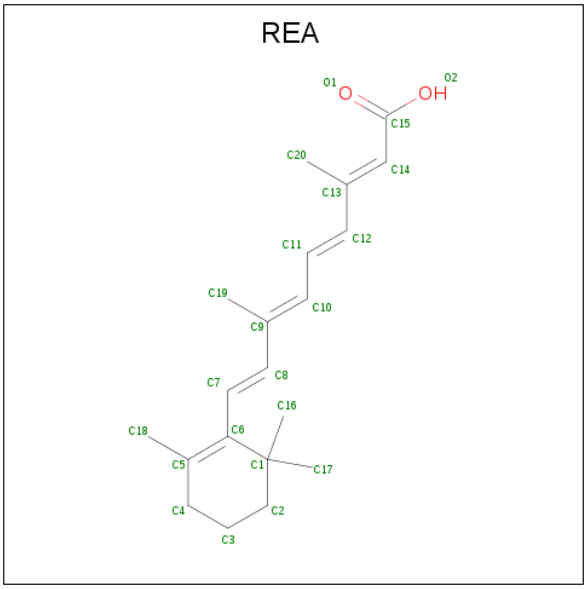
There are 3 unique types of molecules in this entry. The entry contains 1609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINOL BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1423	895	248	270	10	0	0	1

- Molecule 2 is RETINOIC ACID (three-letter code: REA) (formula: $C_{20}H_{28}O_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
3	A	164	164	164		0	0

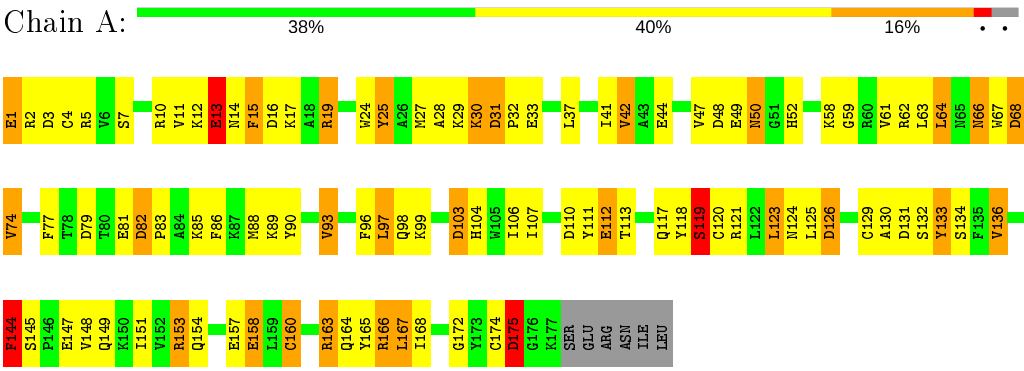
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: RETINOL BINDING PROTEIN

Chain A:



4 Data and refinement statistics (i)

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	46.21Å 48.81Å 75.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1609	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: REA

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	0.85	9/1456 (0.6%)	1.64	38/1966 (1.9%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CD-OE2	7.21	1.33	1.25
1	A	1	GLU	CD-OE2	6.40	1.32	1.25
1	A	158	GLU	CD-OE1	5.72	1.31	1.25
1	A	112	GLU	CD-OE1	5.63	1.31	1.25
1	A	33	GLU	CD-OE2	5.51	1.31	1.25
1	A	49	GLU	CD-OE1	5.42	1.31	1.25
1	A	157	GLU	CD-OE1	5.41	1.31	1.25
1	A	13	GLU	CD-OE2	5.35	1.31	1.25
1	A	44	GLU	CD-OE2	5.02	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	TRP	CB-CA-C	-9.27	91.87	110.40
1	A	67	TRP	N-CA-CB	8.63	126.14	110.60
1	A	110	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	A	67	TRP	CA-CB-CG	7.79	128.50	113.70
1	A	16	ASP	CB-CG-OD2	7.65	125.19	118.30
1	A	110	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	133	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	A	16	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	A	25	TYR	CB-CG-CD1	-6.83	116.90	121.00
1	A	79	ASP	CB-CG-OD1	-6.76	112.21	118.30
1	A	153	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	31	ASP	CB-CG-OD2	-6.70	112.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	SER	N-CA-CB	6.37	120.05	110.50
1	A	131	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	133	TYR	N-CA-CB	6.24	121.83	110.60
1	A	131	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	A	166	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	82	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	31	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	25	TYR	CB-CG-CD2	6.01	124.61	121.00
1	A	82	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	79	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	103	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	15	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	68	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	A	165	TYR	CB-CA-C	-5.82	98.75	110.40
1	A	144	PHE	CB-CA-C	-5.78	98.84	110.40
1	A	3	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	48	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	A	5	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	103	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	72	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	140	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	86	PHE	CB-CA-C	-5.17	100.06	110.40
1	A	68	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	175	ASP	N-CA-CB	5.08	119.74	110.60
1	A	72	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	126	ASP	CB-CG-OD2	-5.03	113.77	118.30

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	A	1423	0	1346	95	0
2	A	22	0	27	8	0
3	A	164	0	0	26	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1609	0	1373	97	2

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 34.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:HH22	1:A:112:GLU:HG2	1.44	0.82
1:A:37:LEU:HD22	1:A:59:GLY:HA3	1.61	0.82
1:A:50:ASN:HB3	1:A:52:HIS:ND1	1.96	0.81
1:A:103:ASP:O	1:A:119:SER:HB3	1.84	0.78
1:A:129:CYS:SG	1:A:132:SER:HB3	2.24	0.78
1:A:154:GLN:O	1:A:158:GLU:HG3	1.84	0.77
1:A:98:GLN:CB	2:A:184:REA:H202	2.18	0.72
1:A:4:CYS:SG	1:A:160:CYS:HB2	2.31	0.70
1:A:98:GLN:HB3	2:A:184:REA:H202	1.72	0.70
1:A:41:ILE:HD12	1:A:168:ILE:HD13	1.74	0.67
1:A:62:ARG:HG2	1:A:68:ASP:OD1	1.95	0.67
1:A:2:ARG:HB3	3:A:197:HOH:O	1.94	0.66
1:A:12:LYS:HA	3:A:264:HOH:O	1.97	0.65
1:A:158:GLU:OE2	3:A:261:HOH:O	2.15	0.64
1:A:29:LYS:NZ	1:A:31:ASP:OD1	2.31	0.63
1:A:47:VAL:HG12	3:A:215:HOH:O	1.98	0.63
1:A:58:LYS:HE3	3:A:236:HOH:O	1.98	0.63
1:A:144:PHE:HB3	1:A:148:VAL:HG11	1.82	0.62
1:A:30:LYS:NZ	3:A:331:HOH:O	2.30	0.62
1:A:120:CYS:SG	1:A:123:LEU:HD12	2.40	0.62
1:A:30:LYS:C	1:A:30:LYS:HD2	2.21	0.61
1:A:99:LYS:HD3	3:A:336:HOH:O	2.01	0.61
1:A:19:ARG:NH2	3:A:341:HOH:O	2.29	0.59
1:A:89:LYS:NZ	3:A:192:HOH:O	2.29	0.59
1:A:144:PHE:HB3	1:A:148:VAL:CG1	2.33	0.58
1:A:145:SER:OG	1:A:148:VAL:HG12	2.05	0.57
1:A:120:CYS:SG	1:A:129:CYS:HB2	2.44	0.57
1:A:172:GLY:O	1:A:175:ASP:HA	2.06	0.56
1:A:11:VAL:HG13	3:A:300:HOH:O	2.06	0.55
1:A:50:ASN:CB	1:A:52:HIS:ND1	2.64	0.55
2:A:184:REA:O2	2:A:184:REA:H201	2.07	0.55
1:A:50:ASN:HB2	3:A:233:HOH:O	2.06	0.55
1:A:124:ASN:HB3	3:A:251:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG22	3:A:300:HOH:O	2.06	0.54
1:A:83:PRO:HD3	3:A:207:HOH:O	2.08	0.53
1:A:117:GLN:HG2	1:A:118:TYR:H	1.75	0.52
1:A:37:LEU:CD2	1:A:59:GLY:HA3	2.36	0.52
1:A:126:ASP:HB3	3:A:302:HOH:O	2.10	0.52
1:A:153:ARG:HG3	3:A:258:HOH:O	2.10	0.51
1:A:144:PHE:CB	1:A:148:VAL:HG13	2.42	0.50
1:A:164:GLN:HB2	3:A:281:HOH:O	2.11	0.49
1:A:70:CYS:SG	1:A:174:CYS:HA	2.53	0.49
1:A:151:ILE:O	1:A:154:GLN:HB3	2.13	0.49
1:A:98:GLN:HB2	2:A:184:REA:C20	2.42	0.49
1:A:77:PHE:HZ	2:A:184:REA:H32	1.78	0.48
1:A:28:ALA:HA	1:A:166:ARG:O	2.14	0.48
1:A:2:ARG:HD3	3:A:197:HOH:O	2.14	0.48
1:A:98:GLN:CB	2:A:184:REA:C20	2.91	0.48
1:A:145:SER:O	1:A:149:GLN:HG3	2.13	0.48
1:A:19:ARG:NH2	1:A:112:GLU:HG2	2.22	0.47
1:A:144:PHE:HB2	1:A:148:VAL:HG13	1.95	0.47
1:A:164:GLN:O	1:A:164:GLN:HG3	2.15	0.47
1:A:25:TYR:CD2	1:A:42:VAL:HG12	2.50	0.47
1:A:13:GLU:O	1:A:14:ASN:HB2	2.14	0.47
1:A:63:LEU:O	1:A:66:ASN:N	2.48	0.47
1:A:139:ARG:HG2	3:A:249:HOH:O	2.15	0.46
1:A:117:GLN:HG2	1:A:118:TYR:N	2.30	0.46
1:A:96:PHE:CE1	1:A:97:LEU:CD1	2.98	0.46
1:A:25:TYR:CD2	1:A:42:VAL:CG1	2.99	0.45
1:A:104:HIS:CE1	1:A:117:GLN:HG3	2.52	0.44
1:A:13:GLU:HA	3:A:317:HOH:O	2.17	0.44
1:A:124:ASN:OD1	1:A:130:ALA:HB2	2.18	0.44
1:A:61:VAL:HG21	2:A:184:REA:C14	2.47	0.44
1:A:19:ARG:NH2	1:A:111:TYR:HB3	2.33	0.44
2:A:184:REA:C20	2:A:184:REA:O2	2.65	0.44
1:A:1:GLU:OE1	1:A:2:ARG:HG2	2.16	0.44
1:A:83:PRO:HG2	3:A:303:HOH:O	2.17	0.44
1:A:72:ASP:O	1:A:93:VAL:HG13	2.18	0.43
1:A:117:GLN:CG	1:A:118:TYR:N	2.81	0.43
1:A:120:CYS:SG	1:A:123:LEU:CD1	3.06	0.43
1:A:172:GLY:O	1:A:175:ASP:N	2.49	0.43
1:A:74:VAL:O	1:A:90:TYR:HA	2.19	0.43
1:A:82:ASP:HB3	1:A:85:LYS:HB2	2.00	0.43
1:A:77:PHE:CD2	1:A:88:MET:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:CYS:SG	1:A:129:CYS:CB	3.06	0.43
1:A:149:GLN:HB3	3:A:258:HOH:O	2.17	0.43
1:A:113:THR:HG21	3:A:265:HOH:O	2.19	0.43
1:A:64:LEU:HD22	1:A:64:LEU:HA	1.73	0.43
1:A:32:PRO:HG3	1:A:133:TYR:CD2	2.53	0.43
1:A:41:ILE:HA	1:A:58:LYS:O	2.19	0.42
1:A:19:ARG:NH2	1:A:111:TYR:CB	2.82	0.42
1:A:64:LEU:C	1:A:66:ASN:H	2.23	0.42
1:A:29:LYS:HD2	1:A:31:ASP:OD1	2.19	0.42
1:A:136:VAL:HG12	1:A:136:VAL:O	2.20	0.42
1:A:140:ASP:OD1	1:A:142:SER:OG	2.29	0.42
1:A:63:LEU:HD21	3:A:338:HOH:O	2.20	0.42
1:A:160:CYS:O	1:A:160:CYS:SG	2.78	0.42
1:A:29:LYS:HZ2	1:A:31:ASP:CG	2.23	0.42
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.67	0.41
1:A:163:ARG:HB3	1:A:163:ARG:HE	1.46	0.41
1:A:144:PHE:CB	1:A:148:VAL:CG1	2.97	0.41
1:A:24:TRP:CH2	1:A:139:ARG:HD2	2.56	0.41
1:A:77:PHE:CZ	1:A:88:MET:SD	3.13	0.41
1:A:164:GLN:NE2	3:A:221:HOH:O	2.33	0.40
1:A:15:PHE:CZ	1:A:106:ILE:HG13	2.56	0.40
1:A:17:LYS:HE3	3:A:342:HOH:O	2.21	0.40
1:A:11:VAL:HG12	1:A:107:ILE:HD13	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:188:HOH:O	3:A:328:HOH:O[4_466]	2.16	0.04
3:A:264:HOH:O	3:A:328:HOH:O[4_466]	2.18	0.02

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	174/183 (95%)	158 (91%)	14 (8%)	2 (1%)	14 5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	A	13	GLU

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	151/158 (96%)	127 (84%)	24 (16%)	2 1

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	10	ARG
1	A	19	ARG
1	A	27	MET
1	A	30	LYS
1	A	42	VAL
1	A	50	ASN
1	A	64	LEU
1	A	66	ASN
1	A	74	VAL
1	A	81	GLU
1	A	93	VAL
1	A	97	LEU
1	A	119	SER
1	A	121	ARG
1	A	123	LEU
1	A	125	LEU
1	A	134	SER

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Mol	Chain	Res	Type
1	A	136	VAL
1	A	139	ARG
1	A	144	PHE
1	A	160	CYS
1	A	163	ARG
1	A	167	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	156	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 carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	REA	A	184	-	19,22,22	2.28	4 (21%)	26,30,30	5.30	17 (65%)

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	REA	A	184	-	-	0/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	184	REA	C14-C13	8.31	1.44	1.35
2	A	184	REA	C1-C6	-2.65	1.50	1.53
2	A	184	REA	C5-C6	2.40	1.38	1.34
2	A	184	REA	C20-C13	2.26	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	184	REA	C11-C10-C9	-11.84	110.42	127.31
2	A	184	REA	C16-C1-C2	-9.31	71.68	108.91
2	A	184	REA	C17-C1-C6	8.21	123.62	110.30
2	A	184	REA	C20-C13-C14	7.87	141.12	124.64
2	A	184	REA	C10-C11-C12	-6.71	102.27	123.22
2	A	184	REA	C7-C8-C9	-6.59	116.27	126.23
2	A	184	REA	C19-C9-C10	6.20	131.61	122.92
2	A	184	REA	C16-C1-C6	6.03	120.07	110.30
2	A	184	REA	C11-C12-C13	-5.80	110.11	126.42
2	A	184	REA	C18-C5-C6	5.79	131.03	124.53
2	A	184	REA	C12-C13-C14	-5.77	103.72	119.11
2	A	184	REA	C8-C9-C10	-5.46	110.56	118.94
2	A	184	REA	C8-C7-C6	-4.72	113.94	127.20
2	A	184	REA	C4-C5-C6	-3.59	117.53	122.73
2	A	184	REA	C1-C6-C7	3.35	125.25	115.78
2	A	184	REA	C1-C6-C5	-3.21	118.09	122.61
2	A	184	REA	C18-C5-C4	-3.04	107.78	113.62

There are no chirality outliers.

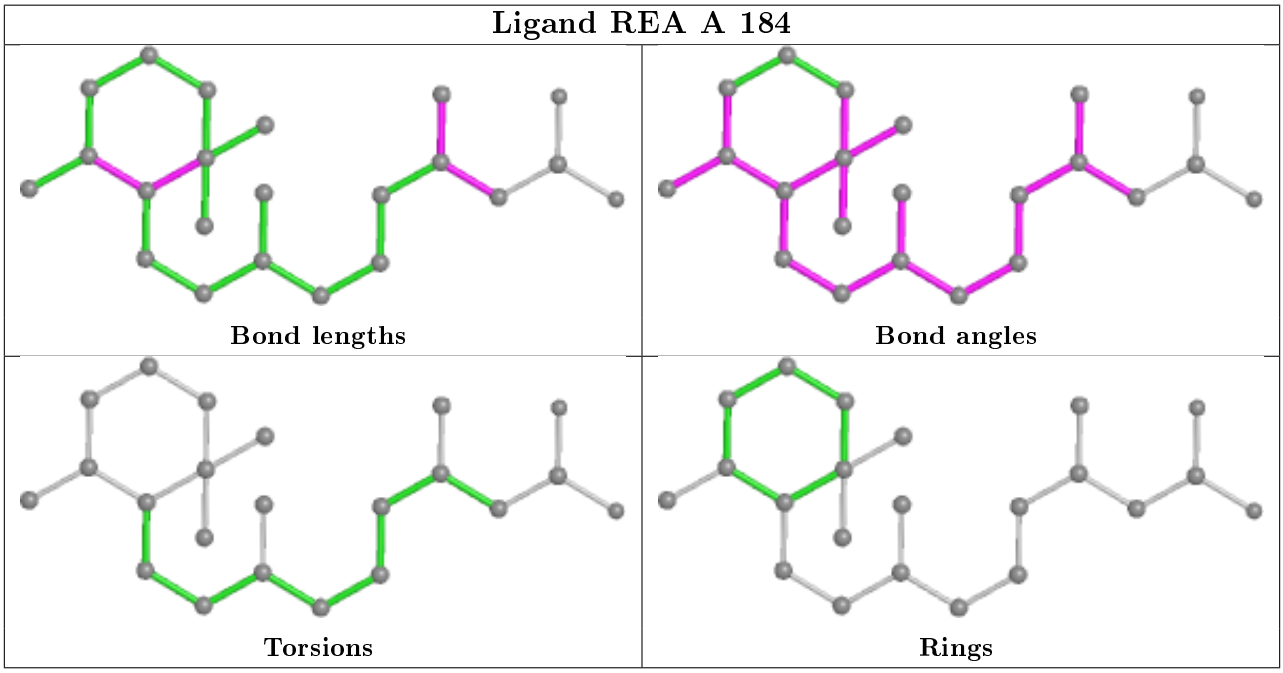
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	184	REA	8	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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	176:GLY	C	177:LYS	N	3.54

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.