wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:00 PM GMT

PDB ID	:	1RLB
Title	:	RETINOL BINDING PROTEIN COMPLEXED WITH TRANSTHYRETIN
Authors	:	Monaco, H.L.; Rizzi, M.; Coda, A.
Deposited on	:	1995-02-20
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

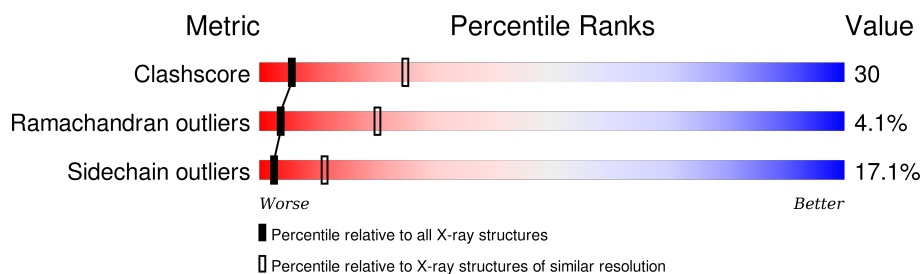|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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	Percentile Ranks	Value
Clashscore		30
Ramachandran outliers		4.1%
Sidechain outliers		17.1%

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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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 <=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	127	52% 30% 13% · ·
1	B	127	43% 41% 9% · 6%
1	C	127	45% 31% 19% · ·
1	D	127	29% 50% 9% 6% 6%
2	E	174	44% 40% 11% 5%
2	F	174	46% 40% 11% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	REA	E	176	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6624 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 TRANSTHYRETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	27	0	0
			950	604	157	187	2			
1	B	120	Total	C	N	O	S	0	0	0
			930	593	154	181	2			
1	C	123	Total	C	N	O	S	0	0	0
			950	604	157	187	2			
1	D	120	Total	C	N	O	S	0	0	0
			930	593	154	181	2			

- Molecule 2 is a protein called RETINOL BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	174	Total	C	N	O	S	68	0	0
			1411	889	246	266	10			
2	F	174	Total	C	N	O	S	116	0	0
			1411	889	246	266	10			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	21	ALA	SER	CONFLICT	UNP P02753
E	50	ASN	THR	CONFLICT	UNP P02753
E	52	HIS	GLN	CONFLICT	UNP P02753
E	107	ILE	VAL	CONFLICT	UNP P02753
E	112	GLU	ASP	CONFLICT	UNP P02753
E	114	PHE	TYR	CONFLICT	UNP P02753
E	138	ALA	SER	CONFLICT	UNP P02753
E	142	SER	ASN	CONFLICT	UNP P02753
E	144	PHE	LEU	CONFLICT	UNP P02753
E	145	SER	PRO	CONFLICT	UNP P02753
E	147	GLN	GLU	CONFLICT	UNP P02753
E	148	VAL	ALA	CONFLICT	UNP P02753

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Chain	Residue	Modelled	Actual	Comment	Reference
E	169	PRO	VAL	CONFLICT	UNP P02753
F	21	ALA	SER	CONFLICT	UNP P02753
F	50	ASN	THR	CONFLICT	UNP P02753
F	52	HIS	GLN	CONFLICT	UNP P02753
F	107	ILE	VAL	CONFLICT	UNP P02753
F	112	GLU	ASP	CONFLICT	UNP P02753
F	114	PHE	TYR	CONFLICT	UNP P02753
F	138	ALA	SER	CONFLICT	UNP P02753
F	142	SER	ASN	CONFLICT	UNP P02753
F	144	PHE	LEU	CONFLICT	UNP P02753
F	145	SER	PRO	CONFLICT	UNP P02753
F	147	GLN	GLU	CONFLICT	UNP P02753
F	148	VAL	ALA	CONFLICT	UNP P02753
F	169	PRO	VAL	CONFLICT	UNP P02753

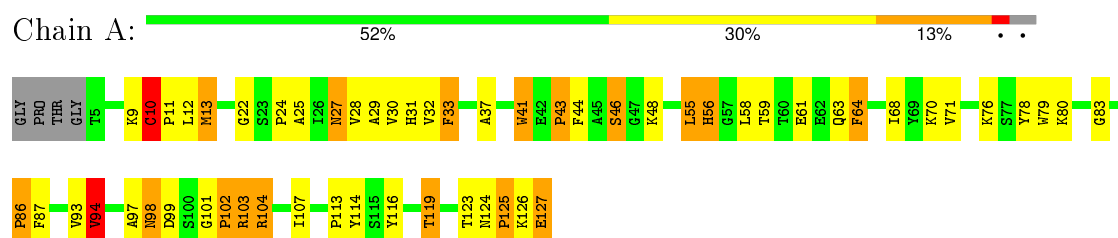- Molecule 3 is RETINOIC ACID (three-letter code: REA) (formula: $C_{20}H_{28}O_2$).
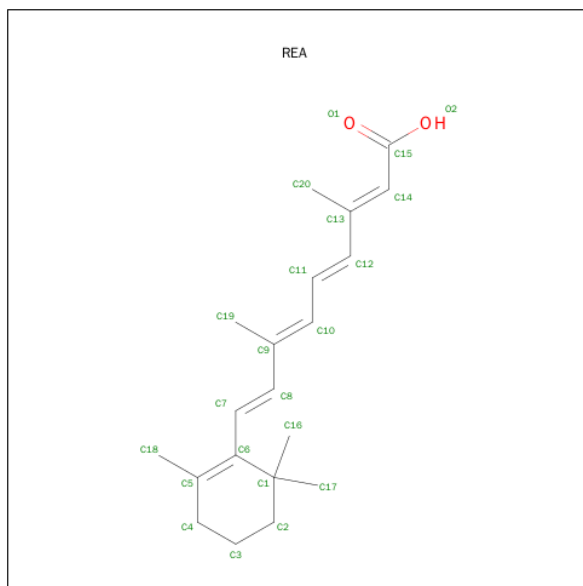
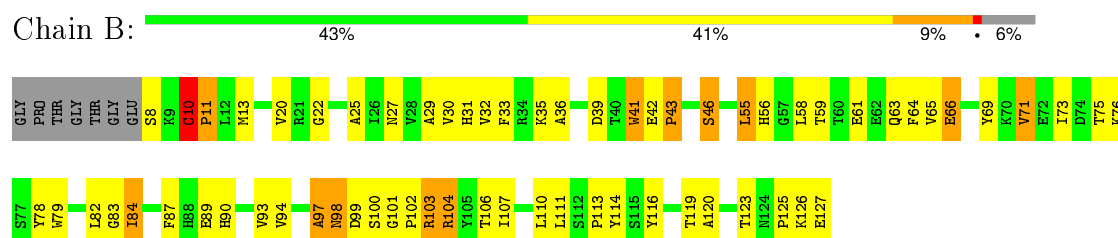| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			21	20	1		
3	F	1	Total	C	O	0	0
			21	20	1		

3 Residue-property plots ⓘ

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.
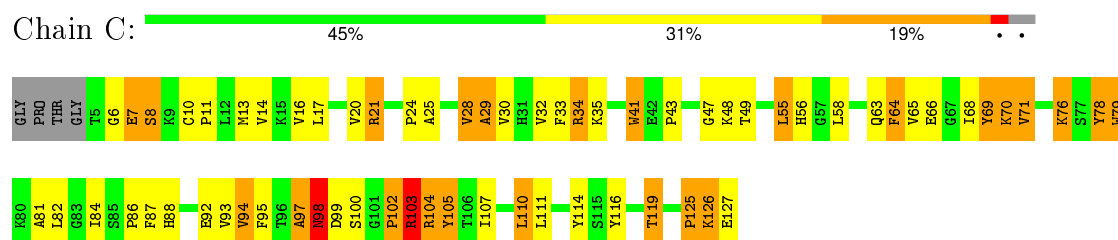
Note EDS was not executed.
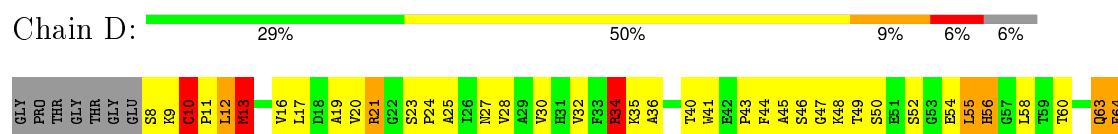
- Molecule 1: TRANSTHYRETIN
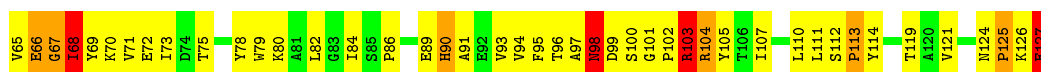

- Molecule 1: TRANSTHYRETIN
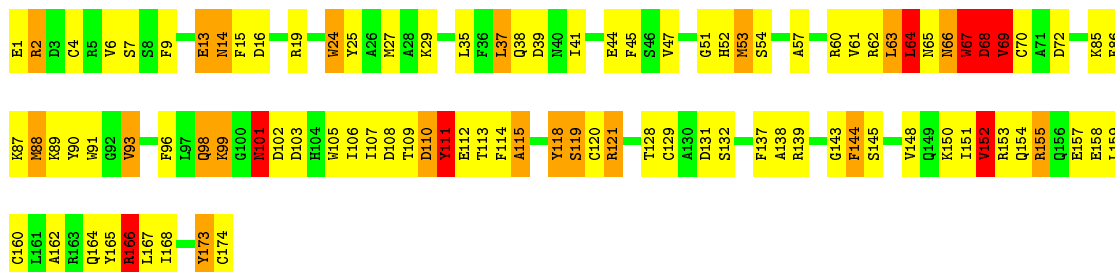

- Molecule 1: TRANSTHYRETIN
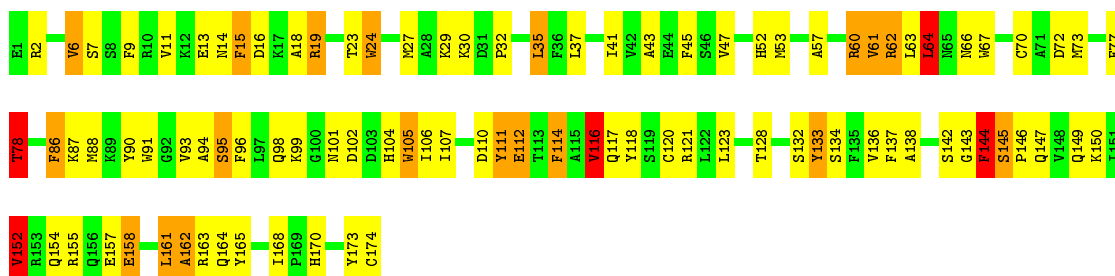

- Molecule 1: TRANSTHYRETIN

V65 E66 G67 I68 Y69 K70 V71 E72 I73 D74 T75 Y78 W79 K80 A81 L82 G83 I84 S85 P86 E89 H90 A91 E92 V93 V94 F95 T96 A97 N98 D99 S100 G101 P102 R103 R104 Y105 T106 I107 L110 L111 S112 P113 Y114 T119 A120 V121 N124 P125 K126 E127

• Molecule 2: RETINOL BINDING PROTEIN

Chain E:

44%   40%   11%   5%

E1 R2 D3 C4 R5 V6 S7 S8 F9 E13 N14 F15 D16 R19 W24 Y25 A26 M27 A28 K29 L35 F36 L37 Q38 D39 N40 I41 E44 F45 S46 V47 G51 H52 M53 S54 A57 R60 V61 R62 L63 L64 N65 N66 W67 D68 V69 C70 A71 D72 K85 F86

K87 M88 K89 Y90 W91 G92 V93 F96 L97 Q98 K99 G100 N101 D102 D103 H104 W105 I106 I107 D108 T109 D110 Y111 E112 T113 F114 A115 Y118 S119 C120 R121 T128 C129 A130 D131 S132 F137 A138 R139 G143 F144 S145 V148 Q149 K150 I151 V152 R153 Q154 R155 Q156 E157 E158 L159

C160 L161 A162 R163 Q164 Y165 R166 L167 I168 Y173 C174

• Molecule 2: RETINOL BINDING PROTEIN

Chain F:

46%   40%   11%   •

E1 R2 V6 S7 S8 F9 R10 V11 K12 E13 N14 F15 D16 K17 A18 R19 T23 W24 M27 A28 K29 K30 D31 P32 L35 F36 L37 I41 V42 A43 E44 F45 S46 V47 H52 M53 A57 R60 V61 R62 L63 L64 N65 N66 W67 C70 A71 D72 M73 F77

T78 F86 K87 M88 K89 Y90 W91 G92 V93 A94 S95 F96 L97 Q98 K99 G100 N101 D102 D103 H104 W105 I106 I107 D110 Y111 E112 T113 F114 A115 V116 Q117 Y118 S119 C120 R121 L122 L123 T128 S132 Y133 S134 F135 V136 F137 A138 S142 G143 F144 S145 P146 Q147 V148 Q149 K150 I151

V152 R153 Q154 R155 Q156 E157 E158 L161 A162 R163 Q164 Y165 I168 P169 H170 Y173 C174

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	222.40Å 163.40Å 55.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.10	Depositor
% Data completeness (in resolution range)	93.5 (6.00-3.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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	1.11	2/974 (0.2%)	1.74	16/1325 (1.2%)
1	B	1.07	0/954	1.82	23/1298 (1.8%)
1	C	1.06	0/974	1.93	28/1325 (2.1%)
1	D	1.04	0/954	1.52	13/1298 (1.0%)
2	E	1.21	5/1445 (0.3%)	2.22	59/1950 (3.0%)
2	F	1.30	3/1445 (0.2%)	2.11	45/1950 (2.3%)
All	All	1.15	10/6746 (0.1%)	1.94	184/9146 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	E	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	162	ALA	C-N	-26.18	0.73	1.34
2	F	163	ARG	N-CA	-13.27	1.19	1.46
1	A	98	ASN	C-O	12.00	1.46	1.23
2	E	69	VAL	N-CA	11.84	1.70	1.46
2	E	99	LYS	N-CA	7.11	1.60	1.46

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	162	ALA	O-C-N	25.37	163.29	122.70
2	F	162	ALA	C-N-CA	-21.22	68.66	121.70
2	E	68	ASP	C-N-CA	18.52	168.01	121.70
2	F	162	ALA	CA-C-N	-17.98	77.66	117.20
2	E	121	ARG	NE-CZ-NH1	17.79	129.19	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	69	TYR	Sidechain
2	E	68	ASP	Peptide

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	950	0	924	47	0
1	B	930	0	908	47	0
1	C	950	0	924	53	0
1	D	930	0	908	103	5
2	E	1411	0	1334	69	0
2	F	1411	0	1334	58	0
3	E	21	0	27	16	0
3	F	21	0	27	7	0
All	All	6624	0	6386	372	5

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 30.

The worst 5 of 372 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:E:69:VAL:CA	2:E:69:VAL:N	1.70	1.51
1:B:66:GLU:HG2	1:B:98:ASN:O	1.14	1.27
1:B:100:SER:O	1:B:102:PRO:HD3	1.41	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLU:OE2	1:A:103:ARG:HD3	1.40	1.19
1:C:97:ALA:HB3	1:C:98:ASN:ND2	1.58	1.18

All (5) 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)
1:D:66:GLU:CD	1:D:66:GLU:OE1[3_655]	0.16	2.04
1:D:66:GLU:OE1	1:D:66:GLU:OE1[3_655]	1.18	1.02
1:D:66:GLU:CD	1:D:66:GLU:CD[3_655]	1.41	0.79
1:D:66:GLU:OE1	1:D:66:GLU:OE2[3_655]	1.43	0.77
1:D:66:GLU:CG	1:D:66:GLU:OE1[3_655]	1.51	0.69

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	121/127 (95%)	100 (83%)	17 (14%)	4 (3%)	5	26
1	B	118/127 (93%)	97 (82%)	16 (14%)	5 (4%)	3	19
1	C	121/127 (95%)	93 (77%)	23 (19%)	5 (4%)	3	20
1	D	118/127 (93%)	89 (75%)	21 (18%)	8 (7%)	1	8
2	E	172/174 (99%)	145 (84%)	20 (12%)	7 (4%)	3	20
2	F	172/174 (99%)	143 (83%)	24 (14%)	5 (3%)	6	29
All	All	822/856 (96%)	667 (81%)	121 (15%)	34 (4%)	3	20

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	A	125	PRO

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Mol	Chain	Res	Type
1	B	98	ASN
1	B	125	PRO
1	C	98	ASN

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	103/105 (98%)	87 (84%)	16 (16%)	3	14
1	B	101/105 (96%)	89 (88%)	12 (12%)	6	25
1	C	103/105 (98%)	83 (81%)	20 (19%)	2	7
1	D	101/105 (96%)	81 (80%)	20 (20%)	1	7
2	E	150/150 (100%)	123 (82%)	27 (18%)	2	10
2	F	150/150 (100%)	124 (83%)	26 (17%)	2	11
All	All	708/720 (98%)	587 (83%)	121 (17%)	2	11

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	46	SER
1	D	127	GLU
2	F	116	VAL
1	D	54	GLU
1	D	68	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	98	ASN
2	E	40	ASN
2	F	104	HIS
1	C	98	ASN
1	D	56	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	$\#|Z| > 2$
3	REA	E	176	-	21,21,22	1.60	3 (14%)	27,28,30	6.09	21 (77%)
3	REA	F	177	-	21,21,22	1.85	5 (23%)	27,28,30	8.97	20 (74%)

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
3	REA	E	176	-	-	1/14/31/32	0/1/1/1
3	REA	F	177	-	-	1/14/31/32	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	177	REA	C11-C10	2.01	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	177	REA	C8-C7	2.28	1.39	1.33
3	F	177	REA	C11-C12	2.42	1.40	1.34
3	E	176	REA	C14-C13	2.43	1.39	1.35
3	E	176	REA	C10-C9	2.45	1.39	1.35

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	177	REA	C18-C5-C6	-30.62	94.54	124.61
3	E	176	REA	C7-C8-C9	-12.79	106.73	126.22
3	F	177	REA	O1-C15-C14	-12.79	107.18	123.65
3	E	176	REA	C20-C13-C14	-11.16	106.41	122.90
3	E	176	REA	O1-C15-C14	-10.87	109.66	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	176	REA	O1-C15-C14-C13
3	F	177	REA	O1-C15-C14-C13

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	176	REA	16	0
3	F	177	REA	7	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.