



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:26 PM GMT

PDB ID : 1FML
Title : CRYSTAL STRUCTURE OF RETINOL DEHYDRATASE IN A COMPLEX WITH RETINOL AND PAP
Authors : Pakhomova, S.; Kobayashi, M.; Buck, J.; Newcomer, M.E.
Deposited on : 2000-08-17
Resolution : 2.75 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

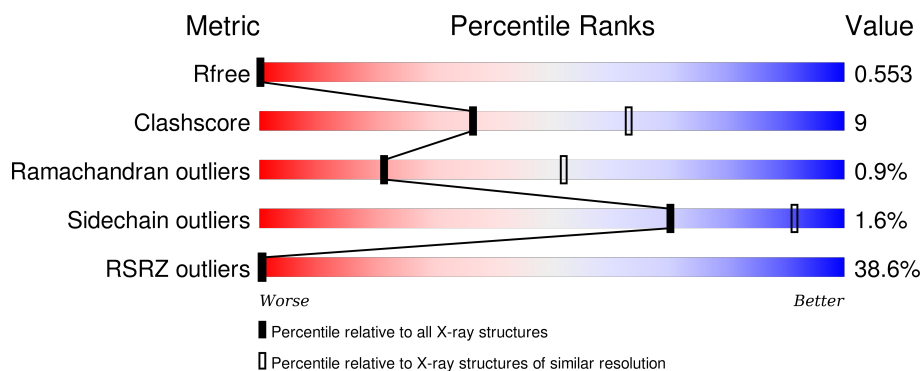
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

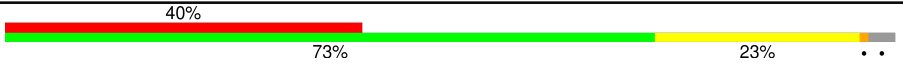

The reported resolution of this entry is 2.75 Å.

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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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.

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	

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	A3P	B	500	-	-	-	X
4	RTL	A	401	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5859 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 DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	1	0
			2838	1837	470	515	16			
1	B	341	Total	C	N	O	S	0	0	0
			2832	1833	468	515	16			

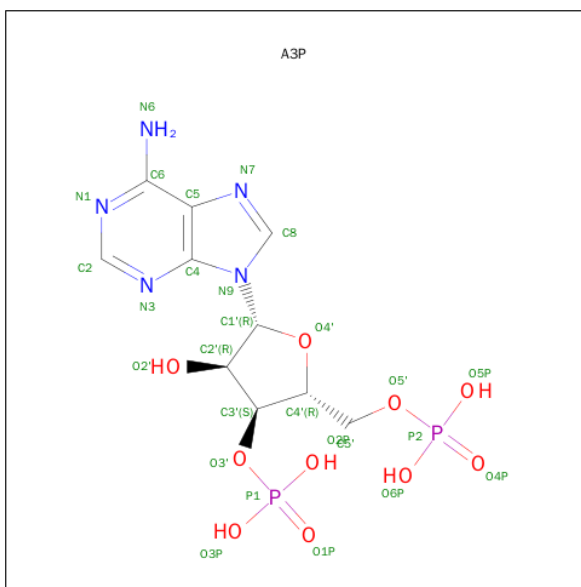
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	PHE	SEE REMARK 999	UNP Q26490
B	142	SER	PHE	SEE REMARK 999	UNP Q26490

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

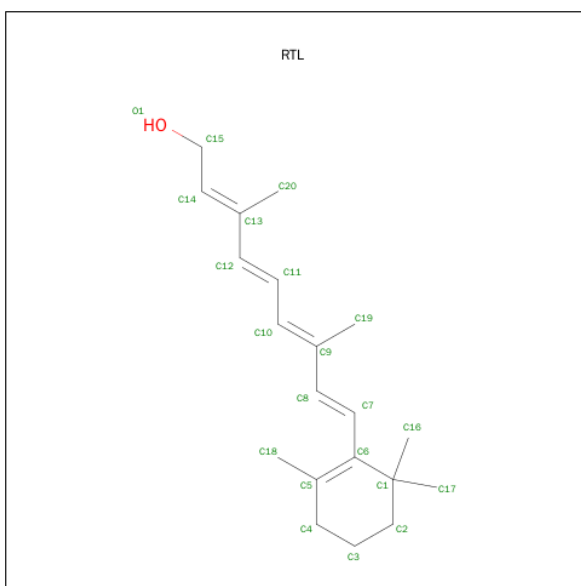
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is RETINOL (three-letter code: RTL) (formula: $C_{20}H_{30}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	20	1		
4	B	1	Total	C	O	0	0
			21	20	1		

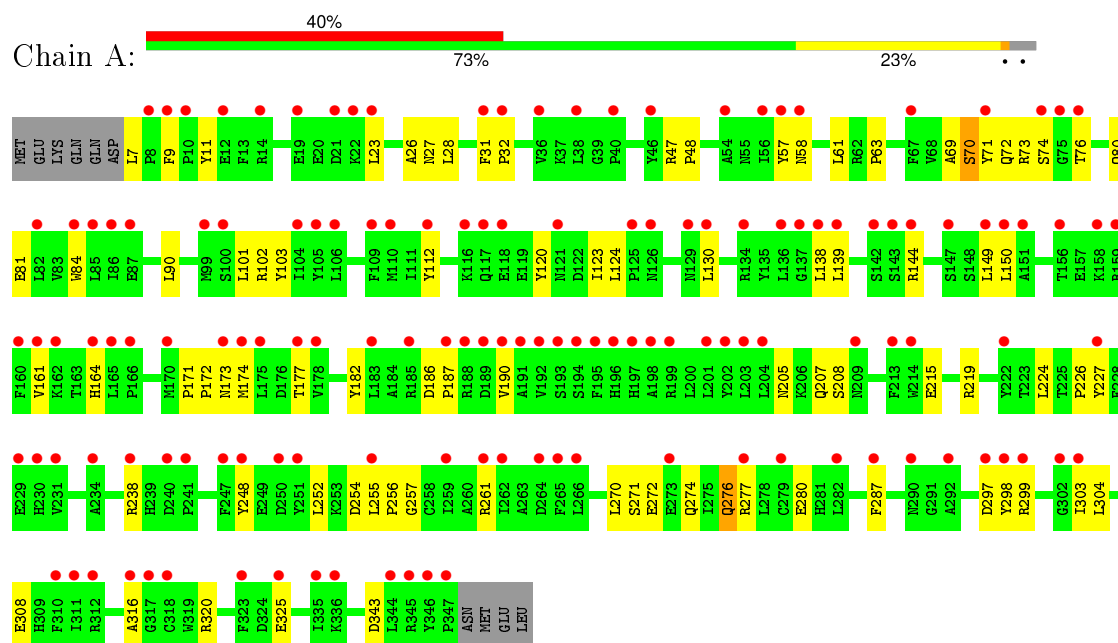
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	0
5	B	45	Total 45	O 45	0	0

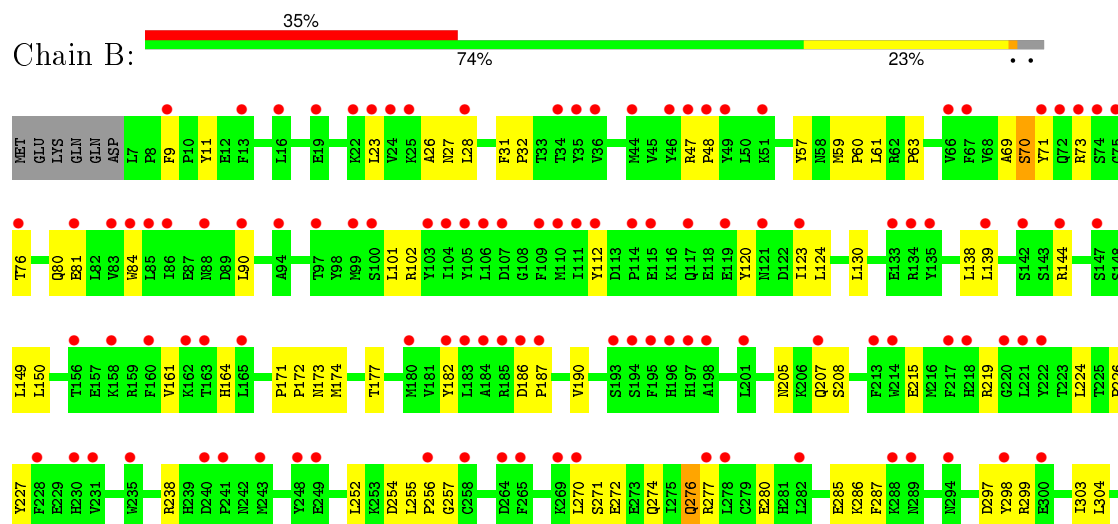
3 Residue-property plots

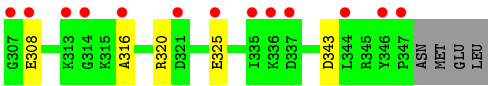
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: RETINOL DEHYDRATASE



• Molecule 1: RETINOL DEHYDRATASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.05Å 66.61Å 84.90Å 90.00° 111.29° 90.00°	Depositor
Resolution (Å)	38.45 – 2.75 76.45 – 2.22	Depositor EDS
% Data completeness (in resolution range)	87.8 (38.45-2.75) 16.6 (76.45-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.55 (at 2.22Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.222 , 0.273 0.562 , 0.553	Depositor DCC
R_{free} test set	299 reflections (4.77%)	DCC
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	1.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 3233.4	EDS
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 7068 reflections	Xtriage
F_o, F_c correlation	0.26	EDS
Total number of atoms	5859	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: RTL, CA, A3P

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	0.39	0/2924	0.62	1/3960 (0.0%)
1	B	0.38	0/2913	0.62	1/3945 (0.0%)
All	All	0.39	0/5837	0.62	2/7905 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	TYR	N-CA-C	-5.36	96.53	111.00
1	B	71	TYR	N-CA-C	-5.11	97.21	111.00

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	2838	0	2765	55	0
1	B	2832	0	2762	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	11	1	0
3	B	27	0	11	1	0
4	A	21	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	30	0	0
5	A	46	0	0	1	0
5	B	45	0	0	2	0
All	All	5859	0	5609	108	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 9.

All (108) 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:120:TYR:O	1:A:123:ILE:HG12	1.84	0.77
1:B:120:TYR:O	1:B:123:ILE:HG12	1.85	0.77
1:A:187:PRO:HG3	1:A:227:TYR:CE2	2.28	0.69
1:B:187:PRO:HG3	1:B:227:TYR:CE2	2.31	0.65
1:A:272:GLU:O	1:A:276:GLN:HB2	1.98	0.63
1:B:272:GLU:O	1:B:276:GLN:HB2	2.00	0.62
1:A:150:LEU:HD21	1:A:161:VAL:HG22	1.82	0.61
1:A:255:LEU:HB3	1:A:256:PRO:HD3	1.84	0.60
1:B:81:GLU:OE2	1:B:81:GLU:HA	2.02	0.60
1:A:298:TYR:HD2	1:A:303:ILE:HD11	1.69	0.58
1:B:238:ARG:NH2	1:B:343:ASP:OD2	2.36	0.58
1:A:238:ARG:NH2	1:A:343:ASP:OD2	2.37	0.58
1:B:150:LEU:HD21	1:B:161:VAL:HG22	1.84	0.58
1:A:69:ALA:O	1:A:70:SER:HB3	2.04	0.58
1:A:252:LEU:HD12	1:A:316:ALA:HB2	1.84	0.57
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.87	0.57
1:B:298:TYR:HD2	1:B:303:ILE:HD11	1.69	0.56
1:B:252:LEU:HD12	1:B:316:ALA:HB2	1.86	0.56
1:B:69:ALA:O	1:B:70:SER:HB3	2.04	0.56
1:B:254:ASP:OD2	1:B:257:GLY:HA3	2.06	0.56
1:B:270:LEU:HA	1:B:274:GLN:OE1	2.07	0.55
1:B:299:ARG:HB2	1:B:304:LEU:HD12	1.88	0.55
1:B:144:ARG:HD3	1:B:149:LEU:HD21	1.88	0.55
1:A:81:GLU:HA	1:A:81:GLU:OE2	2.07	0.55
1:B:47:ARG:HB3	1:B:48:PRO:HD3	1.89	0.54
1:B:76:THR:HG22	1:B:80:GLN:HE21	1.71	0.54
1:A:72:GLN:HG2	5:A:475:HOH:O	2.08	0.54
1:A:270:LEU:HA	1:A:274:GLN:OE1	2.07	0.54
1:A:47:ARG:HB3	1:A:48:PRO:HD3	1.90	0.54
1:A:299:ARG:HB2	1:A:304:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HD3	1:A:149:LEU:HD21	1.89	0.54
1:A:76:THR:HG22	1:A:80:GLN:HE21	1.72	0.54
1:A:254:ASP:OD2	1:A:257:GLY:HA3	2.08	0.54
1:A:270:LEU:HB3	1:A:274:GLN:HB2	1.91	0.53
1:A:277:ARG:HA	1:A:280:GLU:OE1	2.09	0.53
1:B:112:TYR:CE1	1:B:139:LEU:HD22	2.43	0.53
1:A:112:TYR:CE1	1:A:139:LEU:HD22	2.45	0.52
1:B:277:ARG:HA	1:B:280:GLU:OE1	2.10	0.52
1:B:270:LEU:HB3	1:B:274:GLN:HB2	1.91	0.52
1:B:73:ARG:CZ	3:B:500:A3P:H5'1	2.41	0.51
1:A:308:GLU:OE1	1:A:308:GLU:HA	2.11	0.50
1:A:7:LEU:HB2	1:A:58:ASN:OD1	2.11	0.50
1:B:308:GLU:HA	1:B:308:GLU:OE1	2.11	0.50
1:A:73:ARG:CZ	3:A:400:A3P:H5'1	2.41	0.49
1:A:325:GLU:CD	1:A:325:GLU:H	2.16	0.49
1:A:9:PHE:CE2	1:A:11:TYR:HB2	2.46	0.49
1:A:27:ASN:HB2	1:A:28:LEU:HD12	1.94	0.49
1:A:90:LEU:HD21	1:A:274:GLN:HB3	1.94	0.49
1:B:9:PHE:CE2	1:B:11:TYR:HB2	2.47	0.49
1:B:320:ARG:HG2	1:B:320:ARG:NH1	2.28	0.49
1:A:320:ARG:HG2	1:A:320:ARG:NH1	2.28	0.48
1:B:27:ASN:HB2	1:B:28:LEU:HD12	1.94	0.48
1:A:124:LEU:CD1	1:A:130:LEU:HD21	2.44	0.48
1:A:205:ASN:C	1:A:207:GLN:N	2.67	0.48
1:B:325:GLU:CD	1:B:325:GLU:H	2.16	0.48
1:B:90:LEU:HD21	1:B:274:GLN:HB3	1.96	0.48
1:A:215:GLU:O	1:A:219:ARG:HB2	2.13	0.48
1:B:205:ASN:C	1:B:207:GLN:N	2.67	0.47
1:B:124:LEU:CD1	1:B:130:LEU:HD21	2.44	0.47
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.79	0.47
1:B:63:PRO:HA	1:B:177:THR:O	2.15	0.47
1:B:81:GLU:HG2	1:B:287:PHE:HE1	1.79	0.47
1:B:215:GLU:O	1:B:219:ARG:HB2	2.14	0.47
1:A:172:PRO:O	1:A:173:ASN:HB2	2.15	0.46
1:B:70:SER:O	1:B:164:HIS:HA	2.16	0.46
1:B:172:PRO:O	1:B:173:ASN:HB2	2.16	0.46
1:A:61:LEU:CD1	1:A:174:MET:HB2	2.46	0.46
1:B:61:LEU:CD1	1:B:174:MET:HB2	2.46	0.45
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.80	0.45
1:A:63:PRO:HA	1:A:177:THR:O	2.17	0.45
1:A:23:LEU:O	1:A:26:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:O	1:A:164:HIS:HA	2.17	0.45
1:A:299:ARG:NH2	1:A:308:GLU:O	2.50	0.44
1:A:81:GLU:HG2	1:A:287:PHE:HE1	1.80	0.44
1:A:90:LEU:HD12	1:A:90:LEU:N	2.33	0.44
1:B:285:GLU:HG2	5:B:592:HOH:O	2.16	0.44
1:A:320:ARG:HG2	1:A:320:ARG:HH11	1.82	0.44
1:B:205:ASN:C	1:B:207:GLN:H	2.21	0.44
1:B:286:LYS:NZ	5:B:585:HOH:O	2.51	0.43
1:B:299:ARG:NH2	1:B:308:GLU:O	2.49	0.43
1:B:320:ARG:HG2	1:B:320:ARG:HH11	1.82	0.43
1:A:61:LEU:HD11	1:A:174:MET:HB2	2.00	0.43
1:A:186:ASP:O	1:A:190:VAL:HG23	2.18	0.43
1:B:90:LEU:N	1:B:90:LEU:HD12	2.35	0.42
1:A:257:GLY:O	1:A:261:ARG:HG3	2.19	0.42
1:B:23:LEU:O	1:B:26:ALA:HB3	2.19	0.42
1:B:47:ARG:NH1	1:B:47:ARG:HG3	2.34	0.42
1:B:57:TYR:O	1:B:171:PRO:HG3	2.19	0.42
1:A:80:GLN:HB3	1:A:103:TYR:CE1	2.54	0.42
1:A:205:ASN:C	1:A:207:GLN:H	2.22	0.41
1:B:61:LEU:HD11	1:B:174:MET:HB2	2.02	0.41
1:A:57:TYR:O	1:A:171:PRO:HG3	2.20	0.41
1:B:186:ASP:O	1:B:190:VAL:HG23	2.20	0.41
1:A:76:THR:HG22	1:A:80:GLN:NE2	2.34	0.41
1:A:31:PHE:HA	1:A:32:PRO:HD3	1.83	0.41
1:B:124:LEU:HD12	1:B:130:LEU:HD11	2.03	0.41
1:A:74:SER:O	1:A:248:TYR:HB2	2.21	0.41
1:A:255:LEU:N	1:A:256:PRO:CD	2.84	0.41
1:B:69:ALA:O	1:B:182:TYR:HA	2.21	0.41
1:B:76:THR:HG22	1:B:80:GLN:NE2	2.34	0.41
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.36	0.41
1:B:59:MET:HA	1:B:60:PRO:HD3	1.93	0.41
1:A:84:TRP:CE2	1:A:102:ARG:HD2	2.56	0.40
1:B:84:TRP:CE2	1:B:102:ARG:HD2	2.56	0.40
1:A:271:SER:O	1:A:272:GLU:C	2.60	0.40
1:A:69:ALA:O	1:A:182:TYR:HA	2.22	0.40
1:B:271:SER:O	1:B:272:GLU:C	2.59	0.40
1:B:31:PHE:HA	1:B:32:PRO:HD3	1.83	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	340/351 (97%)	315 (93%)	22 (6%)	3 (1%)	21	52
1	B	339/351 (97%)	311 (92%)	25 (7%)	3 (1%)	21	52
All	All	679/702 (97%)	626 (92%)	47 (7%)	6 (1%)	21	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	B	208	SER
1	A	70	SER
1	B	70	SER
1	B	226	PRO
1	A	226	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	A	305/316 (96%)	300 (98%)	5 (2%)	70	91
1	B	304/316 (96%)	299 (98%)	5 (2%)	70	91
All	All	609/632 (96%)	599 (98%)	10 (2%)	70	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	138	LEU
1	A	224	LEU
1	A	276	GLN
1	A	297	ASP
1	B	101	LEU
1	B	138	LEU
1	B	224	LEU
1	B	276	GLN
1	B	297	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	117	GLN
1	A	276	GLN
1	A	330	GLN
1	A	338	ASN
1	B	80	GLN
1	B	276	GLN
1	B	330	GLN
1	B	338	ASN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	A3P	A	400	-	24,29,29	1.49	3 (12%)	28,45,45	1.16	3 (10%)
4	RTL	A	401	-	21,21,21	1.45	2 (9%)	26,28,28	3.24	13 (50%)
3	A3P	B	500	-	24,29,29	1.46	2 (8%)	28,45,45	1.17	3 (10%)
4	RTL	B	501	-	21,21,21	1.38	2 (9%)	26,28,28	3.23	13 (50%)

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	A3P	A	400	-	-	0/11/31/31	0/3/3/3
4	RTL	A	401	-	-	2/14/31/31	0/1/1/1
3	A3P	B	500	-	-	0/11/31/31	0/3/3/3
4	RTL	B	501	-	-	2/14/31/31	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	A3P	C2-N1	2.43	1.38	1.33
4	A	401	RTL	C1-C6	2.59	1.57	1.53
4	B	501	RTL	C1-C6	2.61	1.57	1.53
4	B	501	RTL	C5-C6	3.29	1.39	1.34
4	A	401	RTL	C5-C6	3.37	1.39	1.34
3	B	500	A3P	C2-N3	3.71	1.38	1.32
3	A	400	A3P	C2-N3	4.21	1.39	1.32
3	A	400	A3P	C4-N3	4.22	1.41	1.35
3	B	500	A3P	C4-N3	4.33	1.42	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	RTL	C20-C13-C12	-6.91	106.59	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	RTL	C20-C13-C12	-6.91	106.60	118.10
4	A	401	RTL	C3-C4-C5	-5.24	105.56	113.87
4	B	501	RTL	C3-C4-C5	-5.12	105.74	113.87
3	B	500	A3P	N3-C2-N1	-4.06	125.78	128.89
4	B	501	RTL	C10-C11-C12	-4.02	110.89	123.13
3	A	400	A3P	N3-C2-N1	-4.01	125.82	128.89
4	A	401	RTL	C10-C11-C12	-3.76	111.67	123.13
4	B	501	RTL	C18-C5-C6	-3.19	121.47	124.61
4	A	401	RTL	C18-C5-C6	-3.03	121.63	124.61
4	A	401	RTL	C7-C8-C9	-2.91	121.78	126.22
4	B	501	RTL	C16-C1-C2	-2.55	99.64	108.79
4	B	501	RTL	C7-C8-C9	-2.49	122.41	126.22
4	A	401	RTL	C16-C1-C2	-2.42	100.14	108.79
4	A	401	RTL	C18-C5-C4	-2.23	109.20	113.43
4	B	501	RTL	C18-C5-C4	-2.18	109.30	113.43
3	B	500	A3P	C4-C5-N7	2.05	111.36	109.48
4	A	401	RTL	C16-C1-C6	2.10	113.59	110.30
3	B	500	A3P	O2'-C2'-C3'	2.13	117.31	111.16
3	A	400	A3P	O2'-C2'-C3'	2.26	117.68	111.16
3	A	400	A3P	C4-C5-N7	2.28	111.57	109.48
4	B	501	RTL	C16-C1-C6	2.28	113.89	110.30
4	B	501	RTL	C17-C1-C6	2.74	114.59	110.30
4	A	401	RTL	C17-C1-C6	2.84	114.75	110.30
4	A	401	RTL	C11-C12-C13	3.28	135.96	126.32
4	B	501	RTL	C11-C12-C13	3.34	136.14	126.32
4	B	501	RTL	C2-C1-C6	3.80	116.39	110.36
4	A	401	RTL	C2-C1-C6	3.87	116.49	110.36
4	A	401	RTL	C4-C5-C6	5.01	129.16	122.78
4	B	501	RTL	C4-C5-C6	5.04	129.21	122.78
4	B	501	RTL	C2-C3-C4	8.83	133.80	111.53
4	A	401	RTL	C2-C3-C4	8.96	134.11	111.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	RTL	C15-C14-C13-C12
4	B	501	RTL	C15-C14-C13-C20
4	A	401	RTL	C15-C14-C13-C20
4	A	401	RTL	C15-C14-C13-C12

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	A3P	1	0
3	B	500	A3P	1	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

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	341/351 (97%)	2.52	140 (41%) 0 0	9, 32, 58, 83	0
1	B	341/351 (97%)	2.11	123 (36%) 0 0	11, 31, 55, 71	0
All	All	682/702 (97%)	2.32	263 (38%) 0 0	9, 31, 57, 83	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	ILE	23.9
1	A	161	VAL	21.8
1	A	86	ILE	19.8
1	B	183	LEU	19.0
1	A	192	VAL	17.0
1	B	23	LEU	15.9
1	A	104	ILE	14.5
1	A	189	ASP	14.2
1	A	214	TRP	14.1
1	A	142	SER	13.3
1	A	248	TYR	12.7
1	A	105	TYR	12.1
1	A	230	HIS	11.4
1	A	99	MET	11.3
1	A	106	LEU	11.2
1	B	35	TYR	11.0
1	A	316	ALA	11.0
1	B	193	SER	11.0
1	A	190	VAL	10.6
1	A	57	TYR	10.4
1	B	335	ILE	10.3
1	B	213	PHE	9.9
1	B	111	ILE	9.7
1	B	117	GLN	8.9

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Mol	Chain	Res	Type	RSRZ
1	B	112	TYR	8.9
1	A	302	GLY	8.7
1	B	162	LYS	8.5
1	B	182	TYR	8.5
1	B	147	SER	8.4
1	A	282	LEU	8.3
1	B	85	LEU	8.2
1	A	147	SER	8.1
1	A	346	TYR	7.8
1	A	335	ILE	7.7
1	B	230	HIS	7.7
1	B	336	LYS	7.6
1	B	74	SER	7.5
1	B	36	VAL	7.4
1	A	158	LYS	7.4
1	B	321	ASP	7.3
1	A	150	LEU	7.3
1	A	54	ALA	7.3
1	A	100	SER	7.2
1	A	67	PHE	7.2
1	A	310	PHE	7.2
1	B	156	THR	7.0
1	A	347	PRO	7.0
1	B	278	LEU	7.0
1	A	250	ASP	6.9
1	A	38	LEU	6.6
1	B	119	GLU	6.6
1	B	73	ARG	6.6
1	B	347	PRO	6.5
1	A	203	LEU	6.5
1	B	346	TYR	6.3
1	B	28	LEU	6.1
1	A	292	ALA	6.1
1	B	185	ARG	6.0
1	A	183	LEU	6.0
1	A	32	PRO	5.9
1	A	297	ASP	5.9
1	A	46	TYR	5.8
1	A	262	ILE	5.8
1	A	185	ARG	5.7
1	A	166	PRO	5.6
1	A	164	HIS	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	231	VAL	5.6
1	B	344	LEU	5.6
1	A	318	CYS	5.5
1	A	151	ALA	5.5
1	A	162	LYS	5.4
1	B	24	VAL	5.4
1	A	22	LYS	5.4
1	B	71	TYR	5.4
1	B	100	SER	5.3
1	B	134	ARG	5.2
1	B	214	TRP	5.2
1	A	298	TYR	5.2
1	A	266	LEU	5.2
1	B	106	LEU	5.2
1	A	222	TYR	5.2
1	A	112	TYR	5.1
1	B	294	ASN	5.1
1	B	107	ASP	5.1
1	A	187	PRO	5.0
1	A	84	TRP	5.0
1	A	194	SER	5.0
1	A	130	LEU	5.0
1	A	279	CYS	4.9
1	B	197	HIS	4.9
1	A	76	THR	4.9
1	B	88	ASN	4.9
1	A	117	GLN	4.8
1	B	220	GLY	4.8
1	B	201	LEU	4.8
1	B	196	HIS	4.7
1	A	174	MET	4.7
1	A	238	ARG	4.7
1	B	163	THR	4.7
1	A	303	ILE	4.7
1	B	114	PRO	4.6
1	B	282	LEU	4.6
1	B	115	GLU	4.5
1	B	22	LYS	4.4
1	A	234	ALA	4.4
1	B	194	SER	4.4
1	A	277	ARG	4.4
1	B	34	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	4.3
1	B	67	PHE	4.3
1	A	177	THR	4.3
1	B	47	ARG	4.3
1	A	247	PHE	4.3
1	A	110	MET	4.3
1	A	36	VAL	4.3
1	A	198	ALA	4.3
1	B	25	LYS	4.2
1	B	300	GLU	4.2
1	B	165	LEU	4.2
1	B	104	ILE	4.2
1	B	76	THR	4.2
1	A	273	GLU	4.2
1	A	56	ILE	4.1
1	A	85	LEU	4.1
1	A	109	PHE	4.1
1	A	75	GLY	4.1
1	B	222	TYR	4.1
1	B	184	ALA	4.0
1	A	251	TYR	3.9
1	B	142	SER	3.9
1	A	159	ARG	3.9
1	B	180	MET	3.8
1	B	265	PHE	3.8
1	B	235	TRP	3.8
1	A	265	PHE	3.8
1	B	133	GLU	3.7
1	B	144	ARG	3.7
1	B	231	VAL	3.7
1	A	227	TYR	3.6
1	B	97	THR	3.6
1	A	202	TYR	3.6
1	B	110	MET	3.6
1	A	255	LEU	3.6
1	A	188	ARG	3.6
1	A	259	ILE	3.5
1	A	178	VAL	3.5
1	B	105	TYR	3.5
1	B	83	VAL	3.5
1	A	201	LEU	3.5
1	A	264	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	258	CYS	3.4
1	A	175	LEU	3.4
1	A	116	LYS	3.4
1	A	156	THR	3.4
1	A	40	PRO	3.4
1	B	248	TYR	3.4
1	A	287	PHE	3.3
1	A	71	TYR	3.3
1	A	139	LEU	3.3
1	B	81	GLU	3.3
1	A	344	LEU	3.3
1	B	121	ASN	3.3
1	B	19	GLU	3.3
1	B	51	LYS	3.2
1	B	337	ASP	3.2
1	A	118	GLU	3.2
1	B	270	LEU	3.1
1	A	323	PHE	3.1
1	B	221	LEU	3.1
1	B	288	LYS	3.1
1	A	173	ASN	3.0
1	B	307	GLY	3.0
1	A	19	GLU	3.0
1	A	149	LEU	3.0
1	A	209	ASN	3.0
1	B	139	LEU	3.0
1	A	58	ASN	3.0
1	A	213	PHE	2.9
1	B	99	MET	2.9
1	A	229	GLU	2.9
1	B	9	PHE	2.9
1	B	241	PRO	2.9
1	B	325	GLU	2.9
1	A	336	LYS	2.9
1	A	290	ASN	2.8
1	B	72	GLN	2.8
1	B	298	TYR	2.8
1	A	121	ASN	2.7
1	A	136	LEU	2.7
1	A	31	PHE	2.7
1	B	228	PHE	2.7
1	B	75	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	313	LYS	2.7
1	B	218	HIS	2.7
1	A	317	GLY	2.7
1	A	137	GLY	2.6
1	B	264	ASP	2.6
1	B	84	TRP	2.6
1	A	12	GLU	2.6
1	B	160	PHE	2.6
1	B	269	LYS	2.6
1	B	217	PHE	2.6
1	B	277	ARG	2.6
1	B	46	TYR	2.6
1	B	158	LYS	2.6
1	A	261	ARG	2.6
1	A	195	PHE	2.6
1	B	44	MET	2.5
1	A	345	ARG	2.5
1	B	256	PRO	2.5
1	A	191	ALA	2.5
1	A	299	ARG	2.5
1	A	23	LEU	2.5
1	A	125	PRO	2.5
1	B	66	VAL	2.5
1	A	143	SER	2.5
1	A	312	ARG	2.5
1	B	186	ASP	2.5
1	A	311	ILE	2.5
1	B	289	ASN	2.5
1	A	170	MET	2.4
1	A	74	SER	2.4
1	B	316	ALA	2.4
1	B	48	PRO	2.4
1	B	195	PHE	2.4
1	A	129	ASN	2.4
1	B	109	PHE	2.3
1	A	10	PRO	2.3
1	B	240	ASP	2.3
1	B	90	LEU	2.3
1	A	21	ASP	2.3
1	A	197	HIS	2.3
1	A	240	ASP	2.3
1	B	49	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	204	LEU	2.3
1	A	138	LEU	2.2
1	B	13	PHE	2.2
1	A	199	ARG	2.2
1	A	144	ARG	2.2
1	B	187	PRO	2.2
1	A	196	HIS	2.2
1	B	249	GLU	2.2
1	A	126	ASN	2.2
1	B	308	GLU	2.2
1	A	9	PHE	2.2
1	A	14	ARG	2.2
1	A	87	GLU	2.1
1	B	207	GLN	2.1
1	A	165	LEU	2.1
1	A	193	SER	2.1
1	B	314	GLY	2.1
1	A	134	ARG	2.1
1	A	241	PRO	2.1
1	B	16	LEU	2.1
1	B	243	MET	2.1
1	B	103	TYR	2.1
1	A	8	PRO	2.1
1	B	123	ILE	2.1
1	A	325	GLU	2.1
1	A	160	PHE	2.0
1	B	94	ALA	2.0
1	B	135	TYR	2.0
1	B	198	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 ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	A3P	B	500	27/27	0.54	0.45	0.31	25,25,25,25	0
4	RTL	A	401	21/21	0.61	0.43	-0.34	53,53,53,53	0
4	RTL	B	501	21/21	0.65	0.32	-0.46	65,65,65,65	0
3	A3P	A	400	27/27	0.83	0.19	-0.98	6,6,6,6	0
2	CA	A	450	1/1	0.63	0.26	-	83,83,83,83	0
2	CA	B	550	1/1	0.55	0.39	-	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.