



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:12 AM GMT

PDB ID : 2A3I
Title : Structural and Biochemical Mechanisms for the Specificity of Hormone Binding and Coactivator Assembly by Mineralocorticoid Receptor
Authors : Li, Y.; Suino, K.; Daugherty, J.; Xu, H.E.
Deposited on : 2005-06-24
Resolution : 1.95 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

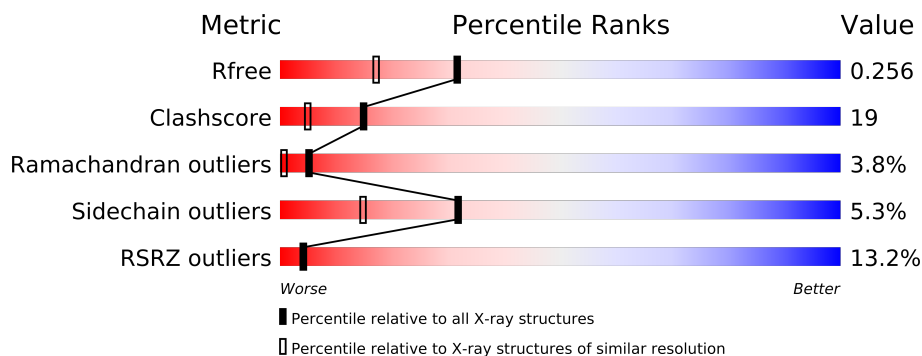
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.95 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}	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	253	
2	B	12	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2349 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	2064	1336	336	378	14	0	0	0

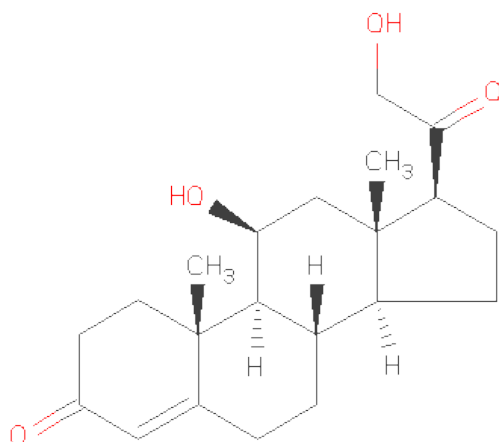
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	808	SER	CYS	ENGINEERED	UNP P08235

- Molecule 2 is a protein called Nuclear receptor coactivator 1, residues 1430-1441.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	12	100	62	17	21	0	0	0

- Molecule 3 is CORTICOSTERONE (three-letter code: C0R) (formula: C₂₁H₃₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		

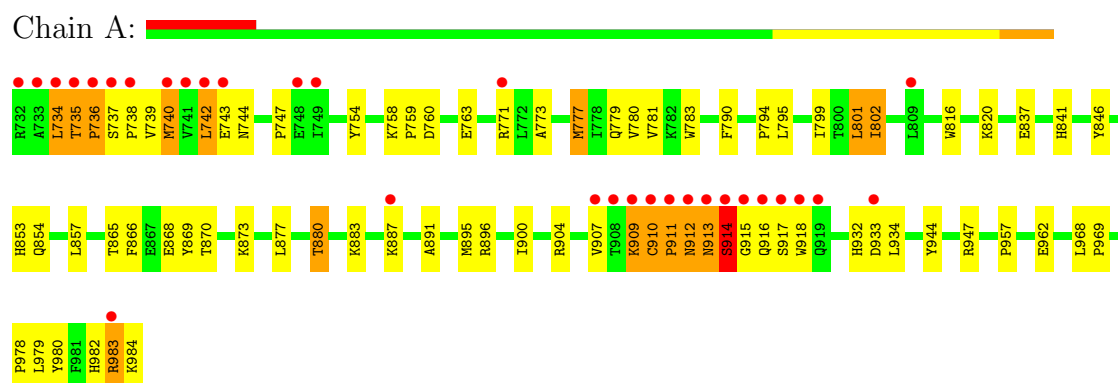
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	5	Total	O	0	0
			5	5		

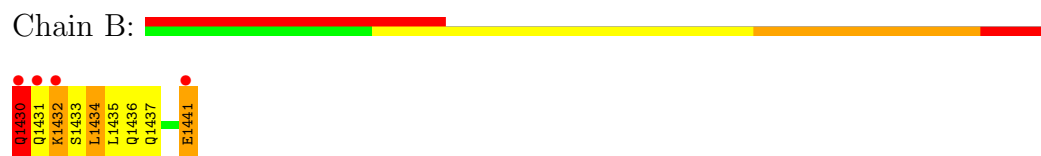
3 Residue-property plots

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: Mineralocorticoid receptor



- Molecule 2: Nuclear receptor coactivator 1, residues 1430-1441



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.65Å 72.26Å 81.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 28.09 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.95) 99.7 (28.09-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.253 0.223 , 0.256	Depositor DCC
R_{free} test set	1540 reflections (7.83%)	DCC
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19661 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2349	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C0R

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	0.94	2/2114 (0.1%)	1.23	6/2858 (0.2%)
2	B	0.38	0/99	1.52	5/130 (3.8%)
All	All	0.92	2/2213 (0.1%)	1.25	11/2988 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	802	ILE	CB-CG2	30.79	2.48	1.52
1	A	801	LEU	CG-CD2	25.84	2.47	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	801	LEU	CB-CG-CD2	-44.98	34.53	111.00
1	A	802	ILE	CG1-CB-CG2	-34.54	35.42	111.40
1	A	795	LEU	CB-CG-CD2	-10.17	93.72	111.00
2	B	1430	GLN	CG-CD-OE1	7.86	137.32	121.60
2	B	1430	GLN	CG-CD-NE2	-7.56	98.55	116.70
2	B	1434	LEU	CB-CG-CD1	-7.50	98.25	111.00
1	A	802	ILE	CA-CB-CG2	-6.64	97.62	110.90
2	B	1434	LEU	CA-CB-CG	-6.11	101.25	115.30
1	A	795	LEU	CB-CG-CD1	5.95	121.12	111.00
2	B	1430	GLN	CA-CB-CG	-5.67	100.92	113.40
1	A	801	LEU	CD1-CG-CD2	-5.25	94.74	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2064	0	2069	75	2
2	B	100	0	106	11	6
3	A	25	0	30	1	0
4	A	155	0	0	9	7
4	B	5	0	0	0	0
All	All	2349	0	2205	84	8

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (84) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1433:SER:HB3	2:B:1436:GLN:HE21	1.19	1.02
1:A:801:LEU:HD21	1:A:877:LEU:O	1.71	0.91
1:A:980:TYR:H	1:A:984:LYS:HE2	1.38	0.86
1:A:734:LEU:CD2	1:A:735:THR:H	1.95	0.80
2:B:1433:SER:CB	2:B:1436:GLN:HE21	1.97	0.77
1:A:738:PRO:O	1:A:742:LEU:HD23	1.90	0.71
1:A:947:ARG:HD2	4:A:19:HOH:O	1.92	0.70
1:A:865:THR:HG23	1:A:868:GLU:H	1.58	0.69
1:A:734:LEU:HD23	1:A:735:THR:H	1.57	0.69
1:A:880:THR:HG23	4:A:55:HOH:O	1.95	0.66
1:A:968:LEU:HB3	1:A:969:PRO:HD3	1.79	0.65
1:A:794:PRO:HG3	1:A:887:LYS:HG2	1.80	0.62
1:A:758:LYS:HB2	1:A:759:PRO:HD2	1.83	0.61
1:A:777:MET:HE3	1:A:780:VAL:HG21	1.84	0.60
2:B:1431:GLN:HG3	2:B:1432:LYS:HG3	1.83	0.59
1:A:865:THR:HG22	1:A:868:GLU:OE1	2.02	0.59
1:A:913:ASN:HB2	1:A:916:GLN:HG2	1.84	0.59
1:A:790:PHE:HA	1:A:895:MET:HE1	1.84	0.59
1:A:734:LEU:HD22	1:A:735:THR:H	1.68	0.58
1:A:980:TYR:HB2	1:A:984:LYS:HG3	1.84	0.58
1:A:982:HIS:O	1:A:983:ARG:C	2.44	0.56
1:A:747:PRO:HG3	4:A:148:HOH:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:801:LEU:CD2	1:A:877:LEU:O	2.50	0.55
1:A:983:ARG:HD2	1:A:983:ARG:O	2.07	0.55
1:A:773:ALA:HB2	3:A:301:C0R:H11A	1.89	0.55
1:A:841:HIS:HD2	4:A:9:HOH:O	1.90	0.55
1:A:911:PRO:O	1:A:912:ASN:HB3	2.08	0.54
1:A:912:ASN:OD1	1:A:913:ASN:N	2.41	0.54
1:A:739:VAL:HG13	1:A:740:MET:N	2.23	0.53
1:A:979:LEU:HA	1:A:984:LYS:HE2	1.91	0.53
2:B:1433:SER:HB3	2:B:1436:GLN:NE2	2.04	0.52
1:A:841:HIS:HE1	4:A:98:HOH:O	1.92	0.52
1:A:980:TYR:N	1:A:984:LYS:HE2	2.15	0.51
1:A:913:ASN:O	1:A:914:SER:C	2.48	0.51
1:A:865:THR:HG22	1:A:868:GLU:CD	2.31	0.51
1:A:904:ARG:O	1:A:907:VAL:HG12	2.12	0.50
1:A:865:THR:HG22	1:A:868:GLU:CG	2.42	0.50
1:A:865:THR:CG2	1:A:868:GLU:HG3	2.42	0.50
1:A:968:LEU:C	1:A:968:LEU:HD23	2.31	0.50
1:A:891:ALA:O	1:A:895:MET:HG3	2.12	0.49
1:A:896:ARG:O	1:A:900:ILE:HG13	2.12	0.49
2:B:1432:LYS:O	2:B:1433:SER:HB3	2.13	0.49
1:A:853:HIS:HD2	4:A:114:HOH:O	1.95	0.49
2:B:1431:GLN:HA	2:B:1431:GLN:OE1	2.13	0.48
1:A:880:THR:HG21	4:A:74:HOH:O	2.13	0.48
1:A:734:LEU:CD2	1:A:735:THR:N	2.73	0.48
1:A:743:GLU:HG2	1:A:866:PHE:CE2	2.50	0.47
1:A:754:TYR:OH	1:A:760:ASP:OD1	2.25	0.47
2:B:1431:GLN:O	2:B:1432:LYS:HB2	2.15	0.47
1:A:982:HIS:O	1:A:984:LYS:N	2.47	0.47
1:A:909:LYS:HG2	1:A:910:CYS:N	2.29	0.46
1:A:783:TRP:CZ2	1:A:873:LYS:HE2	2.50	0.46
1:A:854:GLN:NE2	1:A:857:LEU:HD12	2.30	0.46
1:A:912:ASN:O	1:A:913:ASN:C	2.52	0.46
1:A:910:CYS:HB3	1:A:911:PRO:HD3	1.97	0.46
1:A:909:LYS:O	1:A:910:CYS:C	2.54	0.46
1:A:802:ILE:HG23	1:A:877:LEU:HD11	1.97	0.45
1:A:913:ASN:O	1:A:915:GLY:N	2.49	0.45
1:A:866:PHE:O	1:A:870:THR:HG23	2.16	0.45
1:A:837:GLU:OE2	1:A:846:TYR:OH	2.21	0.45
1:A:983:ARG:HG3	4:A:100:HOH:O	2.15	0.44
1:A:758:LYS:HE2	1:A:758:LYS:HB3	1.83	0.44
1:A:820:LYS:HB3	1:A:820:LYS:NZ	2.32	0.44
1:A:739:VAL:O	1:A:743:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:913:ASN:HB2	1:A:916:GLN:CG	2.47	0.43
1:A:816:TRP:HB2	1:A:869:TYR:CE2	2.54	0.42
1:A:980:TYR:HB2	1:A:984:LYS:CG	2.49	0.42
1:A:962:GLU:OE2	2:B:1434:LEU:HG	2.18	0.42
1:A:747:PRO:HB3	1:A:779:GLN:HB3	2.01	0.42
1:A:737:SER:OG	1:A:739:VAL:HG12	2.19	0.42
2:B:1437:GLN:O	2:B:1441:GLU:N	2.53	0.41
1:A:933:ASP:OD1	1:A:934:LEU:N	2.52	0.41
1:A:777:MET:O	1:A:781:VAL:HG23	2.20	0.41
1:A:771:ARG:HD3	1:A:957:PRO:HB3	2.01	0.41
1:A:880:THR:HG22	1:A:932:HIS:HE1	1.85	0.41
1:A:739:VAL:CG1	1:A:740:MET:N	2.84	0.41
2:B:1431:GLN:O	2:B:1432:LYS:CB	2.68	0.41
1:A:909:LYS:O	1:A:911:PRO:N	2.53	0.41
1:A:799:ILE:HG23	2:B:1435:LEU:HD23	2.02	0.41
1:A:763:GLU:HG2	4:A:136:HOH:O	2.20	0.41
1:A:912:ASN:O	1:A:913:ASN:O	2.38	0.41
1:A:854:GLN:NE2	1:A:854:GLN:HA	2.36	0.40
1:A:820:LYS:HB3	1:A:820:LYS:HZ2	1.87	0.40
1:A:932:HIS:CE1	1:A:978:PRO:HB3	2.56	0.40

All (8) 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	Distance(Å)	Clash(Å)
2:B:1430:GLN:CG	4:A:140:HOH:O[4.575]	0.63	1.57
2:B:1430:GLN:CD	4:A:140:HOH:O[4.575]	1.00	1.20
2:B:1430:GLN:OE1	4:A:140:HOH:O[4.575]	1.94	0.26
1:A:914:SER:OG	1:A:944:TYR:OH[2.574]	1.96	0.24
2:B:1430:GLN:NE2	4:A:140:HOH:O[4.575]	1.97	0.23
2:B:1430:GLN:CB	4:A:140:HOH:O[4.575]	2.09	0.11
2:B:1431:GLN:NE2	4:A:156:HOH:O[1.655]	2.15	0.05
1:A:916:GLN:NE2	4:A:126:HOH:O[4.465]	2.19	0.01

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	251/253 (99%)	236 (94%)	6 (2%)	9 (4%)	5	1
2	B	10/12 (83%)	8 (80%)	1 (10%)	1 (10%)	1	0
All	All	261/265 (98%)	244 (94%)	7 (3%)	10 (4%)	5	1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	909	LYS
1	A	912	ASN
1	A	983	ARG
1	A	736	PRO
1	A	911	PRO
1	A	914	SER
2	B	1432	LYS
1	A	910	CYS
1	A	913	ASN
1	A	917	SER

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	232/233 (100%)	221 (95%)	11 (5%)	36	18
2	B	12/12 (100%)	10 (83%)	2 (17%)	3	0
All	All	244/245 (100%)	231 (95%)	13 (5%)	32	15

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	734	LEU
1	A	735	THR
1	A	736	PRO
1	A	740	MET
1	A	742	LEU
1	A	744	ASN
1	A	777	MET

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Mol	Chain	Res	Type
1	A	880	THR
1	A	883	LYS
1	A	914	SER
1	A	918	TRP
2	B	1430	GLN
2	B	1441	GLU

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	841	HIS
1	A	842	GLN
1	A	850	GLN
1	A	854	GLN
1	A	913	ASN
1	A	975	ASN
2	B	1430	GLN
2	B	1436	GLN
2	B	1437	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
3	C0R	A	301	-	28,28,28	2.39	10 (35%)	45,45,45	2.24	14 (31%)

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	C0R	A	301	-	-	0/6/67/67	0/0/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	C0R	C1-C2	-6.99	1.37	1.53
3	A	301	C0R	C12-C13	4.10	1.61	1.54
3	A	301	C0R	C4-C3	3.83	1.54	1.45
3	A	301	C0R	C18-C13	3.60	1.61	1.54
3	A	301	C0R	C9-C11	3.15	1.59	1.54
3	A	301	C0R	C8-C9	3.05	1.58	1.54
3	A	301	C0R	C17-C20	2.81	1.57	1.52
3	A	301	C0R	C6-C5	2.54	1.54	1.50
3	A	301	C0R	O3-C20	2.17	1.25	1.21
3	A	301	C0R	C19-C10	2.09	1.58	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	C0R	C2-C1-C10	8.51	125.37	113.39
3	A	301	C0R	C19-C10-C1	-5.11	101.31	109.45
3	A	301	C0R	C19-C10-C5	-4.07	101.84	108.39
3	A	301	C0R	C1-C10-C9	3.59	115.03	109.32
3	A	301	C0R	C1-C2-C3	3.29	118.08	111.63
3	A	301	C0R	C6-C5-C4	-3.18	116.94	120.93
3	A	301	C0R	C21-C20-C17	3.09	121.75	116.36
3	A	301	C0R	C5-C4-C3	-2.94	120.14	123.77
3	A	301	C0R	C13-C17-C20	-2.58	111.82	115.56
3	A	301	C0R	C6-C7-C8	2.28	115.51	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	C0R	C1-C10-C5	2.26	113.04	108.81
3	A	301	C0R	C10-C9-C11	-2.19	112.11	114.36
3	A	301	C0R	C19-C10-C9	2.06	115.81	112.63
3	A	301	C0R	C6-C5-C10	2.06	119.00	116.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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(Å ²)	Q<0.9
1	A	253/253 (100%)	0.97	31 (12%) 5 5	21, 32, 87, 101	0
2	B	12/12 (100%)	2.24	4 (33%) 1 0	40, 43, 59, 63	0
All	All	265/265 (100%)	1.03	35 (13%) 4 4	21, 32, 85, 101	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	914	SER	14.9
1	A	915	GLY	12.5
2	B	1430	GLN	12.0
1	A	733	ALA	10.4
1	A	734	LEU	10.3
1	A	736	PRO	9.3
1	A	910	CYS	9.2
1	A	913	ASN	9.1
1	A	735	THR	7.9
1	A	912	ASN	7.1
2	B	1431	GLN	5.3
1	A	738	PRO	5.3
1	A	918	TRP	5.2
1	A	911	PRO	4.9
1	A	737	SER	4.8
1	A	917	SER	4.4
1	A	909	LYS	4.1
1	A	908	THR	3.9
1	A	732	ARG	3.9
1	A	907	VAL	3.7
1	A	740	MET	3.3
1	A	916	GLN	3.3
2	B	1441	GLU	3.1
1	A	983	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	743	GLU	3.0
1	A	742	LEU	2.9
1	A	749	ILE	2.9
2	B	1432	LYS	2.8
1	A	933	ASP	2.5
1	A	887	LYS	2.5
1	A	748	GLU	2.3
1	A	771	ARG	2.3
1	A	919	GLN	2.2
1	A	741	VAL	2.2
1	A	809	LEU	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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q < 0.9
3	C0R	A	301	25/25	0.18	1.77	19,22,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.