



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:36 PM UTC

PDB ID : 1Y9R / pdb_00001y9r
Title : Crystal structure of the human mineralocorticoid receptor ligand-binding domain bound to deoxycorticosterone and harboring the S810L mutation responsible for a severe form of hypertension
Authors : Fagart, J.; Huyet, J.; Pinon, G.M.; Rochel, M.; Mayer, C.; Rafestin-Oblin, M.E.
Deposited on : 2004-12-16
Resolution : 1.96 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

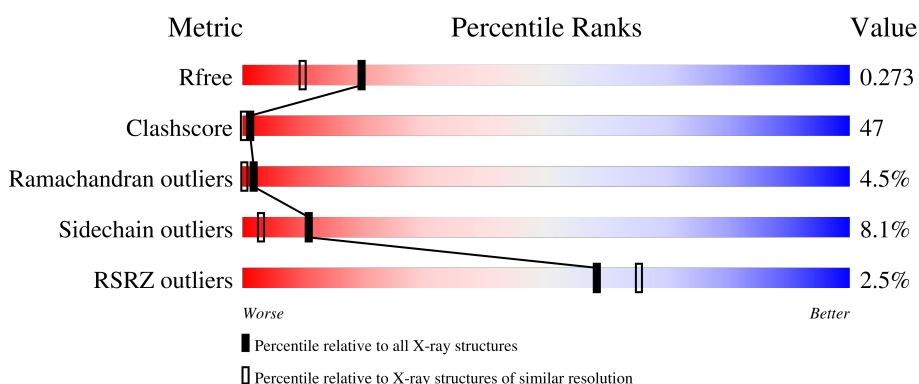
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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 $\leq 5\%$. 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	255	3% 26% 56% 11% 6%
1	B	255	2% 32% 53% 9% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4394 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.

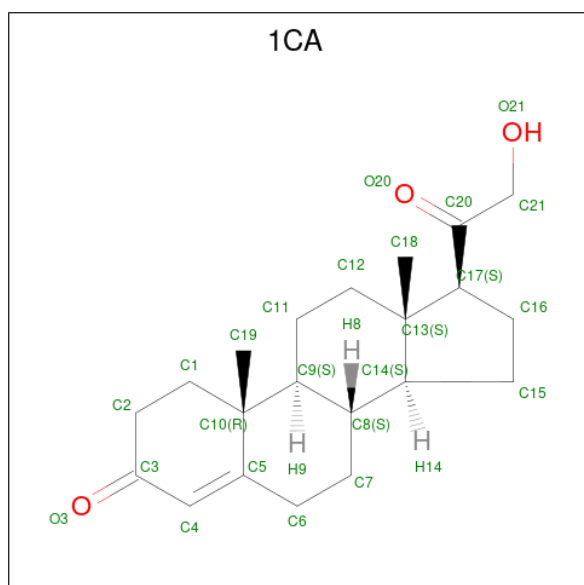
- Molecule 1 is a protein called Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1952	1270	317	351	14			
1	B	238	Total	C	N	O	S	0	0	0
			1933	1255	311	354	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	SER	-	cloning artifact	UNP P08235
A	810	LEU	SER	engineered mutation	UNP P08235
A	910	ALA	CYS	engineered mutation	UNP P08235
B	730	SER	-	cloning artifact	UNP P08235
B	810	LEU	SER	engineered mutation	UNP P08235
B	910	ALA	CYS	engineered mutation	UNP P08235

- Molecule 2 is DESOXYCORTICOSTERONE (CCD ID: 1CA) (formula: $C_{21}H_{30}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 24	C 21	O 3	0	0
2	B	1	Total 24	C 21	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total 236	O 236	0	0
3	B	225	Total 225	O 225	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	120.28Å 120.28Å 41.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.30 – 1.96 18.30 – 1.96	Depositor EDS
% Data completeness (in resolution range)	84.1 (18.30-1.96) 84.1 (18.30-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.96Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.267 0.239 , 0.273	Depositor DCC
R_{free} test set	4101 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 153.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l 0.118 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4394	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8957e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 1CA

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	0.41	0/1998	1.01	11/2701 (0.4%)
1	B	0.41	0/1976	0.95	8/2668 (0.3%)
All	All	0.41	0/3974	0.98	19/5369 (0.4%)

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	A	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	900	ILE	N-CA-C	-7.51	103.01	110.30
1	B	777	MET	CG-SD-CE	-6.95	85.61	100.90
1	A	848	LEU	N-CA-C	-6.39	105.61	113.41
1	A	972	GLU	N-CA-C	-6.33	105.27	112.87
1	B	757	SER	N-CA-C	-6.13	105.96	113.50
1	A	877	LEU	N-CA-C	-6.09	104.72	111.36
1	A	843	SER	N-CA-C	-5.80	105.53	113.30
1	B	843	SER	N-CA-C	-5.78	106.27	113.38
1	B	838	GLU	N-CA-C	-5.71	106.40	113.19
1	A	766	LEU	N-CA-C	5.63	117.41	111.28
1	A	905	LYS	N-CA-C	-5.54	105.14	111.07
1	B	746	GLU	CA-C-N	5.43	126.63	119.84
1	B	746	GLU	C-N-CA	5.43	126.63	119.84
1	A	945	THR	N-CA-C	-5.39	106.20	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	874	VAL	N-CA-C	-5.23	105.44	110.72
1	B	866	PHE	N-CA-C	5.18	117.00	111.36
1	B	824	SER	N-CA-C	5.17	121.82	110.80
1	A	835	PHE	N-CA-C	5.04	117.19	109.07
1	A	887	LYS	N-CA-C	-5.03	105.48	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	944	TYR	Sidechain

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	1952	0	1961	195	0
1	B	1933	0	1936	174	0
2	A	24	0	30	5	0
2	B	24	0	30	5	0
3	A	236	0	0	19	0
3	B	225	0	0	26	0
All	All	4394	0	3957	371	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 47.

All (371) 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:836:ASN:HD22	1:A:837:GLU:N	1.43	1.15
1:A:812:PHE:HB2	1:A:931:MET:HE1	1.30	1.11
1:B:872:MET:HA	1:B:875:LEU:HD12	1.35	1.06
1:B:755:ASP:HB2	1:B:758:LYS:HG2	1.37	1.03
1:A:836:ASN:ND2	1:A:837:GLU:N	2.10	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:878:LEU:HD11	1:B:895:MET:HE2	1.42	0.99
1:A:806:TRP:HA	1:A:809:LEU:HD12	1.46	0.96
1:A:807:MET:HE1	2:A:2001:1CA:H191	1.51	0.92
1:B:848:LEU:HD23	1:B:938:LEU:HD23	1.52	0.90
1:B:964:ILE:HG23	1:B:968:LEU:HD12	1.55	0.89
1:A:983:ARG:NH1	1:A:983:ARG:HB2	1.88	0.88
1:A:777:MET:HE3	1:A:780:VAL:HB	1.57	0.87
1:B:861:ARG:HD3	3:B:1016:HOH:O	1.75	0.86
1:A:853:HIS:CE1	1:A:857:LEU:HD21	2.12	0.83
1:B:950:HIS:NE2	3:B:1110:HOH:O	2.11	0.83
1:A:782:LYS:HA	1:A:785:LYS:HE2	1.61	0.83
1:A:761:THR:HG22	1:A:762:ALA:H	1.44	0.83
1:A:825:GLN:NE2	3:A:1270:HOH:O	2.13	0.81
1:A:903:LEU:O	1:A:907:VAL:HG23	1.82	0.80
1:B:845:MET:HG3	1:B:848:LEU:HD13	1.61	0.80
1:A:836:ASN:ND2	1:A:837:GLU:H	1.76	0.80
1:A:790:PHE:HA	1:A:895:MET:HE1	1.64	0.80
1:A:802:ILE:HG13	3:A:1130:HOH:O	1.84	0.78
1:A:876:LEU:HD13	1:A:931:MET:SD	2.24	0.77
1:A:738:PRO:O	1:A:741:VAL:HG22	1.84	0.77
1:A:846:TYR:O	1:A:847:GLU:HG2	1.82	0.77
1:B:942:CYS:HA	2:B:3001:1CA:O20	1.85	0.77
1:B:871:ILE:O	1:B:875:LEU:HG	1.85	0.77
1:A:943:PHE:HB2	1:A:968:LEU:HD13	1.67	0.77
1:A:775:LYS:O	1:A:778:ILE:HG22	1.85	0.76
1:B:749:ILE:HD12	1:B:749:ILE:H	1.49	0.76
1:B:795:LEU:HD12	1:B:795:LEU:O	1.86	0.76
1:B:946:PHE:CD1	1:B:964:ILE:HG21	2.22	0.76
1:A:787:LEU:HD21	1:A:874:VAL:HG13	1.67	0.75
1:B:964:ILE:HG23	1:B:968:LEU:CD1	2.15	0.75
1:A:768:THR:HA	3:A:1078:HOH:O	1.86	0.75
1:B:833:LEU:HG	1:B:835:PHE:HE1	1.52	0.74
1:B:926:LYS:HG3	1:B:927:LEU:N	2.01	0.74
1:B:934:LEU:HD23	1:B:935:VAL:N	2.04	0.73
1:B:975:ASN:HB3	3:B:1226:HOH:O	1.88	0.73
1:A:802:ILE:HD13	1:A:877:LEU:HD11	1.70	0.72
1:B:772:LEU:HD21	1:B:776:GLN:NE2	2.04	0.72
1:B:871:ILE:HD11	1:B:899:TYR:O	1.88	0.72
1:B:871:ILE:HD13	1:B:903:LEU:HB2	1.71	0.71
1:B:937:ASP:O	1:B:940:GLU:HG3	1.90	0.71
1:A:847:GLU:OE1	1:A:847:GLU:HA	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:VAL:HG11	1:A:976:ALA:HB2	1.73	0.71
1:A:806:TRP:CZ3	1:A:960:LEU:HD11	2.26	0.71
1:B:738:PRO:O	1:B:742:LEU:HG	1.91	0.71
1:B:946:PHE:CG	1:B:964:ILE:HG21	2.26	0.71
1:B:878:LEU:HD11	1:B:895:MET:CE	2.20	0.70
1:A:836:ASN:HD22	1:A:836:ASN:C	1.99	0.70
1:A:867:GLU:O	1:A:870:THR:HG22	1.90	0.70
1:A:967:GLN:C	1:A:969:PRO:HD2	2.16	0.69
1:A:775:LYS:HE2	3:A:1162:HOH:O	1.91	0.69
1:B:785:LYS:HG3	1:B:786:VAL:HG23	1.75	0.69
1:B:857:LEU:HA	1:B:860:VAL:HG23	1.75	0.69
1:B:845:MET:HG2	1:B:848:LEU:HB2	1.75	0.68
1:A:786:VAL:HA	1:A:791:LYS:HE2	1.75	0.68
2:B:3001:1CA:H72	3:B:1255:HOH:O	1.92	0.68
1:A:761:THR:HG22	1:A:762:ALA:N	2.08	0.68
1:A:837:GLU:O	1:A:841:HIS:HB2	1.93	0.68
1:A:839:LYS:O	1:A:843:SER:HB3	1.94	0.68
1:A:802:ILE:HD13	1:A:877:LEU:CD1	2.24	0.68
1:A:939:LEU:HD22	1:A:967:GLN:HE22	1.57	0.67
1:A:872:MET:HB3	1:A:928:LEU:HD21	1.77	0.67
1:A:939:LEU:HD22	1:A:967:GLN:NE2	2.10	0.67
1:B:772:LEU:HD12	1:B:833:LEU:HD23	1.76	0.67
1:B:856:SER:O	1:B:859:PHE:HB2	1.95	0.66
1:B:944:TYR:HA	3:B:1366:HOH:O	1.94	0.66
1:A:876:LEU:HD21	1:A:928:LEU:HD22	1.78	0.66
1:B:739:VAL:HG23	1:B:740:MET:N	2.11	0.65
1:B:964:ILE:HG22	1:B:965:SER:N	2.10	0.65
1:B:786:VAL:HG12	1:B:786:VAL:O	1.96	0.65
1:A:761:THR:N	1:A:764:ASN:OD1	2.29	0.65
1:A:742:LEU:HA	1:A:745:ILE:HG12	1.78	0.65
1:A:765:LEU:HD22	1:A:765:LEU:H	1.61	0.65
1:A:932:HIS:CE1	1:A:978:PRO:HB3	2.32	0.65
1:B:740:MET:HA	1:B:740:MET:HE2	1.78	0.65
1:A:972:GLU:OE2	1:A:972:GLU:HA	1.97	0.64
1:B:773:ALA:HB3	1:B:960:LEU:HD11	1.79	0.64
1:A:853:HIS:HE1	1:A:857:LEU:HD21	1.60	0.64
1:A:854:GLN:O	1:A:858:GLN:HG3	1.99	0.63
1:A:773:ALA:HB2	2:A:2001:1CA:H193	1.79	0.63
1:B:739:VAL:HG23	1:B:740:MET:H	1.64	0.63
1:A:881:ILE:HG23	3:A:1364:HOH:O	1.99	0.62
1:A:776:GLN:O	1:A:779:GLN:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:LYS:HD3	3:A:1205:HOH:O	2.00	0.62
1:A:801:LEU:HD21	1:A:892:PHE:CE1	2.35	0.62
1:B:872:MET:HA	1:B:875:LEU:CD1	2.22	0.62
1:A:894:GLU:O	1:A:897:THR:HG22	2.00	0.62
1:B:854:GLN:NE2	3:B:1273:HOH:O	2.33	0.61
1:B:749:ILE:HD12	1:B:749:ILE:N	2.15	0.61
1:A:797:ASP:O	1:A:801:LEU:HD13	2.00	0.61
1:B:772:LEU:HD21	1:B:776:GLN:HE21	1.63	0.61
1:B:866:PHE:HZ	3:B:1274:HOH:O	1.81	0.61
1:B:879:SER:O	1:B:979:LEU:HG	2.01	0.61
1:B:901:LYS:O	1:B:905:LYS:HG3	2.01	0.61
1:B:972:GLU:CD	3:B:1146:HOH:O	2.43	0.61
1:B:907:VAL:CG1	1:B:920:ARG:HB3	2.30	0.60
1:A:928:LEU:O	1:A:931:MET:HB3	2.01	0.60
1:B:972:GLU:HB2	3:B:1430:HOH:O	2.00	0.60
1:A:860:VAL:O	1:A:863:GLN:HG3	2.02	0.60
1:B:794:PRO:HB2	3:B:1263:HOH:O	2.01	0.60
1:A:983:ARG:HB2	1:A:983:ARG:CZ	2.32	0.60
1:B:968:LEU:N	1:B:969:PRO:HD2	2.17	0.60
1:A:820:LYS:HE3	1:A:820:LYS:HA	1.82	0.59
1:B:755:ASP:HB2	1:B:758:LYS:CG	2.25	0.59
1:B:808:CYS:HB3	1:B:876:LEU:HD13	1.85	0.59
1:A:954:VAL:HG21	3:A:1045:HOH:O	2.02	0.59
1:A:971:VAL:C	1:A:973:SER:N	2.60	0.59
1:B:853:HIS:CE1	1:B:857:LEU:HD21	2.38	0.58
1:B:944:TYR:HD1	3:B:1366:HOH:O	1.85	0.58
1:B:983:ARG:O	1:B:984:LYS:HB2	2.02	0.58
1:A:907:VAL:HG13	1:A:920:ARG:HB3	1.85	0.58
1:A:823:ASN:HA	3:A:1103:HOH:O	2.04	0.58
1:B:764:ASN:HB3	3:B:1009:HOH:O	2.02	0.58
1:A:823:ASN:O	1:A:824:SER:HB2	2.03	0.58
1:B:776:GLN:O	1:B:780:VAL:HG23	2.03	0.58
1:A:812:PHE:CB	1:A:931:MET:HE1	2.20	0.57
1:B:772:LEU:HD23	1:B:772:LEU:O	2.05	0.57
1:A:798:GLN:O	1:A:802:ILE:HG12	2.04	0.57
1:A:942:CYS:HA	2:A:2001:1CA:O20	2.04	0.57
1:A:971:VAL:C	1:A:973:SER:H	2.10	0.57
1:B:817:ARG:HD3	3:B:1014:HOH:O	2.05	0.57
1:A:983:ARG:HB2	1:A:983:ARG:HH11	1.65	0.57
1:A:968:LEU:N	1:A:969:PRO:HD2	2.19	0.56
1:B:794:PRO:HG2	1:B:797:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:LYS:HD2	3:A:1311:HOH:O	2.06	0.56
1:A:964:ILE:HD11	3:A:1108:HOH:O	2.04	0.56
1:A:976:ALA:O	1:A:978:PRO:HD3	2.06	0.56
1:A:848:LEU:HD23	1:A:938:LEU:HD23	1.88	0.56
1:A:875:LEU:O	1:A:879:SER:HB2	2.05	0.56
1:A:941:PHE:O	1:A:945:THR:HG23	2.06	0.55
1:B:761:THR:OG1	1:B:763:GLU:HG3	2.05	0.55
1:B:836:ASN:CG	1:B:837:GLU:H	2.14	0.55
1:A:968:LEU:N	1:A:969:PRO:CD	2.70	0.55
1:A:853:HIS:O	1:A:857:LEU:HG	2.06	0.55
1:A:908:THR:HG23	3:A:1342:HOH:O	2.06	0.55
1:B:748:GLU:O	1:B:779:GLN:NE2	2.39	0.55
1:B:926:LYS:HD3	3:B:1265:HOH:O	2.07	0.54
2:B:3001:1CA:H152	3:B:1255:HOH:O	2.07	0.54
1:A:744:ASN:C	1:A:744:ASN:ND2	2.65	0.54
1:B:901:LYS:HG2	1:B:904:ARG:HH22	1.72	0.54
1:B:920:ARG:O	1:B:924:LEU:HG	2.06	0.54
1:A:854:GLN:HA	1:A:857:LEU:HD12	1.89	0.54
1:A:761:THR:CG2	1:A:762:ALA:H	2.18	0.54
1:A:748:GLU:OE1	3:A:1282:HOH:O	2.18	0.54
1:B:888:SER:HB3	1:B:891:ALA:HB3	1.89	0.54
1:B:818:SER:HB3	3:B:1228:HOH:O	2.07	0.54
1:A:876:LEU:HD22	1:A:931:MET:SD	2.48	0.54
1:A:744:ASN:C	1:A:744:ASN:HD22	2.15	0.53
1:A:758:LYS:HB3	1:A:759:PRO:HD2	1.89	0.53
1:A:777:MET:HE2	3:A:1030:HOH:O	2.09	0.53
1:A:943:PHE:CB	1:A:968:LEU:HD13	2.36	0.53
1:B:780:VAL:O	1:B:783:TRP:HB3	2.08	0.53
1:A:737:SER:N	1:A:738:PRO:CD	2.72	0.53
1:A:745:ILE:HG22	3:A:1307:HOH:O	2.08	0.53
1:B:836:ASN:CG	1:B:837:GLU:N	2.66	0.53
1:B:845:MET:CG	1:B:848:LEU:HD13	2.34	0.53
1:B:858:GLN:HB2	3:B:1379:HOH:O	2.07	0.53
1:B:943:PHE:CD1	1:B:968:LEU:HD13	2.42	0.53
1:A:776:GLN:OE1	1:A:810:LEU:HD22	2.09	0.53
1:B:769:LEU:HD23	1:B:833:LEU:HD21	1.89	0.53
1:A:920:ARG:O	1:A:921:PHE:C	2.52	0.53
1:A:939:LEU:CD2	1:A:967:GLN:HE22	2.21	0.53
1:B:737:SER:OG	1:B:738:PRO:HD3	2.09	0.53
1:B:772:LEU:CD2	1:B:776:GLN:NE2	2.70	0.53
1:A:820:LYS:HA	1:A:820:LYS:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:GLN:O	1:A:854:GLN:HG2	2.08	0.53
1:A:876:LEU:CD1	1:A:931:MET:SD	2.96	0.53
1:B:772:LEU:HD22	2:B:3001:1CA:H21	1.89	0.52
1:B:901:LYS:HG2	1:B:904:ARG:NH2	2.23	0.52
1:A:971:VAL:HG12	1:A:971:VAL:O	2.09	0.52
1:A:737:SER:N	1:A:738:PRO:HD2	2.25	0.52
1:B:793:LEU:HB3	1:B:794:PRO:HD2	1.91	0.52
1:A:765:LEU:HD22	1:A:765:LEU:N	2.25	0.52
1:A:934:LEU:O	1:A:937:ASP:HB2	2.08	0.52
1:B:934:LEU:HD23	1:B:934:LEU:C	2.34	0.52
1:B:845:MET:HE2	1:B:849:CYS:SG	2.50	0.52
1:B:895:MET:HE3	1:B:899:TYR:HE2	1.75	0.52
1:B:907:VAL:HG11	1:B:920:ARG:HB3	1.91	0.52
1:A:886:LEU:O	1:A:889:GLN:HB2	2.10	0.51
1:A:739:VAL:HG13	1:A:740:MET:H	1.74	0.51
1:B:776:GLN:OE1	1:B:810:LEU:HD22	2.09	0.51
1:A:804:TYR:CE2	1:A:882:PRO:HG3	2.45	0.51
1:A:906:MET:SD	1:A:906:MET:C	2.94	0.51
1:A:756:SER:O	1:A:757:SER:HB2	2.11	0.51
1:A:816:TRP:CE2	1:A:820:LYS:HG3	2.45	0.51
1:B:808:CYS:SG	1:B:935:VAL:HG21	2.50	0.51
1:B:837:GLU:C	1:B:839:LYS:H	2.19	0.51
1:B:938:LEU:HB3	3:B:1255:HOH:O	2.10	0.51
1:A:784:ALA:HB1	1:A:790:PHE:CE2	2.46	0.51
1:B:775:LYS:O	1:B:778:ILE:HG13	2.11	0.51
1:A:805:SER:O	1:A:809:LEU:HG	2.11	0.51
1:A:742:LEU:HD12	1:A:870:THR:HG23	1.93	0.51
1:A:983:ARG:HH11	1:A:983:ARG:CB	2.23	0.51
1:B:755:ASP:C	1:B:757:SER:H	2.17	0.51
1:B:848:LEU:HD23	1:B:938:LEU:HA	1.92	0.51
1:A:931:MET:HB2	3:A:1119:HOH:O	2.11	0.51
1:B:749:ILE:H	1:B:749:ILE:CD1	2.23	0.51
1:B:840:MET:O	1:B:846:TYR:HB2	2.11	0.51
1:A:819:TYR:CE1	1:A:860:VAL:HA	2.45	0.50
1:A:868:GLU:HG2	1:A:924:LEU:CD1	2.42	0.50
1:A:801:LEU:HD11	1:A:886:LEU:HD11	1.94	0.50
1:A:742:LEU:HB3	1:A:870:THR:OG1	2.12	0.50
1:B:878:LEU:HD21	1:B:895:MET:HE1	1.93	0.50
1:A:780:VAL:HG11	1:A:809:LEU:HD13	1.93	0.50
1:B:871:ILE:HD12	1:B:902:GLU:HB3	1.94	0.50
1:A:846:TYR:CD1	1:A:846:TYR:C	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:GLN:O	1:B:806:TRP:HD1	1.95	0.49
1:B:871:ILE:CD1	1:B:902:GLU:HB3	2.42	0.49
1:A:956:PHE:O	1:A:957:PRO:O	2.31	0.49
1:B:855:ILE:HG23	3:B:1379:HOH:O	2.13	0.49
1:B:873:LYS:HE2	3:B:1141:HOH:O	2.11	0.49
1:B:827:LEU:HD12	1:B:840:MET:HE2	1.95	0.49
1:B:946:PHE:CE1	1:B:964:ILE:HG21	2.47	0.49
1:B:983:ARG:O	3:B:1077:HOH:O	2.19	0.49
1:A:807:MET:HE2	1:A:807:MET:HA	1.94	0.49
1:A:932:HIS:ND1	1:A:978:PRO:HB3	2.28	0.49
1:B:851:GLY:O	1:B:854:GLN:HB3	2.13	0.49
1:B:778:ILE:O	1:B:781:VAL:HG23	2.12	0.48
1:A:812:PHE:HB2	1:A:931:MET:CE	2.21	0.48
1:A:747:PRO:HB2	1:A:779:GLN:NE2	2.28	0.48
1:A:868:GLU:HG2	1:A:924:LEU:HD11	1.94	0.48
1:B:841:HIS:C	1:B:843:SER:H	2.21	0.48
1:A:895:MET:O	1:A:898:ASN:HB2	2.12	0.48
1:B:788:PRO:HB2	1:B:899:TYR:OH	2.14	0.48
1:A:971:VAL:CG1	1:A:976:ALA:HB2	2.40	0.48
1:A:836:ASN:C	1:A:838:GLU:H	2.22	0.48
1:A:889:GLN:O	1:A:892:PHE:HB3	2.14	0.47
1:A:738:PRO:O	1:A:739:VAL:C	2.56	0.47
1:B:819:TYR:HA	1:B:824:SER:OG	2.14	0.47
1:B:768:THR:HG21	3:B:1373:HOH:O	2.12	0.47
1:B:771:ARG:HA	1:B:957:PRO:HG3	1.96	0.47
1:B:897:THR:O	1:B:901:LYS:HG3	2.15	0.47
1:B:943:PHE:HD1	1:B:968:LEU:HD13	1.78	0.47
1:A:846:TYR:O	1:A:847:GLU:CG	2.57	0.47
1:B:878:LEU:CD1	1:B:895:MET:HE2	2.30	0.47
1:A:950:HIS:CG	1:A:951:ALA:N	2.83	0.47
1:B:902:GLU:O	1:B:905:LYS:HB2	2.15	0.47
1:B:807:MET:HB3	1:B:935:VAL:HG13	1.97	0.47
1:A:871:ILE:HG21	1:A:903:LEU:HB2	1.98	0.46
1:B:895:MET:HE3	1:B:899:TYR:CE2	2.50	0.46
1:A:765:LEU:H	1:A:765:LEU:CD2	2.27	0.46
1:A:741:VAL:HG23	1:A:742:LEU:HD23	1.96	0.46
1:A:818:SER:OG	1:A:827:LEU:HA	2.15	0.46
1:B:741:VAL:O	1:B:745:ILE:HG12	2.14	0.46
1:A:860:VAL:HG13	3:A:1103:HOH:O	2.13	0.46
1:A:983:ARG:O	1:A:983:ARG:HG3	2.14	0.46
1:B:814:LEU:HD22	2:B:3001:1CA:H4	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:GLY:C	1:A:895:MET:SD	2.99	0.46
1:B:871:ILE:CG2	1:B:903:LEU:HD13	2.45	0.46
1:B:816:TRP:O	1:B:820:LYS:N	2.38	0.46
1:A:944:TYR:CE1	1:A:948:GLU:HG3	2.51	0.46
1:A:739:VAL:HG13	1:A:740:MET:N	2.31	0.46
1:A:818:SER:HB3	1:A:826:PHE:O	2.16	0.45
1:A:983:ARG:NH1	1:A:983:ARG:CB	2.71	0.45
1:A:864:LEU:HD11	1:A:872:MET:SD	2.56	0.45
1:B:920:ARG:HA	1:B:923:GLN:OE1	2.17	0.45
1:A:814:LEU:HD13	1:A:829:PHE:HA	1.99	0.45
1:A:897:THR:O	1:A:901:LYS:HD3	2.16	0.45
1:A:743:GLU:HA	1:A:866:PHE:HE2	1.82	0.45
1:A:754:TYR:O	1:A:756:SER:N	2.48	0.45
1:B:859:PHE:CE2	1:B:864:LEU:HD22	2.51	0.45
1:A:743:GLU:HA	1:A:866:PHE:CE2	2.51	0.45
1:A:808:CYS:SG	1:A:935:VAL:HG21	2.56	0.45
1:A:940:GLU:HB2	3:A:1246:HOH:O	2.16	0.45
1:B:833:LEU:HG	1:B:835:PHE:CE1	2.41	0.45
1:A:897:THR:O	1:A:900:ILE:HB	2.15	0.45
1:B:907:VAL:HG13	1:B:920:ARG:HB3	1.98	0.45
1:B:772:LEU:HD23	1:B:772:LEU:C	2.41	0.45
1:B:829:PHE:HB2	1:B:833:LEU:O	2.16	0.45
1:B:945:THR:HB	1:B:954:VAL:HG11	1.98	0.45
1:B:794:PRO:HG2	1:B:797:ASP:CG	2.42	0.44
1:A:746:GLU:OE2	1:A:747:PRO:HD2	2.17	0.44
1:A:814:LEU:HB2	2:A:2001:1CA:O3	2.16	0.44
1:A:950:HIS:ND1	1:A:951:ALA:N	2.65	0.44
1:B:857:LEU:HA	1:B:860:VAL:CG2	2.46	0.44
1:B:927:LEU:HD11	3:B:1379:HOH:O	2.16	0.44
1:A:746:GLU:OE2	1:A:873:LYS:NZ	2.42	0.44
1:A:930:SER:O	1:A:933:ASP:HB2	2.17	0.44
1:B:946:PHE:CD2	1:B:964:ILE:HG21	2.53	0.44
1:B:970:LYS:O	1:B:975:ASN:HB2	2.18	0.44
1:A:781:VAL:O	1:A:785:LYS:HG2	2.18	0.44
1:A:897:THR:HA	1:A:900:ILE:HD12	1.99	0.44
1:A:777:MET:CE	1:A:780:VAL:HB	2.39	0.44
1:A:774:GLY:O	1:A:959:MET:SD	2.76	0.44
1:B:933:ASP:HB3	3:B:1207:HOH:O	2.17	0.44
1:A:777:MET:HE3	1:A:780:VAL:CB	2.40	0.44
1:A:812:PHE:HE1	1:A:927:LEU:HD21	1.82	0.44
1:A:836:ASN:C	1:A:838:GLU:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:LEU:HD13	1:A:981:PHE:CZ	2.53	0.44
1:B:771:ARG:HA	1:B:957:PRO:CG	2.47	0.44
1:B:778:ILE:HG13	1:B:778:ILE:H	1.62	0.44
1:B:895:MET:O	1:B:898:ASN:HB3	2.17	0.44
1:A:770:ASN:OD1	2:A:2001:1CA:H211	2.18	0.43
1:B:867:GLU:HB2	1:B:906:MET:CE	2.48	0.43
1:A:894:GLU:O	1:A:897:THR:CG2	2.65	0.43
1:B:772:LEU:HD12	1:B:833:LEU:CD2	2.47	0.43
1:B:819:TYR:CD2	1:B:859:PHE:HD2	2.35	0.43
1:B:876:LEU:CD2	1:B:928:LEU:HD22	2.48	0.43
1:A:964:ILE:HG23	1:A:968:LEU:HD12	2.00	0.43
1:B:835:PHE:CD2	1:B:839:LYS:HB3	2.53	0.43
1:B:784:ALA:HB1	1:B:790:PHE:CE2	2.53	0.43
1:B:946:PHE:HE1	1:B:961:VAL:HA	1.83	0.43
1:A:801:LEU:HD21	1:A:892:PHE:HE1	1.80	0.43
1:A:806:TRP:HA	1:A:809:LEU:CD1	2.33	0.43
1:A:840:MET:O	1:A:846:TYR:HB2	2.19	0.43
1:A:758:LYS:HB3	1:A:759:PRO:CD	2.48	0.43
1:A:843:SER:O	1:A:844:ALA:HB3	2.19	0.43
1:A:836:ASN:O	1:A:838:GLU:N	2.52	0.43
1:A:876:LEU:CD2	1:A:928:LEU:HD22	2.44	0.43
1:B:811:SER:O	1:B:814:LEU:HB3	2.19	0.43
1:A:902:GLU:O	1:A:905:LYS:HB3	2.18	0.43
1:B:876:LEU:HD21	1:B:928:LEU:HD22	2.00	0.43
1:A:869:TYR:HE2	1:A:873:LYS:HZ3	1.64	0.43
1:A:870:THR:O	1:A:874:VAL:HG23	2.19	0.42
1:B:934:LEU:HD21	1:B:938:LEU:CD1	2.49	0.42
1:B:965:SER:O	1:B:969:PRO:HG3	2.19	0.42
1:A:927:LEU:C	1:A:927:LEU:HD23	2.43	0.42
1:B:739:VAL:CG2	1:B:740:MET:N	2.80	0.42
1:B:929:ASP:OD2	1:B:980:TYR:HD1	2.02	0.42
1:A:747:PRO:HB2	1:A:779:GLN:CD	2.44	0.42
1:B:871:ILE:HG21	1:B:903:LEU:HD13	2.01	0.42
1:B:894:GLU:O	1:B:898:ASN:HB2	2.19	0.42
1:B:895:MET:SD	3:B:1261:HOH:O	2.61	0.42
1:A:742:LEU:HD12	1:A:870:THR:CG2	2.49	0.42
1:B:755:ASP:OD1	1:B:758:LYS:HE3	2.19	0.42
1:B:786:VAL:O	1:B:786:VAL:CG1	2.66	0.42
1:B:950:HIS:O	1:B:951:ALA:HB2	2.18	0.42
1:B:952:LEU:O	1:B:953:LYS:HB2	2.19	0.42
1:B:837:GLU:C	1:B:839:LYS:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:MET:HE3	1:A:777:MET:HA	2.02	0.42
1:B:906:MET:C	1:B:908:THR:H	2.25	0.42
1:A:787:LEU:HB3	1:A:790:PHE:HB3	2.00	0.42
1:A:856:SER:O	1:A:859:PHE:HB2	2.20	0.42
1:B:868:GLU:N	1:B:906:MET:HE1	2.34	0.42
1:A:896:ARG:O	1:A:900:ILE:HG13	2.20	0.41
1:B:759:PRO:O	1:B:764:ASN:CG	2.62	0.41
1:B:787:LEU:HA	1:B:788:PRO:HD3	1.98	0.41
1:A:784:ALA:CB	3:A:1088:HOH:O	2.68	0.41
1:A:965:SER:O	1:A:969:PRO:HG3	2.20	0.41
1:A:906:MET:SD	1:A:906:MET:O	2.78	0.41
1:B:838:GLU:O	1:B:838:GLU:HG2	2.20	0.41
1:A:737:SER:O	1:A:738:PRO:C	2.64	0.41
1:A:919:GLN:O	1:A:923:GLN:HG3	2.20	0.41
1:A:958:ALA:O	1:A:961:VAL:HB	2.19	0.41
1:B:787:LEU:HB3	1:B:790:PHE:HB3	2.01	0.41
1:B:843:SER:C	1:B:845:MET:N	2.76	0.41
1:A:784:ALA:HB3	3:A:1088:HOH:O	2.21	0.41
1:B:907:VAL:O	1:B:908:THR:HG23	2.20	0.41
1:A:840:MET:HE3	1:A:849:CYS:HB3	2.02	0.41
1:A:955:GLU:HG2	1:A:956:PHE:N	2.35	0.41
1:B:854:GLN:O	1:B:858:GLN:HG2	2.21	0.41
1:B:946:PHE:CE1	1:B:961:VAL:HG13	2.56	0.41
1:B:823:ASN:O	1:B:824:SER:HB2	2.21	0.41
1:B:967:GLN:C	1:B:969:PRO:HD2	2.46	0.41
1:A:846:TYR:O	1:A:847:GLU:CB	2.69	0.41
1:B:777:MET:O	1:B:781:VAL:HG22	2.21	0.41
1:B:872:MET:HB3	1:B:928:LEU:HD21	2.03	0.41
1:A:806:TRP:CG	1:A:807:MET:N	2.88	0.40
1:A:854:GLN:NE2	1:A:857:LEU:HD12	2.36	0.40
1:B:847:GLU:OE1	1:B:847:GLU:HA	2.21	0.40
1:A:905:LYS:HE3	1:A:905:LYS:HB2	1.96	0.40
1:B:960:LEU:O	1:B:963:ILE:N	2.55	0.40
1:B:781:VAL:C	1:B:783:TRP:N	2.79	0.40
1:B:814:LEU:HD23	1:B:852:MET:SD	2.61	0.40
1:A:864:LEU:HD12	1:A:868:GLU:OE1	2.22	0.40
1:B:755:ASP:C	1:B:757:SER:N	2.79	0.40
1:B:866:PHE:CZ	3:B:1274:HOH:O	2.57	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	235/255 (92%)	196 (83%)	29 (12%)	10 (4%)	2	0
1	B	234/255 (92%)	197 (84%)	26 (11%)	11 (5%)	2	0
All	All	469/510 (92%)	393 (84%)	55 (12%)	21 (4%)	2	0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	SER
1	A	949	SER
1	A	957	PRO
1	B	820	LYS
1	B	951	ALA
1	B	957	PRO
1	A	847	GLU
1	A	980	TYR
1	B	837	GLU
1	B	971	VAL
1	A	747	PRO
1	A	837	GLU
1	B	983	ARG
1	B	842	GLN
1	B	907	VAL
1	A	738	PRO
1	B	974	GLY
1	A	739	VAL
1	B	747	PRO
1	A	968	LEU
1	B	789	GLY

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	218/234 (93%)	198 (91%)	20 (9%)	8	2
1	B	215/234 (92%)	200 (93%)	15 (7%)	14	4
All	All	433/468 (92%)	398 (92%)	35 (8%)	11	3

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	738	PRO
1	A	741	VAL
1	A	760	ASP
1	A	777	MET
1	A	782	LYS
1	A	786	VAL
1	A	807	MET
1	A	820	LYS
1	A	823	ASN
1	A	836	ASN
1	A	847	GLU
1	A	849	CYS
1	A	860	VAL
1	A	888	SER
1	A	893	GLU
1	A	906	MET
1	A	926	LYS
1	A	962	GLU
1	A	965	SER
1	A	970	LYS
1	B	781	VAL
1	B	822	THR
1	B	825	GLN
1	B	856	SER
1	B	864	LEU
1	B	868	GLU
1	B	873	LYS

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Mol	Chain	Res	Type
1	B	887	LYS
1	B	894	GLU
1	B	908	THR
1	B	926	LYS
1	B	929	ASP
1	B	944	TYR
1	B	948	GLU
1	B	962	GLU

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

Mol	Chain	Res	Type
1	A	744	ASN
1	A	803	GLN
1	A	825	GLN
1	A	836	ASN
1	A	853	HIS
1	A	854	GLN
1	B	764	ASN
1	B	853	HIS
1	B	858	GLN

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 oligosaccharides 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$
2	1CA	A	2001	-	27,27,27	4.88	17 (62%)	42,43,43	1.99	12 (28%)
2	1CA	B	3001	-	27,27,27	4.74	19 (70%)	42,43,43	1.82	10 (23%)

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	1CA	A	2001	-	-	0/6/64/64	0/4/4/4
2	1CA	B	3001	-	-	0/6/64/64	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	1CA	C8-C9	10.12	1.72	1.53
2	A	2001	1CA	C10-C5	9.49	1.71	1.52
2	B	3001	1CA	C10-C9	9.04	1.70	1.56
2	A	2001	1CA	C2-C3	8.80	1.68	1.50
2	B	3001	1CA	C4-C5	8.54	1.46	1.34
2	A	2001	1CA	C12-C13	8.32	1.68	1.54
2	B	3001	1CA	C12-C13	8.13	1.68	1.54
2	B	3001	1CA	C10-C5	7.80	1.67	1.52
2	A	2001	1CA	C1-C2	7.50	1.68	1.53
2	B	3001	1CA	C8-C9	7.34	1.67	1.53
2	A	2001	1CA	C11-C9	7.26	1.65	1.53
2	A	2001	1CA	C1-C10	6.35	1.65	1.54
2	B	3001	1CA	C18-C13	6.20	1.64	1.54
2	B	3001	1CA	C1-C2	6.11	1.65	1.53
2	B	3001	1CA	C8-C14	5.99	1.64	1.53
2	A	2001	1CA	C18-C13	5.71	1.63	1.54
2	A	2001	1CA	C6-C5	5.39	1.59	1.50
2	B	3001	1CA	C6-C5	5.29	1.59	1.50
2	B	3001	1CA	C1-C10	4.62	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	1CA	C13-C14	4.49	1.63	1.55
2	B	3001	1CA	C13-C14	4.34	1.63	1.55
2	B	3001	1CA	C2-C3	4.01	1.58	1.50
2	B	3001	1CA	C11-C9	3.84	1.60	1.53
2	B	3001	1CA	C7-C8	3.84	1.60	1.53
2	B	3001	1CA	O20-C20	3.45	1.27	1.21
2	A	2001	1CA	C4-C3	-3.27	1.38	1.45
2	A	2001	1CA	C17-C20	3.20	1.57	1.52
2	B	3001	1CA	O3-C3	-3.14	1.18	1.23
2	A	2001	1CA	C4-C5	3.11	1.38	1.34
2	A	2001	1CA	C10-C9	3.00	1.60	1.56
2	A	2001	1CA	C13-C17	2.85	1.60	1.56
2	A	2001	1CA	O20-C20	2.56	1.25	1.21
2	B	3001	1CA	C12-C11	2.32	1.58	1.53
2	A	2001	1CA	O21-C21	2.22	1.49	1.41
2	B	3001	1CA	C13-C17	2.22	1.59	1.56
2	B	3001	1CA	C15-C14	2.15	1.58	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	1CA	C17-C13-C14	-4.72	94.80	99.72
2	B	3001	1CA	C17-C13-C14	-4.51	95.01	99.72
2	B	3001	1CA	C2-C3-C4	4.31	123.27	116.73
2	A	2001	1CA	C2-C3-C4	4.09	122.94	116.73
2	A	2001	1CA	C1-C10-C9	3.75	113.70	108.74
2	A	2001	1CA	C15-C16-C17	3.65	111.19	105.25
2	A	2001	1CA	O21-C21-C20	3.44	121.84	112.73
2	A	2001	1CA	C19-C10-C5	-3.10	103.65	108.38
2	A	2001	1CA	C6-C5-C4	-3.05	115.99	120.86
2	A	2001	1CA	C15-C14-C13	3.03	107.40	103.84
2	B	3001	1CA	C18-C13-C14	3.01	117.14	111.68
2	A	2001	1CA	O3-C3-C4	-2.98	116.29	121.65
2	B	3001	1CA	C6-C7-C8	2.91	116.74	111.64
2	A	2001	1CA	C18-C13-C14	2.69	116.56	111.68
2	B	3001	1CA	C16-C17-C13	2.55	106.50	104.21
2	B	3001	1CA	C19-C10-C1	-2.55	105.55	109.43
2	B	3001	1CA	C19-C10-C5	-2.49	104.59	108.38
2	B	3001	1CA	C19-C10-C9	2.48	114.44	111.66
2	B	3001	1CA	O21-C21-C20	2.28	118.77	112.73
2	A	2001	1CA	C6-C7-C8	2.26	115.62	111.64
2	B	3001	1CA	O3-C3-C2	-2.12	117.36	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	1CA	C19-C10-C1	-2.04	106.33	109.43

There are no chirality outliers.

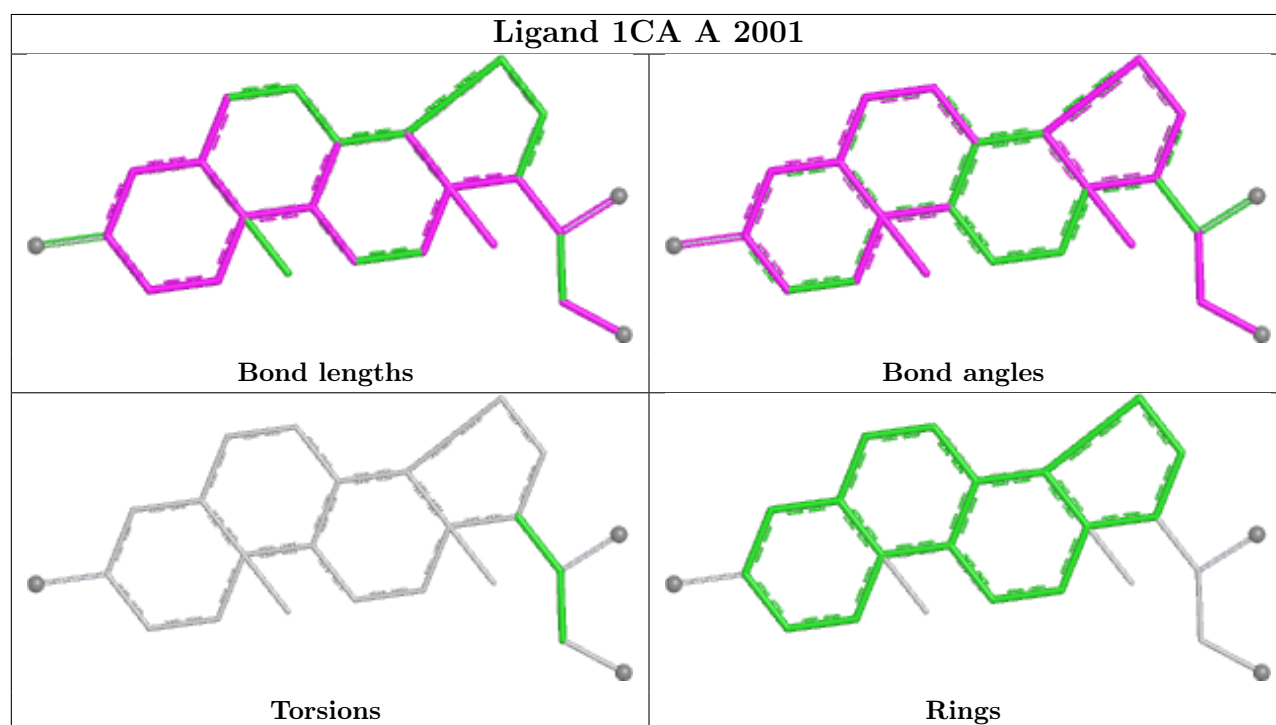
There are no torsion outliers.

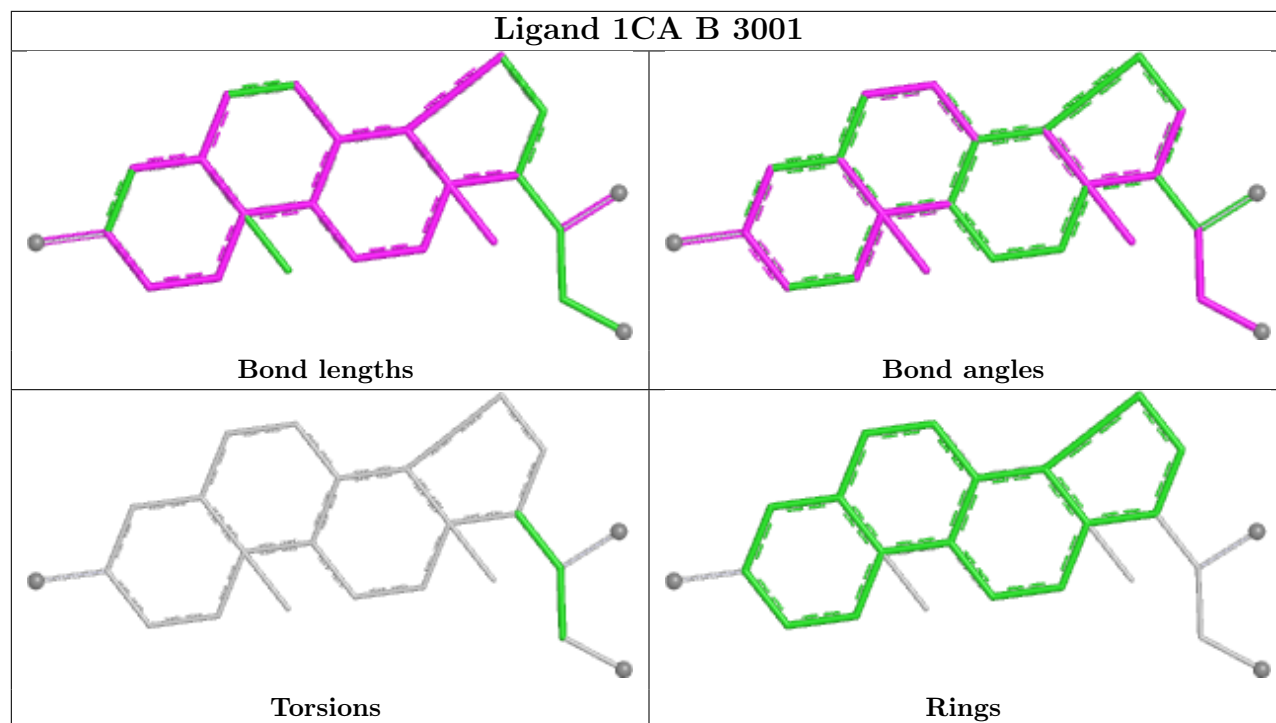
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	1CA	5	0
2	B	3001	1CA	5	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 than 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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	239/255 (93%)	0.39	7 (2%) 53 60	12, 23, 35, 38	0
1	B	238/255 (93%)	0.42	5 (2%) 63 70	11, 25, 36, 40	0
All	All	477/510 (93%)	0.40	12 (2%) 58 65	11, 24, 36, 40	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	761	THR	2.9
1	A	750	VAL	2.8
1	A	754	TYR	2.8
1	B	833	LEU	2.8
1	B	983	ARG	2.7
1	A	745	ILE	2.5
1	B	835	PHE	2.2
1	A	971	VAL	2.2
1	A	960	LEU	2.2
1	B	969	PRO	2.1
1	A	742	LEU	2.0
1	B	834	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

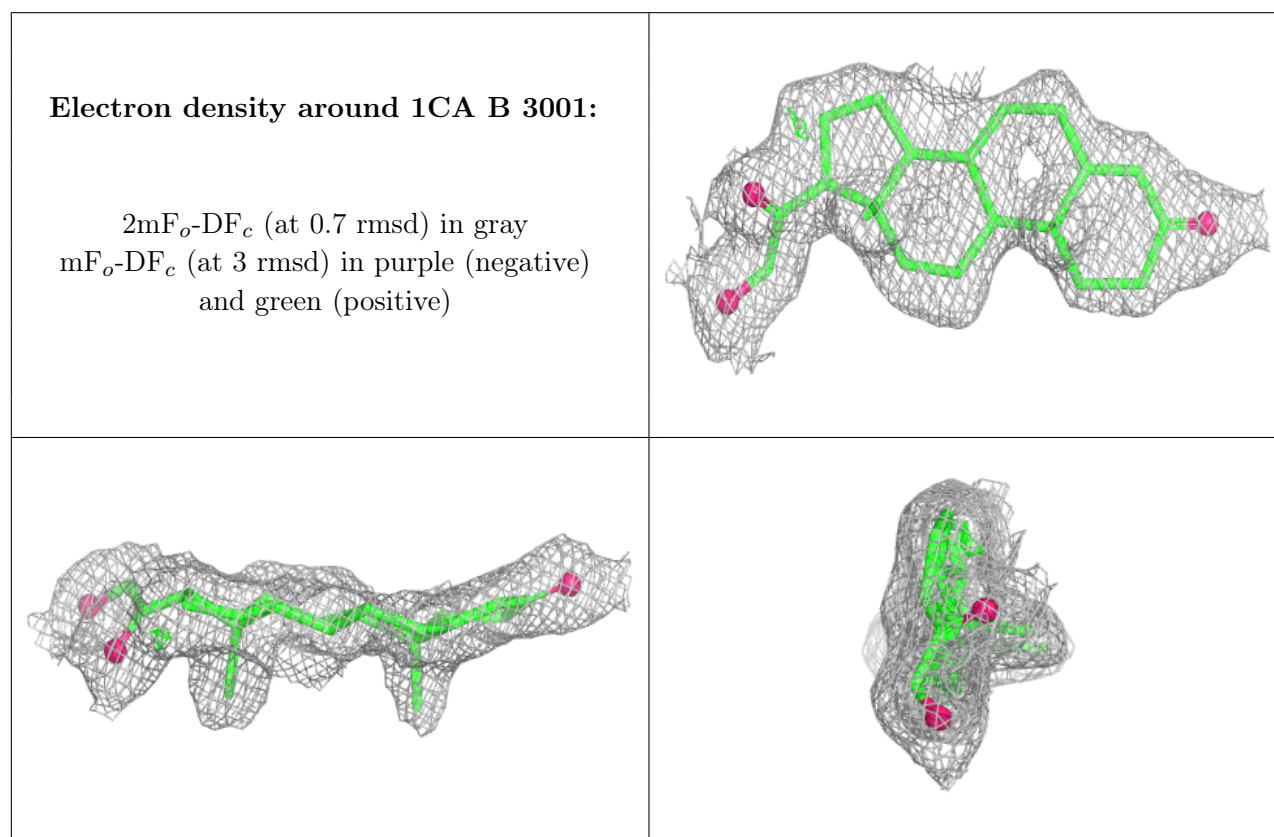
There are no oligosaccharides in this entry.

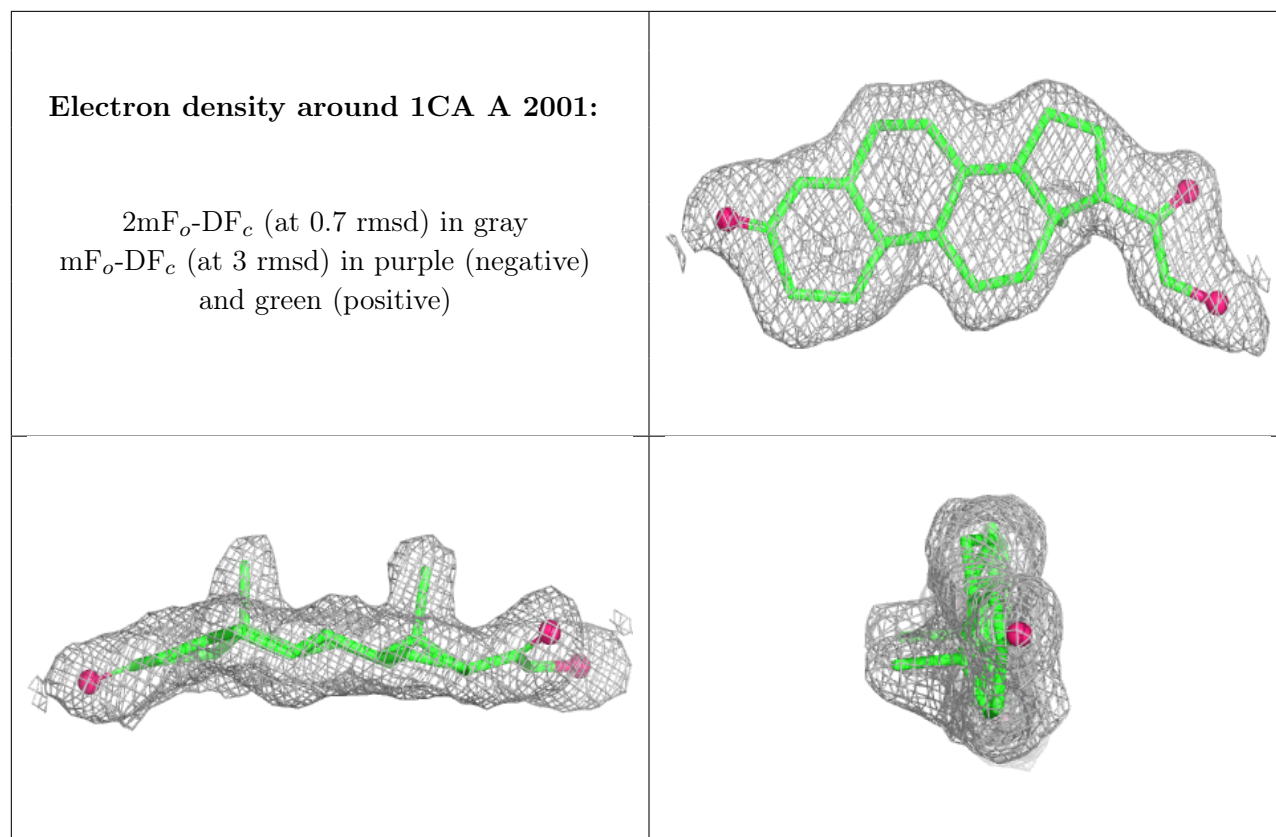
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	1CA	B	3001	24/24	0.87	0.10	15,19,23,23	0
2	1CA	A	2001	24/24	0.91	0.08	18,21,24,27	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.