



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:41 am GMT

PDB ID : 1Y9R  
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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

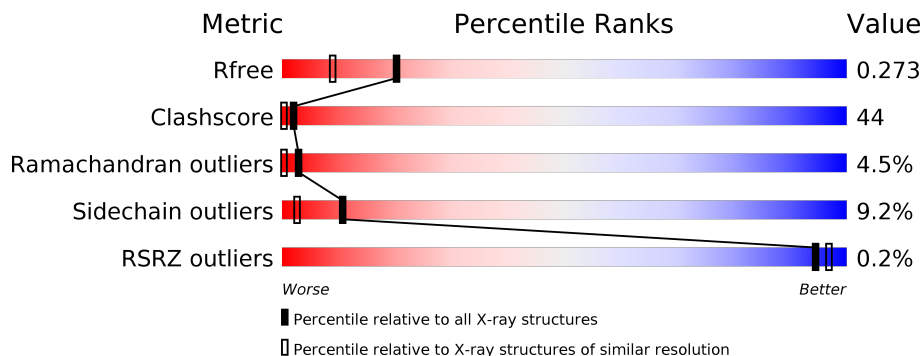
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (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  $\geq 3$ , 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	255	
1	B	255	

## 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.

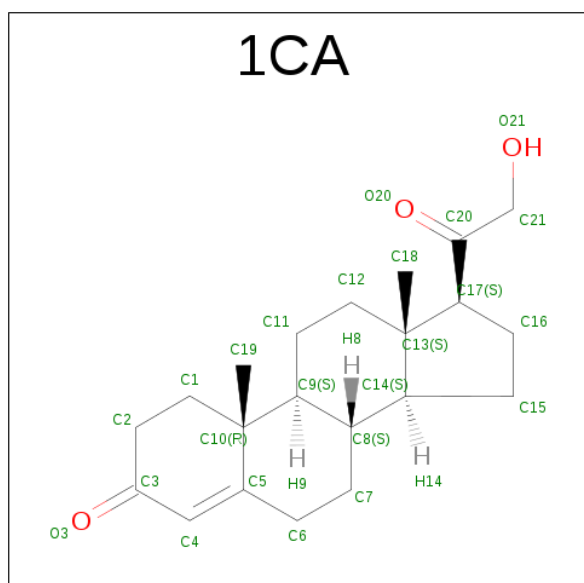
- Molecule 1 is a protein called Mineralocorticoid receptor.

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	UNP P08235
A	910	ALA	CYS	ENGINEERED	UNP P08235
B	730	SER	-	CLONING ARTIFACT	UNP P08235
B	810	LEU	SER	ENGINEERED	UNP P08235
B	910	ALA	CYS	ENGINEERED	UNP P08235

- Molecule 2 is DESOXYCORTICOSTERONE (three-letter code: 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, $\alpha$ , $\beta$ , $\gamma$	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) 84.2 (18.30-1.96)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 151.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.35	0/1998	0.63	0/2701
1	B	0.34	0/1976	0.63	2/2668 (0.1%)
All	All	0.35	0/3974	0.63	2/5369 (0.0%)

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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	777	MET	CG-SD-CE	-9.12	85.61	100.20
1	B	807	MET	CG-SD-CE	6.03	109.85	100.20

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	187	0
1	B	1933	0	1936	162	0
2	A	24	0	30	6	0
2	B	24	0	30	5	0
3	A	236	0	0	18	0
3	B	225	0	0	26	0
All	All	4394	0	3957	351	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 44.

All (351) 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: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:812:PHE:HB2	1:A:931:MET:HE1	1.37	1.03
1:A:836:ASN:ND2	1:A:837:GLU:N	2.10	0.99
1:A:806:TRP:HA	1:A:809:LEU:HD12	1.46	0.96
1:B:878:LEU:HD11	1:B:895:MET:HE2	1.48	0.95
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: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: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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:749:ILE:HD12	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:HA	1:A:847:GLU:OE1	1.89	0.71
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:867:GLU:O	1:A:870:THR:HG22	1.90	0.70
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ASN:HD22	1:A:836:ASN:C	1.99	0.65
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:O	1:B:786:VAL:HG12	1.96	0.65
1:A:761:THR:N	1:A:764:ASN:OD1	2.29	0.65
1:A:967:GLN:C	1:A:969:PRO:HD2	2.16	0.65
1:A:742:LEU:HA	1:A:745:ILE:HG12	1.78	0.65
1:A:765:LEU:H	1:A:765:LEU:HD22	1.61	0.65
1:A:932:HIS:CE1	1:A:978:PRO:HB3	2.32	0.65
1:A:812:PHE:HB2	1:A:931:MET:CE	2.21	0.64
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
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:N	1:B:749:ILE:HD12	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: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:B:853:HIS:CE1	1:B:857:LEU:HD21	2.38	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:817:ARG:HD3	3:B:1014:HOH:O	2.05	0.57
1:A:983:ARG:HH11	1:A:983:ARG:HB2	1.65	0.57
1:B:878:LEU:HD21	1:B:895:MET:HE1	1.87	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
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:B:972:GLU:CD	3:B:1146:HOH:O	2.43	0.56
1:A:976:ALA:O	1:A:978:PRO:HD3	2.06	0.56
1:A:875:LEU:O	1:A:879:SER:HB2	2.05	0.56
1:A:848:LEU:HD23	1:A:938:LEU:HD23	1.88	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:A:968:LEU:N	1:A:969:PRO:CD	2.70	0.55
1:A:807:MET:HE1	2:A:2001:1CA:H191	1.87	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
2:B:3001:1CA:H152	3:B:1255:HOH:O	2.07	0.54
1:B:926:LYS:HD3	3:B:1265:HOH:O	2.07	0.54
1:B:901:LYS:HG2	1:B:904:ARG:HH22	1.72	0.54
1:A:971:VAL:C	1:A:973:SER:N	2.60	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:758:LYS:HB3	1:A:759:PRO:HD2	1.89	0.53
1:A:943:PHE:CB	1:A:968:LEU:HD13	2.36	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:867:GLU:HB2	1:B:906:MET:HE1	1.90	0.53
1:A:820:LYS:CE	1:A:820:LYS:HA	2.39	0.53
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:A:971:VAL:C	1:A:973:SER:H	2.10	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:O	1:A:971:VAL:HG12	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:N	1:A:765:LEU:HD22	2.25	0.52
1:A:777:MET:CE	1:A:780:VAL:HB	2.39	0.52
1:A:934:LEU:O	1:A:937:ASP:HB2	2.08	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: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: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: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:CD1	1:B:749:ILE:H	2.23	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:ASN:CG	1:B:837:GLU:H	2.14	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:744:ASN:C	1:A:744:ASN:ND2	2.65	0.50
1:A:742:LEU:HB3	1:A:870:THR:OG1	2.12	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: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:744:ASN:C	1:A:744:ASN:HD22	2.15	0.49
1:A:956:PHE:O	1:A:957:PRO:O	2.31	0.49
1:A:777:MET:HE3	1:A:780:VAL:HB	1.95	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:A:807:MET:CE	2:A:2001:1CA:H191	2.42	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: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:B:836:ASN:CG	1:B:837:GLU:N	2.66	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:A:920:ARG:O	1:A:921:PHE:C	2.52	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:889:GLN:O	1:A:892:PHE:HB3	2.14	0.47
1:B:819:TYR:HA	1:B:824:SER:OG	2.14	0.47
1:B:934:LEU:C	1:B:934:LEU:HD23	2.34	0.47
1:B:943:PHE:HD1	1:B:968:LEU:HD13	1.78	0.47
1:B:768:THR:HG21	3:B:1373:HOH:O	2.12	0.47
1:B:897:THR:O	1:B:901:LYS:HG3	2.15	0.47
1:B:771:ARG:HA	1:B:957:PRO:HG3	1.96	0.47
1:A:846:TYR:O	1:A:847:GLU:CG	2.57	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:906:MET:C	1:A:906:MET:SD	2.94	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ILE:HG21	1:A:903:LEU:HB2	1.98	0.46
1:B:837:GLU:C	1:B:839:LYS:H	2.19	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:HG3	1:A:983:ARG:O	2.14	0.46
1:B:814:LEU:HD22	2:B:3001:1CA:H4	1.97	0.46
1:B:755:ASP:C	1:B:757:SER:H	2.17	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:B:895:MET:HE3	1:B:899:TYR:HE2	1.80	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:808:CYS:SG	1:A:935:VAL:HG21	2.56	0.45
1:A:743:GLU:HA	1:A:866:PHE:CE2	2.51	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:A:777:MET:HE1	1:A:780:VAL:CB	2.46	0.45
1:A:846:TYR:C	1:A:846:TYR:CD1	2.89	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:812:PHE:HE1	1:A:927:LEU:HD21	1.82	0.44
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:841:HIS:C	1:B:843:SER:H	2.21	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:836:ASN:C	1:A:838:GLU:H	2.22	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:738:PRO:O	1:A:739:VAL:C	2.56	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:B:950:HIS:O	1:B:951:ALA:HB2	2.18	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: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:B:871:ILE:HG21	1:B:903:LEU:HD13	2.01	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:895:MET:SD	3:B:1261:HOH:O	2.61	0.42
1:B:894:GLU:O	1:B:898:ASN:HB2	2.19	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:952:LEU:O	1:B:953:LYS:HB2	2.19	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:925:THR:HG1	1:B:982:HIS:CE1	2.37	0.42
1:A:896:ARG:O	1:A:900:ILE:HG13	2.20	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:O	1:A:906:MET:SD	2.78	0.41
1:B:838:GLU:HG2	1:B:838:GLU:O	2.20	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:A:789:GLY:C	1:A:895:MET:SD	2.99	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: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:A:869:TYR:HE2	1:A:873:LYS:HZ3	1.65	0.41
1:B:823:ASN:O	1:B:824:SER:HB2	2.21	0.41
1:B:777:MET:O	1:B:781:VAL:HG22	2.21	0.41
1:A:846:TYR:O	1:A:847:GLU:CB	2.69	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:HA	1:B:847:GLU:OE1	2.21	0.40
1:A:905:LYS:HB2	1:A:905:LYS:HE3	1.96	0.40
1:B:895:MET:HE3	1:B:899:TYR:CE2	2.56	0.40
1:B:960:LEU:O	1:B:963:ILE:N	2.55	0.40
1:B:814:LEU:HD23	1:B:852:MET:SD	2.61	0.40
1:A:777:MET:HE1	1:A:780:VAL:HG21	2.02	0.40
1:A:864:LEU:HD12	1:A:868:GLU:OE1	2.22	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%)	3	0
1	B	234/255 (92%)	197 (84%)	26 (11%)	11 (5%)	3	0
All	All	469/510 (92%)	393 (84%)	55 (12%)	21 (4%)	3	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%)	194 (89%)	24 (11%)	7	1
1	B	215/234 (92%)	199 (93%)	16 (7%)	16	5
All	All	433/468 (92%)	393 (91%)	40 (9%)	11	3

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	738	PRO
1	A	741	VAL
1	A	744	ASN
1	A	760	ASP
1	A	771	ARG
1	A	777	MET
1	A	782	LYS
1	A	786	VAL
1	A	791	LYS
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	920	ARG
1	A	962	GLU
1	A	965	SER
1	A	970	LYS
1	A	983	ARG
1	B	760	ASP
1	B	781	VAL
1	B	797	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	822	THR
1	B	825	GLN
1	B	856	SER
1	B	864	LEU
1	B	868	GLU
1	B	894	GLU
1	B	908	THR
1	B	926	LYS
1	B	929	ASP
1	B	940	GLU
1	B	944	TYR
1	B	948	GLU
1	B	962	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	744	ASN
1	A	792	ASN
1	A	803	GLN
1	A	823	ASN
1	A	825	GLN
1	A	836	ASN
1	A	854	GLN
1	A	950	HIS
1	A	967	GLN
1	A	975	ASN
1	B	764	ASN
1	B	821	HIS
1	B	853	HIS
1	B	854	GLN
1	B	858	GLN
1	B	932	HIS
1	B	975	ASN

### 5.3.3 RNA ⓘ

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	$\# Z  > 2$
2	1CA	A	2001	-	27,27,27	4.64	17 (62%)	42,43,43	1.91	11 (26%)
2	1CA	B	3001	-	27,27,27	4.51	19 (70%)	42,43,43	1.75	9 (21%)

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	C4-C3	-3.07	1.38	1.45
2	B	3001	1CA	O3-C3	-2.97	1.18	1.23
2	B	3001	1CA	C13-C17	2.03	1.59	1.56
2	B	3001	1CA	C15-C14	2.07	1.58	1.54
2	A	2001	1CA	O21-C21	2.09	1.49	1.41
2	B	3001	1CA	C12-C11	2.15	1.58	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	1CA	O20-C20	2.45	1.25	1.21
2	A	2001	1CA	C13-C17	2.62	1.60	1.56
2	A	2001	1CA	C10-C9	2.80	1.60	1.56
2	A	2001	1CA	C17-C20	3.00	1.57	1.52
2	A	2001	1CA	C4-C5	3.07	1.38	1.34
2	B	3001	1CA	O20-C20	3.30	1.27	1.21
2	B	3001	1CA	C7-C8	3.65	1.60	1.53
2	B	3001	1CA	C11-C9	3.65	1.60	1.53
2	B	3001	1CA	C2-C3	3.85	1.58	1.49
2	B	3001	1CA	C13-C14	4.07	1.63	1.55
2	A	2001	1CA	C13-C14	4.21	1.63	1.55
2	B	3001	1CA	C1-C10	4.43	1.62	1.54
2	A	2001	1CA	C18-C13	5.21	1.63	1.54
2	B	3001	1CA	C6-C5	5.24	1.59	1.50
2	A	2001	1CA	C6-C5	5.35	1.59	1.50
2	B	3001	1CA	C18-C13	5.66	1.64	1.54
2	B	3001	1CA	C8-C14	5.78	1.64	1.53
2	B	3001	1CA	C1-C2	5.82	1.65	1.53
2	A	2001	1CA	C1-C10	6.09	1.65	1.54
2	A	2001	1CA	C11-C9	6.90	1.65	1.53
2	B	3001	1CA	C8-C9	7.07	1.67	1.53
2	A	2001	1CA	C1-C2	7.14	1.68	1.53
2	B	3001	1CA	C10-C5	7.35	1.67	1.52
2	B	3001	1CA	C12-C13	7.55	1.68	1.54
2	A	2001	1CA	C12-C13	7.73	1.68	1.54
2	A	2001	1CA	C2-C3	8.39	1.68	1.49
2	B	3001	1CA	C4-C5	8.40	1.46	1.34
2	B	3001	1CA	C10-C9	8.47	1.70	1.56
2	A	2001	1CA	C10-C5	8.94	1.71	1.52
2	A	2001	1CA	C8-C9	9.76	1.72	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	1CA	C17-C13-C14	-4.63	94.80	99.71
2	B	3001	1CA	C17-C13-C14	-4.43	95.01	99.71
2	A	2001	1CA	C6-C5-C4	-2.95	115.99	120.87
2	A	2001	1CA	C19-C10-C5	-2.84	103.65	108.34
2	A	2001	1CA	O3-C3-C4	-2.75	116.29	121.61
2	B	3001	1CA	C19-C10-C1	-2.40	105.55	109.41
2	B	3001	1CA	C19-C10-C5	-2.27	104.59	108.34
2	A	2001	1CA	C6-C7-C8	2.12	115.62	111.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3001	1CA	C19-C10-C9	2.24	114.44	111.68
2	B	3001	1CA	O21-C21-C20	2.27	118.77	112.66
2	A	2001	1CA	C18-C13-C14	2.55	116.56	111.73
2	B	3001	1CA	C16-C17-C13	2.63	106.50	104.17
2	B	3001	1CA	C6-C7-C8	2.73	116.74	111.71
2	B	3001	1CA	C18-C13-C14	2.86	117.14	111.73
2	A	2001	1CA	C15-C14-C13	2.89	107.40	103.83
2	A	2001	1CA	O21-C21-C20	3.41	121.84	112.66
2	A	2001	1CA	C1-C10-C9	3.50	113.70	108.68
2	A	2001	1CA	C15-C16-C17	3.53	111.19	105.38
2	A	2001	1CA	C2-C3-C4	3.93	122.94	116.74
2	B	3001	1CA	C2-C3-C4	4.14	123.27	116.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	1CA	6	0
2	B	3001	1CA	5	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	239/255 (93%)	-0.07	0 <a href="#">100</a> <a href="#">100</a>	12, 23, 35, 38	0
1	B	238/255 (93%)	-0.08	1 (0%) <a href="#">92</a> <a href="#">95</a>	11, 25, 36, 40	0
All	All	477/510 (93%)	-0.07	1 (0%) <a href="#">94</a> <a href="#">97</a>	11, 24, 36, 40	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	983	ARG	2.1

### 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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	1CA	B	3001	24/24	0.91	0.13	1.41	15,19,23,23	0
2	1CA	A	2001	24/24	0.91	0.12	0.88	18,21,24,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.