



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 04:27 AM GMT

PDB ID : 4K5Y  
Title : Crystal structure of human corticotropin-releasingfactor receptor 1 (CRF1R)  
in complex with the antagonist CP-376395  
Authors : Hollenstein, K.; Kean, J.; Bortolato, A.; Cheng, R.K.Y.; Dore, A.S.; Jazayeri,  
A.; Cooke, R.M.; Weir, M.; Marshall, F.H.  
Deposited on : 2013-04-15  
Resolution : 2.98 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

---

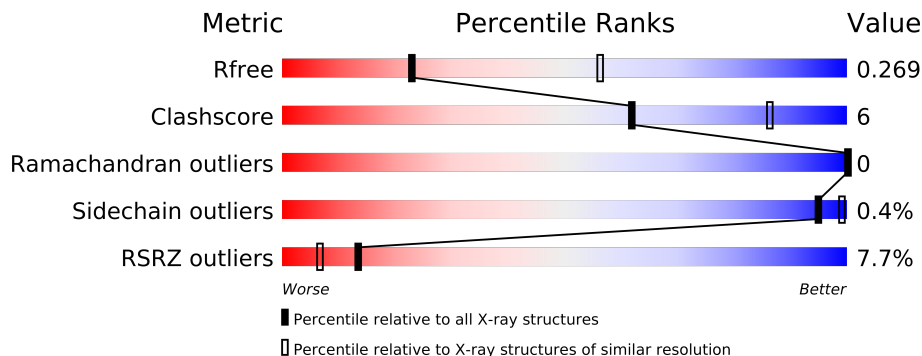
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.98 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	1468 (3.00-2.96)
Clashscore	79885	1894 (3.00-2.96)
Ramachandran outliers	78287	1826 (3.00-2.96)
Sidechain outliers	78261	1829 (3.00-2.96)
RSRZ outliers	66119	1469 (3.00-2.96)

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. 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	441	
1	B	441	
1	C	441	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	OLC	A	503	-	X
4	OLC	B	501	-	X
6	PGW	B	502	-	X
6	PGW	B	504	-	X
7	1PE	B	505	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8823 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 Corticotropin-releasingfactor receptor 1, T4-Lysozyme chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3278	2145	562	554	17			
1	B	396	Total	C	N	O	S	0	0	0
			3194	2091	547	539	17			
1	C	248	Total	C	N	O	S	0	0	0
			2005	1341	330	321	13			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	INITIATING METHIONINE	UNP P34998
A	120	ALA	VAL	ENGINEERED MUTATION	UNP P34998
A	144	ALA	LEU	ENGINEERED MUTATION	UNP P34998
A	156	ALA	TRP	ENGINEERED MUTATION	UNP P34998
A	160	ALA	SER	ENGINEERED MUTATION	UNP P34998
A	1040	SER	ASN	ENGINEERED MUTATION	UNP P00720
A	1041	VAL	ALA	ENGINEERED MUTATION	UNP P00720
A	1054	SER	CYS	ENGINEERED MUTATION	UNP P00720
A	1097	SER	CYS	ENGINEERED MUTATION	UNP P00720
A	1151	ALA	THR	ENGINEERED MUTATION	UNP P00720
A	228	ALA	LYS	ENGINEERED MUTATION	UNP P34998
A	260	ALA	PHE	ENGINEERED MUTATION	UNP P34998
A	277	ALA	ILE	ENGINEERED MUTATION	UNP P34998
A	309	ALA	TYR	ENGINEERED MUTATION	UNP P34998
A	330	ALA	PHE	ENGINEERED MUTATION	UNP P34998
A	349	ALA	SER	ENGINEERED MUTATION	UNP P34998
A	363	ALA	TYR	ENGINEERED MUTATION	UNP P34998
A	374	ALA	-	EXPRESSION TAG	UNP P34998
A	375	ALA	-	EXPRESSION TAG	UNP P34998
A	376	ALA	-	EXPRESSION TAG	UNP P34998
A	377	HIS	-	EXPRESSION TAG	UNP P34998
A	378	HIS	-	EXPRESSION TAG	UNP P34998

*Continued on next page...*

*Continued from previous page...*

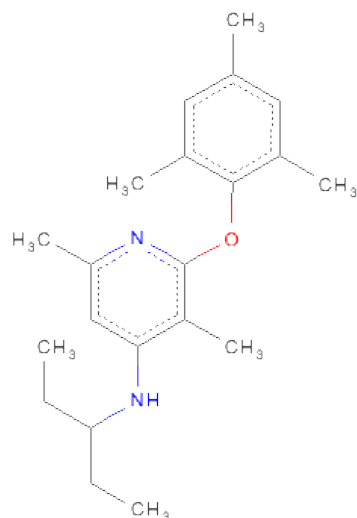
Chain	Residue	Modelled	Actual	Comment	Reference
A	379	HIS	-	EXPRESSION TAG	UNP P34998
A	380	HIS	-	EXPRESSION TAG	UNP P34998
A	381	HIS	-	EXPRESSION TAG	UNP P34998
A	382	HIS	-	EXPRESSION TAG	UNP P34998
A	383	HIS	-	EXPRESSION TAG	UNP P34998
A	384	HIS	-	EXPRESSION TAG	UNP P34998
A	385	HIS	-	EXPRESSION TAG	UNP P34998
A	386	HIS	-	EXPRESSION TAG	UNP P34998
B	103	MET	-	INITIATING METHIONINE	UNP P34998
B	120	ALA	VAL	ENGINEERED MUTATION	UNP P34998
B	144	ALA	LEU	ENGINEERED MUTATION	UNP P34998
B	156	ALA	TRP	ENGINEERED MUTATION	UNP P34998
B	160	ALA	SER	ENGINEERED MUTATION	UNP P34998
B	1040	SER	ASN	ENGINEERED MUTATION	UNP P00720
B	1041	VAL	ALA	ENGINEERED MUTATION	UNP P00720
B	1054	SER	CYS	ENGINEERED MUTATION	UNP P00720
B	1097	SER	CYS	ENGINEERED MUTATION	UNP P00720
B	1151	ALA	THR	ENGINEERED MUTATION	UNP P00720
B	228	ALA	LYS	ENGINEERED MUTATION	UNP P34998
B	260	ALA	PHE	ENGINEERED MUTATION	UNP P34998
B	277	ALA	ILE	ENGINEERED MUTATION	UNP P34998
B	309	ALA	TYR	ENGINEERED MUTATION	UNP P34998
B	330	ALA	PHE	ENGINEERED MUTATION	UNP P34998
B	349	ALA	SER	ENGINEERED MUTATION	UNP P34998
B	363	ALA	TYR	ENGINEERED MUTATION	UNP P34998
B	374	ALA	-	EXPRESSION TAG	UNP P34998
B	375	ALA	-	EXPRESSION TAG	UNP P34998
B	376	ALA	-	EXPRESSION TAG	UNP P34998
B	377	HIS	-	EXPRESSION TAG	UNP P34998
B	388	HIS	-	EXPRESSION TAG	UNP P34998
B	389	HIS	-	EXPRESSION TAG	UNP P34998
B	390	HIS	-	EXPRESSION TAG	UNP P34998
B	391	HIS	-	EXPRESSION TAG	UNP P34998
B	392	HIS	-	EXPRESSION TAG	UNP P34998
B	393	HIS	-	EXPRESSION TAG	UNP P34998
B	394	HIS	-	EXPRESSION TAG	UNP P34998
B	395	HIS	-	EXPRESSION TAG	UNP P34998
B	396	HIS	-	EXPRESSION TAG	UNP P34998
C	103	MET	-	INITIATING METHIONINE	UNP P34998
C	120	ALA	VAL	ENGINEERED MUTATION	UNP P34998
C	144	ALA	LEU	ENGINEERED MUTATION	UNP P34998
C	156	ALA	TRP	ENGINEERED MUTATION	UNP P34998

*Continued on next page...*

*Continued from previous page...*

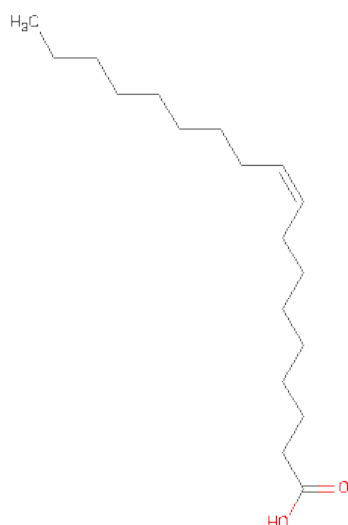
Chain	Residue	Modelled	Actual	Comment	Reference
C	160	ALA	SER	ENGINEERED MUTATION	UNP P34998
C	1040	SER	ASN	ENGINEERED MUTATION	UNP P00720
C	1041	VAL	ALA	ENGINEERED MUTATION	UNP P00720
C	1054	SER	CYS	ENGINEERED MUTATION	UNP P00720
C	1097	SER	CYS	ENGINEERED MUTATION	UNP P00720
C	1151	ALA	THR	ENGINEERED MUTATION	UNP P00720
C	228	ALA	LYS	ENGINEERED MUTATION	UNP P34998
C	260	ALA	PHE	ENGINEERED MUTATION	UNP P34998
C	277	ALA	ILE	ENGINEERED MUTATION	UNP P34998
C	309	ALA	TYR	ENGINEERED MUTATION	UNP P34998
C	330	ALA	PHE	ENGINEERED MUTATION	UNP P34998
C	349	ALA	SER	ENGINEERED MUTATION	UNP P34998
C	363	ALA	TYR	ENGINEERED MUTATION	UNP P34998
C	374	ALA	-	EXPRESSION TAG	UNP P34998
C	375	ALA	-	EXPRESSION TAG	UNP P34998
C	376	ALA	-	EXPRESSION TAG	UNP P34998
C	377	HIS	-	EXPRESSION TAG	UNP P34998
C	378	HIS	-	EXPRESSION TAG	UNP P34998
C	379	HIS	-	EXPRESSION TAG	UNP P34998
C	380	HIS	-	EXPRESSION TAG	UNP P34998
C	381	HIS	-	EXPRESSION TAG	UNP P34998
C	382	HIS	-	EXPRESSION TAG	UNP P34998
C	383	HIS	-	EXPRESSION TAG	UNP P34998
C	384	HIS	-	EXPRESSION TAG	UNP P34998
C	385	HIS	-	EXPRESSION TAG	UNP P34998
C	386	HIS	-	EXPRESSION TAG	UNP P34998

- Molecule 2 is 3,6-DIMETHYL-N-(PENTAN-3-YL)-2-(2,4,6-TRIMETHYLPHENOXY)PYRIDIN-4-AMINE (three-letter code: 1Q5) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>2</sub>O).



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

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula:  $C_{18}H_{34}O_2$ ).



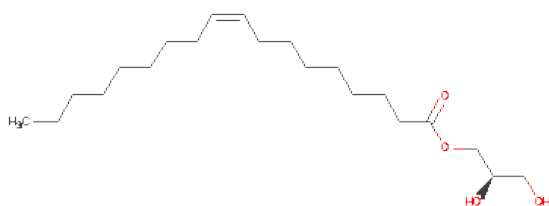
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			13	13		

*Continued on next page...*

*Continued from previous page...*

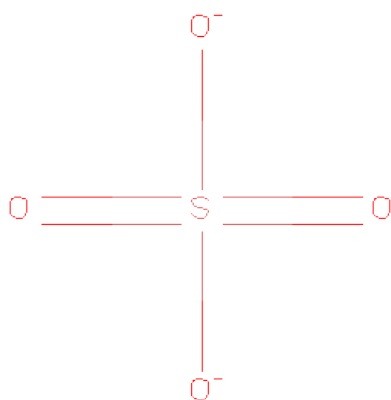
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is (2R)-2,3-DIHYDROXYPROPYL(9Z)-OCTADEC-9-ENOATE (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



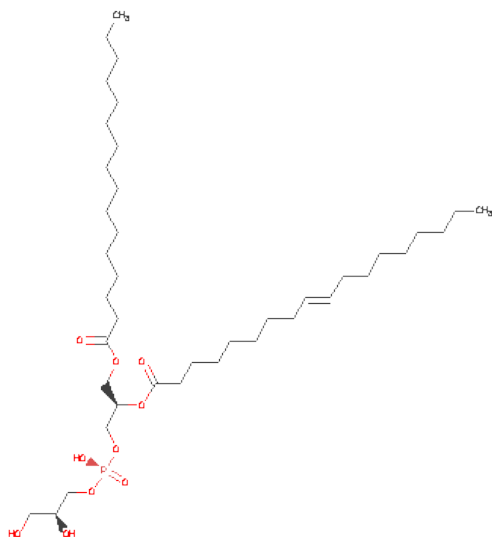
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

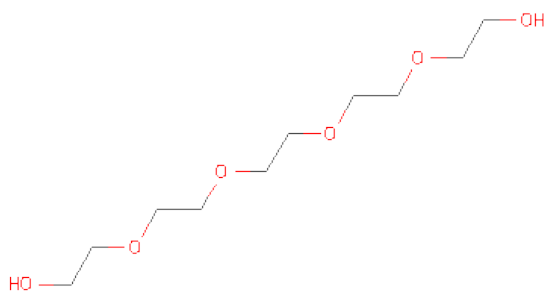
- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(HEXADECANOYLOXY)METHYL]ETHYL(9Z)-OCTADEC-9-ENOATE (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			39	30	8	1		
6	B	1	Total	C	O	P	0	0
			46	37	8	1		
6	B	1	Total	C	O		0	0
			37	32	5			

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).

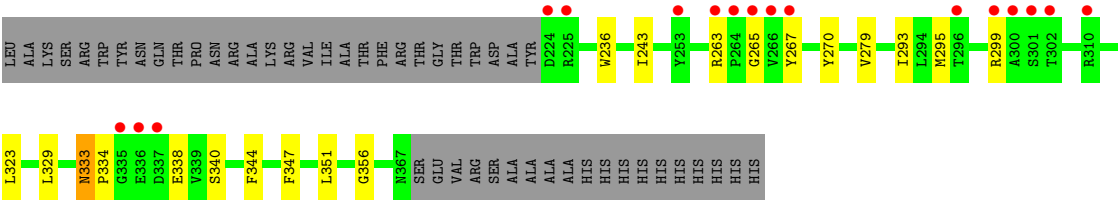


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is water.

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.56Å 123.97Å 166.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.14 – 2.98 34.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	85.7 (34.14-2.98) 85.7 (34.15-2.98)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.242 , 0.265 0.245 , 0.269	Depositor DCC
$R_{free}$ test set	1586 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 32121 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: OLA, OLC, 1PE, 1Q5, PGW, SO4

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	0.62	0/3358	0.68	3/4556 (0.1%)
1	B	0.65	0/3271	0.65	1/4435 (0.0%)
1	C	0.60	0/2063	0.69	0/2810
All	All	0.63	0/8692	0.67	4/11801 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LYS	N-CA-C	-7.98	89.46	111.00
1	B	296	THR	N-CA-C	6.72	129.15	111.00
1	A	1048	LYS	CD-CE-NZ	-6.53	96.68	111.70
1	A	1007	LEU	CB-CG-CD2	-5.55	101.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	GLU	Mainchain

## 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	3278	0	3333	40	1
1	B	3194	0	3247	40	1
1	C	2005	0	2038	19	1
2	A	24	0	30	2	0
2	B	24	0	30	5	0
2	C	24	0	30	3	0
3	A	13	0	23	1	0
3	C	20	0	33	1	0
4	A	50	0	80	4	0
4	B	25	0	40	2	0
5	A	5	0	0	1	1
5	B	15	0	0	0	1
6	B	122	0	174	10	0
7	B	16	0	22	0	0
8	A	4	0	0	0	0
8	B	4	0	0	1	0
All	All	8823	0	9080	102	3

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 6.

The worst 5 of 102 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:338:GLU:HB2	1:C:340:SER:H	1.44	0.82
1:B:329:LEU:HB3	1:B:344:PHE:HE1	1.48	0.77
1:A:1006:MET:HG2	1:A:1007:LEU:HD12	1.69	0.75
1:A:263:ARG:O	1:A:265:GLY:HA3	1.87	0.74
1:C:263:ARG:O	1:C:265:GLY:HA3	1.92	0.70

All (3) 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)
1:A:1137:ARG:NH1	5:B:506:SO4:O1[1_655]	2.16	0.04

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1137:ARG:NH1	5:A:504:SO4:O2[1_455]	2.17	0.03
1:C:270:TYR:OH	1:C:338:GLU:OE1[2_556]	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	403/441 (91%)	394 (98%)	9 (2%)	0	100	100
1	B	390/441 (88%)	383 (98%)	7 (2%)	0	100	100
1	C	244/441 (55%)	240 (98%)	4 (2%)	0	100	100
All	All	1037/1323 (78%)	1017 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	345/374 (92%)	344 (100%)	1 (0%)	96	99
1	B	335/374 (90%)	333 (99%)	2 (1%)	92	98
1	C	211/374 (56%)	210 (100%)	1 (0%)	94	99
All	All	891/1122 (79%)	887 (100%)	4 (0%)	95	99

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	TYR
1	B	283	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	354	PHE
1	C	333	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	367	ASN
1	C	333	ASN

### 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 ⓘ

16 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	1Q5	A	401	-	25,25,25	1.61	4 (16%)	35,35,35	1.90	9 (25%)
3	OLA	A	501	-	12,12,19	1.41	1 (8%)	11,11,19	2.49	1 (9%)
4	OLC	A	502	-	24,24,24	0.76	2 (8%)	25,25,25	1.00	1 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OLC	A	503	-	24,24,24	0.79	2 (8%)	25,25,25	1.00	1 (4%)
5	SO4	A	504	-	4,4,4	0.20	0	6,6,6	0.10	0
2	1Q5	B	401	-	25,25,25	1.58	4 (16%)	35,35,35	1.83	7 (20%)
4	OLC	B	501	-	24,24,24	0.76	2 (8%)	25,25,25	0.99	1 (4%)
6	PGW	B	502	-	38,38,50	1.25	5 (13%)	43,43,56	1.28	4 (9%)
6	PGW	B	503	-	45,45,50	0.94	4 (8%)	50,50,56	1.16	2 (4%)
6	PGW	B	504	-	36,36,50	1.29	5 (13%)	38,38,56	1.36	5 (13%)
7	1PE	B	505	-	15,15,15	0.52	0	14,14,14	0.86	0
5	SO4	B	506	-	4,4,4	0.20	0	6,6,6	0.07	0
5	SO4	B	507	-	4,4,4	0.26	0	6,6,6	0.19	0
5	SO4	B	508	-	4,4,4	0.13	0	6,6,6	0.09	0
2	1Q5	C	401	-	25,25,25	1.58	4 (16%)	35,35,35	1.79	7 (20%)
3	OLA	C	501	-	19,19,19	0.46	0	19,19,19	1.02	0

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	1Q5	A	401	-	-	0/12/12/12	0/2/2/2
3	OLA	A	501	-	-	0/10/10/17	0/0/0/0
4	OLC	A	502	-	-	0/24/24/24	0/0/0/0
4	OLC	A	503	-	-	0/24/24/24	0/0/0/0
5	SO4	A	504	-	-	0/0/0/0	0/0/0/0
2	1Q5	B	401	-	-	0/12/12/12	0/2/2/2
4	OLC	B	501	-	-	0/24/24/24	0/0/0/0
6	PGW	B	502	-	-	0/40/40/55	0/0/0/0
6	PGW	B	503	-	-	0/47/47/55	0/0/0/0
6	PGW	B	504	-	-	0/38/38/55	0/0/0/0
7	1PE	B	505	-	-	0/13/13/13	0/0/0/0
5	SO4	B	506	-	-	0/0/0/0	0/0/0/0
5	SO4	B	507	-	-	0/0/0/0	0/0/0/0
5	SO4	B	508	-	-	0/0/0/0	0/0/0/0
2	1Q5	C	401	-	-	0/12/12/12	0/2/2/2
3	OLA	C	501	-	-	0/17/17/17	0/0/0/0

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	OLA	C6-C7	-4.79	1.53	1.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	PGW	C27-C26	-4.41	1.53	1.55
2	A	401	1Q5	C1-C6	4.19	1.47	1.40
2	B	401	1Q5	C1-C6	4.19	1.47	1.40
6	B	504	PGW	C11-C09	-4.16	1.53	1.55

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	OLA	C6-C7-C8	-7.89	109.75	117.97
2	A	401	1Q5	C15-N19-C20	-5.59	119.61	125.56
2	B	401	1Q5	C15-N19-C20	-5.15	120.07	125.56
2	C	401	1Q5	C15-N19-C20	-4.81	120.43	125.56
2	B	401	1Q5	C11-N12-C13	4.19	121.61	117.28

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, 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	407/441 (92%)	0.25	34 (8%) 11 6	32, 56, 112, 131	0
1	B	396/441 (89%)	0.05	20 (5%) 27 12	28, 50, 92, 116	0
1	C	248/441 (56%)	0.44	28 (11%) 6 3	37, 66, 115, 139	0
All	All	1051/1323 (79%)	0.22	82 (7%) 13 6	28, 55, 109, 139	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	TYR	6.9
1	C	300	ALA	6.3
1	C	264	PRO	6.2
1	C	117	HIS	5.6
1	A	1054	SER	5.0

### 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	1PE	B	505	16/16	0.29	3.46	45,56,64,66	0
6	PGW	B	504	37/51	0.25	2.96	41,54,75,81	0
4	OLC	A	503	25/25	0.22	2.94	28,50,67,70	0
6	PGW	B	502	39/51	0.30	2.77	31,53,90,114	0
4	OLC	B	501	25/25	0.28	2.60	25,58,79,83	0
5	SO4	B	508	5/5	0.17	0.90	69,80,92,103	0
3	OLA	C	501	20/20	0.19	0.58	35,47,79,79	0
2	1Q5	A	401	24/24	0.19	0.49	43,52,58,60	0
2	1Q5	B	401	24/24	0.18	0.49	35,47,52,54	0
6	PGW	B	503	46/51	0.24	0.45	29,49,93,111	0
3	OLA	A	501	13/20	0.16	0.21	28,39,47,47	0
2	1Q5	C	401	24/24	0.19	0.19	47,52,58,69	0
4	OLC	A	502	25/25	0.20	0.12	41,53,77,82	0
5	SO4	B	507	5/5	0.17	-0.56	40,48,54,55	0
5	SO4	B	506	5/5	0.11	-1.75	62,64,72,76	0
5	SO4	A	504	5/5	0.09	-4.85	61,62,73,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.