



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:57 PM GMT

PDB ID : 3V6O  
Title : Leptin Receptor-antibody complex  
Authors : Carpenter, B.; Hemsworth, G.R.; Ross, R.J.; Artymiuk, P.J.  
Deposited on : 2011-12-20  
Resolution : 1.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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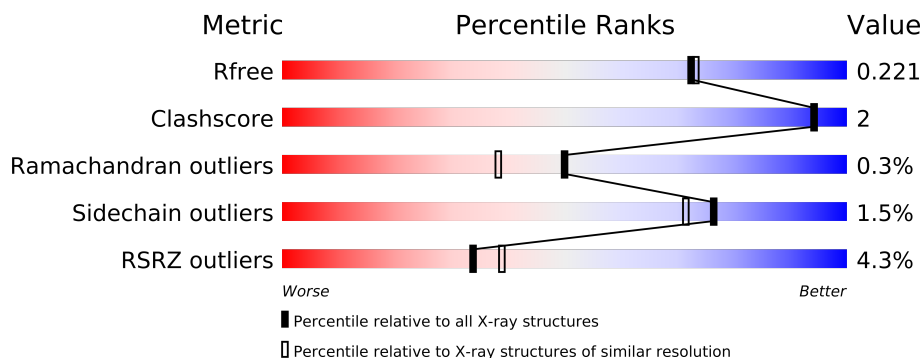
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	206	
1	B	206	
2	C	221	
2	D	221	
3	E	215	
3	F	215	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	A	709	-	X
5	EDO	B	1002	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	C	303	-	X
5	EDO	C	304	-	X
5	EDO	D	303	-	X
5	EDO	D	304	-	X
5	EDO	D	305	-	X
5	EDO	F	304	-	X
5	EDO	F	305	-	X
5	EDO	F	306	-	X
5	EDO	F	308	-	X
5	EDO	F	309	-	X
6	ACT	C	302	-	X
6	ACT	F	302	-	X
8	NAG	F	301	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10514 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 Leptin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1450	937	235	267	11			
1	B	184	Total	C	N	O	S	0	0	0
			1466	942	240	273	11			

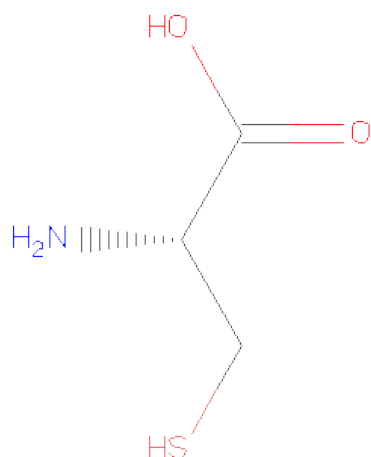
- Molecule 2 is a protein called Monoclonal antibody 9F8 fab fragment Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	220	Total	C	N	O	S	0	0	1
			1640	1034	267	330	9			
2	D	215	Total	C	N	O	S	0	0	0
			1610	1018	260	323	9			

- Molecule 3 is a protein called Monoclonal antibody 9F8 fab fragment Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1663	1037	286	332	8			
3	F	212	Total	C	N	O	S	0	0	0
			1657	1034	285	330	8			

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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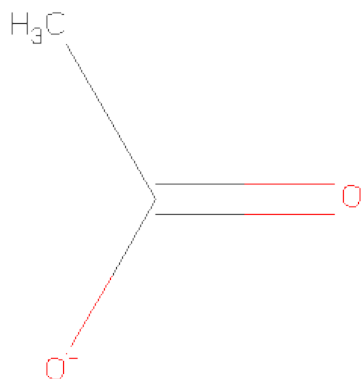
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

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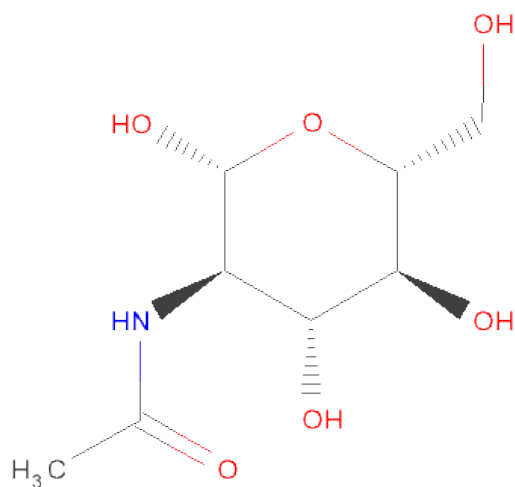
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Na	0	0
			1	1		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	101	Total	O	0	0
			101	101		

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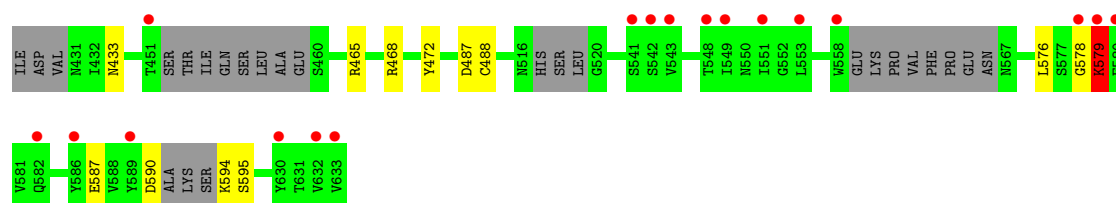
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	89	Total 89	O 89	0	0
9	C	186	Total 186	O 186	0	0
9	D	133	Total 133	O 133	0	0
9	E	168	Total 168	O 168	0	0
9	F	174	Total 174	O 174	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

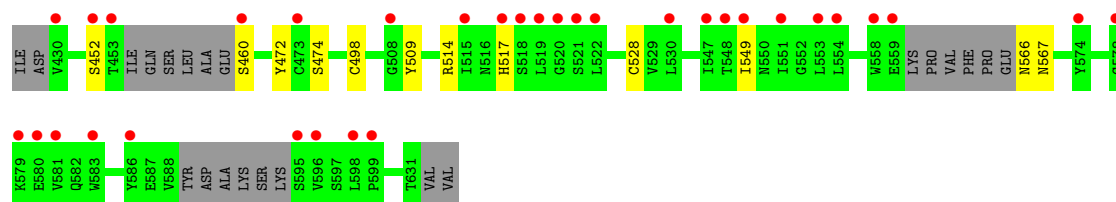
- Molecule 1: Leptin receptor

Chain A: 



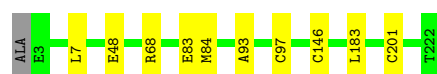
- Molecule 1: Leptin receptor

Chain B: 



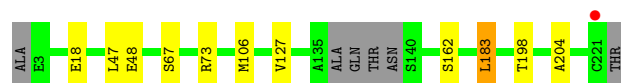
- Molecule 2: Monoclonal antibody 9F8 fab fragment Heavy chain

Chain C: 



- Molecule 2: Monoclonal antibody 9F8 fab fragment Heavy chain

Chain D: 



- Molecule 3: Monoclonal antibody 9F8 fab fragment Light chain

Chain E: 



- Molecule 3: Monoclonal antibody 9F8 fab fragment Light chain

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.81Å 118.83Å 171.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 1.95 44.65 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-1.95) 99.9 (44.65-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.171 , 0.213 0.180 , 0.221	Depositor DCC
$R_{free}$ test set	6724 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 133779 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: NA, ACT, EDO, NAG

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	1.01	1/1488 (0.1%)	0.87	1/2025 (0.0%)
1	B	0.94	2/1505 (0.1%)	0.85	1/2050 (0.0%)
2	C	1.19	6/1683 (0.4%)	0.93	2/2303 (0.1%)
2	D	1.08	2/1652 (0.1%)	0.89	3/2258 (0.1%)
3	E	1.09	3/1701 (0.2%)	0.96	5/2310 (0.2%)
3	F	1.09	2/1694 (0.1%)	0.94	4/2298 (0.2%)
All	All	1.07	16/9723 (0.2%)	0.91	16/13244 (0.1%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	97	CYS	CB-SG	-7.99	1.68	1.82
2	C	201	CYS	CB-SG	-7.27	1.69	1.82
3	E	196	CYS	CB-SG	-6.72	1.70	1.82
2	C	146	CYS	CB-SG	-6.69	1.70	1.82
1	B	498	CYS	CB-SG	6.30	1.93	1.82
2	C	83	GLU	CG-CD	6.25	1.61	1.51
3	F	196	CYS	CB-SG	-6.15	1.71	1.82
3	F	25	CYS	CB-SG	-5.96	1.72	1.81
3	E	86	ALA	CA-CB	5.76	1.64	1.52
2	D	204	ALA	CA-CB	5.52	1.64	1.52
2	C	93	ALA	CA-CB	5.47	1.64	1.52
2	C	48	GLU	CB-CG	-5.28	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	48	GLU	CG-CD	5.19	1.59	1.51
3	E	197	GLU	CG-CD	5.10	1.59	1.51
1	A	468	ARG	CB-CG	-5.09	1.38	1.52
1	B	509	TYR	CD1-CE1	5.04	1.47	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	177	MET	CG-SD-CE	-8.10	87.24	100.20
2	C	68	ARG	NE-CZ-NH1	6.99	123.80	120.30
3	F	32	ARG	NE-CZ-NH1	6.70	123.65	120.30
3	E	32	ARG	NE-CZ-NH2	-6.54	117.03	120.30
3	F	56	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	C	84	MET	CG-SD-CE	-6.13	90.39	100.20
3	F	110	ARG	NE-CZ-NH1	5.97	123.29	120.30
3	E	32	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	D	183	LEU	CA-CB-CG	5.80	128.64	115.30
3	E	63	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	514	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	D	73	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	F	56	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	D	106	MET	CG-SD-CE	5.35	108.76	100.20
1	A	465	ARG	NE-CZ-NH1	-5.17	117.71	120.30
3	E	87	ASP	CB-CG-OD2	5.15	122.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	LYS	Peptide

## 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	1450	0	0	5	0
1	B	1466	0	0	3	0
2	C	1640	0	0	0	0
2	D	1610	0	0	3	0
3	E	1663	0	0	2	0
3	F	1657	0	0	3	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
5	A	32	0	48	3	0
5	B	20	0	30	3	0
5	C	8	0	12	0	0
5	D	28	0	42	3	0
5	E	12	0	18	1	0
5	F	24	0	36	1	0
6	C	8	0	6	0	0
6	D	4	0	3	0	0
6	E	4	0	3	0	0
6	F	8	0	6	1	0
7	C	1	0	0	0	0
8	F	14	0	13	0	0
9	A	101	0	0	0	0
9	B	89	0	0	0	0
9	C	186	0	0	0	0
9	D	133	0	0	0	0
9	E	168	0	0	1	0
9	F	174	0	0	0	0
All	All	10514	0	217	15	0

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 2.

All (15) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:67:SER:N	5:D:306:EDO:HO2	1.76	0.84
2:D:127:VAL:N	5:D:307:EDO:HO2	2.02	0.58
5:A:704:EDO:HO2	1:B:472:TYR:N	2.08	0.52
3:F:119:ILE:N	5:F:309:EDO:HO1	2.07	0.52
1:B:567:ASN:N	5:B:1003:EDO:HO1	2.08	0.51
1:B:528:CYS:N	5:B:1006:EDO:HO2	2.09	0.51
3:E:148:VAL:N	5:E:302:EDO:HO1	2.09	0.50
1:A:487:ASP:N	5:A:702:EDO:HO2	2.10	0.50
1:A:472:TYR:N	5:B:1005:EDO:HO1	2.14	0.46
3:F:57:HIS:ND1	6:F:303:ACT:OXT	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:433:ASN:OD1	3:F:56:ARG:NH2	2.52	0.43
3:E:158:GLN:N	9:E:501:HOH:O	2.52	0.42
1:A:587:GLU:N	1:A:587:GLU:CD	2.73	0.41
2:D:47:LEU:N	5:D:302:EDO:HO2	2.19	0.41
1:A:488:CYS:O	5:A:707:EDO:H12	2.22	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	171/206 (83%)	166 (97%)	3 (2%)	2 (1%)	19	6
1	B	176/206 (85%)	167 (95%)	8 (4%)	1 (1%)	33	19
2	C	218/221 (99%)	213 (98%)	5 (2%)	0	100	100
2	D	211/221 (96%)	203 (96%)	8 (4%)	0	100	100
3	E	211/215 (98%)	207 (98%)	4 (2%)	0	100	100
3	F	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
All	All	1195/1284 (93%)	1158 (97%)	34 (3%)	3 (0%)	50	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	LYS
1	B	452	SER
1	A	578	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	168/191 (88%)	163 (97%)	5 (3%)	53	39
1	B	170/191 (89%)	165 (97%)	5 (3%)	55	41
2	C	191/193 (99%)	189 (99%)	2 (1%)	85	84
2	D	188/193 (97%)	184 (98%)	4 (2%)	66	57
3	E	190/191 (100%)	190 (100%)	0	100	100
3	F	189/191 (99%)	188 (100%)	1 (0%)	94	93
All	All	1096/1150 (95%)	1079 (98%)	17 (2%)	76	69

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	576	LEU
1	A	579	LYS
1	A	590	ASP
1	A	594	LYS
1	A	595	SER
1	B	460	SER
1	B	474	SER
1	B	517	HIS
1	B	549	ILE
1	B	566	ASN
2	C	7	LEU
2	C	183	LEU
2	D	18	GLU
2	D	162	SER
2	D	183	LEU
2	D	198	THR
3	F	72	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 41 ligands modelled in this entry, 1 is monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	CYS	A	701	1	6,6,6	0.99	0	7,7,7	1.92	2 (28%)
5	EDO	A	702	-	3,3,3	0.51	0	2,2,2	0.35	0
5	EDO	A	703	-	3,3,3	0.83	0	2,2,2	0.32	0
5	EDO	A	704	-	3,3,3	0.31	0	2,2,2	0.46	0
5	EDO	A	705	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	A	706	-	3,3,3	0.55	0	2,2,2	0.36	0
5	EDO	A	707	-	3,3,3	0.39	0	2,2,2	0.77	0
5	EDO	A	708	-	3,3,3	0.40	0	2,2,2	0.78	0
5	EDO	A	709	-	3,3,3	0.95	0	2,2,2	0.70	0
4	CYS	B	1001	1	6,6,6	0.97	0	7,7,7	1.13	1 (14%)
5	EDO	B	1002	-	3,3,3	0.46	0	2,2,2	0.90	0
5	EDO	B	1003	-	3,3,3	0.53	0	2,2,2	0.70	0
5	EDO	B	1004	-	3,3,3	0.74	0	2,2,2	0.50	0
5	EDO	B	1005	-	3,3,3	0.53	0	2,2,2	0.76	0
5	EDO	B	1006	-	3,3,3	0.39	0	2,2,2	0.38	0
6	ACT	C	301	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
6	ACT	C	302	-	1,3,3	0.02	0	0,3,3	0.00	-
5	EDO	C	303	-	3,3,3	0.86	0	2,2,2	0.08	0
5	EDO	C	304	-	3,3,3	0.55	0	2,2,2	0.56	0
6	ACT	D	301	-	1,3,3	3.38	1 (100%)	0,3,3	0.00	-
5	EDO	D	302	-	3,3,3	0.78	0	2,2,2	0.17	0
5	EDO	D	303	-	3,3,3	0.55	0	2,2,2	1.07	0
5	EDO	D	304	-	3,3,3	0.63	0	2,2,2	0.80	0
5	EDO	D	305	-	3,3,3	0.46	0	2,2,2	0.91	0
5	EDO	D	306	-	3,3,3	0.47	0	2,2,2	0.51	0
5	EDO	D	307	-	3,3,3	0.63	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	308	-	3,3,3	0.55	0	2,2,2	0.85	0
6	ACT	E	301	-	1,3,3	0.78	0	0,3,3	0.00	-
5	EDO	E	302	-	3,3,3	0.48	0	2,2,2	0.42	0
5	EDO	E	303	-	3,3,3	0.67	0	2,2,2	0.28	0
5	EDO	E	304	-	3,3,3	0.57	0	2,2,2	0.36	0
8	NAG	F	301	3	12,14,15	1.06	1 (8%)	15,19,21	1.95	4 (26%)
6	ACT	F	302	-	1,3,3	1.25	0	0,3,3	0.00	-
6	ACT	F	303	-	1,3,3	1.09	0	0,3,3	0.00	-
5	EDO	F	304	-	3,3,3	0.57	0	2,2,2	0.68	0
5	EDO	F	305	-	3,3,3	0.71	0	2,2,2	0.24	0
5	EDO	F	306	-	3,3,3	1.09	0	2,2,2	0.31	0
5	EDO	F	307	-	3,3,3	0.75	0	2,2,2	0.35	0
5	EDO	F	308	-	3,3,3	0.66	0	2,2,2	0.93	0
5	EDO	F	309	-	3,3,3	0.39	0	2,2,2	0.18	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
4	CYS	A	701	1	-	0/6/6/6	0/0/0/0
5	EDO	A	702	-	-	0/1/1/1	0/0/0/0
5	EDO	A	703	-	-	0/1/1/1	0/0/0/0
5	EDO	A	704	-	-	0/1/1/1	0/0/0/0
5	EDO	A	705	-	-	0/1/1/1	0/0/0/0
5	EDO	A	706	-	-	0/1/1/1	0/0/0/0
5	EDO	A	707	-	-	0/1/1/1	0/0/0/0
5	EDO	A	708	-	-	0/1/1/1	0/0/0/0
5	EDO	A	709	-	-	0/1/1/1	0/0/0/0
4	CYS	B	1001	1	-	0/6/6/6	0/0/0/0
5	EDO	B	1002	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1003	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1004	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1005	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1006	-	-	0/1/1/1	0/0/0/0
6	ACT	C	301	-	-	0/0/0/0	0/0/0/0
6	ACT	C	302	-	-	0/0/0/0	0/0/0/0
5	EDO	C	303	-	-	0/1/1/1	0/0/0/0
5	EDO	C	304	-	-	0/1/1/1	0/0/0/0
6	ACT	D	301	-	-	0/0/0/0	0/0/0/0
5	EDO	D	302	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	303	-	-	0/1/1/1	0/0/0/0
5	EDO	D	304	-	-	0/1/1/1	0/0/0/0
5	EDO	D	305	-	-	0/1/1/1	0/0/0/0
5	EDO	D	306	-	-	0/1/1/1	0/0/0/0
5	EDO	D	307	-	-	0/1/1/1	0/0/0/0
5	EDO	D	308	-	-	0/1/1/1	0/0/0/0
6	ACT	E	301	-	-	0/0/0/0	0/0/0/0
5	EDO	E	302	-	-	0/1/1/1	0/0/0/0
5	EDO	E	303	-	-	0/1/1/1	0/0/0/0
5	EDO	E	304	-	-	0/1/1/1	0/0/0/0
8	NAG	F	301	3	-	0/6/23/26	0/1/1/1
6	ACT	F	302	-	-	0/0/0/0	0/0/0/0
6	ACT	F	303	-	-	0/0/0/0	0/0/0/0
5	EDO	F	304	-	-	0/1/1/1	0/0/0/0
5	EDO	F	305	-	-	0/1/1/1	0/0/0/0
5	EDO	F	306	-	-	0/1/1/1	0/0/0/0
5	EDO	F	307	-	-	0/1/1/1	0/0/0/0
5	EDO	F	308	-	-	0/1/1/1	0/0/0/0
5	EDO	F	309	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	ACT	CH3-C	3.38	1.53	1.48
6	C	301	ACT	CH3-C	2.57	1.52	1.48
8	F	301	NAG	C2-N2	2.51	1.49	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	301	NAG	C2-N2-C7	4.68	130.94	123.09
8	F	301	NAG	O5-C5-C4	-3.59	106.10	110.65
4	A	701	CYS	OXT-C-CA	3.51	124.77	116.88
8	F	301	NAG	O5-C5-C6	2.75	109.87	106.98
4	A	701	CYS	OXT-C-O	-2.63	118.13	124.07
4	B	1001	CYS	OXT-C-CA	2.12	121.64	116.88
8	F	301	NAG	O7-C7-N2	2.10	126.28	121.90

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	181/206 (87%)	0.55	18 (9%) 8 10	20, 38, 77, 107	0
1	B	184/206 (89%)	0.96	33 (17%) 2 2	19, 43, 88, 107	0
2	C	220/221 (99%)	-0.27	0 100 100	18, 30, 48, 63	0
2	D	215/221 (97%)	-0.11	1 (0%) 88 94	19, 32, 63, 94	0
3	E	213/215 (99%)	-0.19	1 (0%) 88 94	21, 35, 54, 65	0
3	F	212/215 (98%)	-0.28	1 (0%) 88 94	19, 32, 48, 79	0
All	All	1225/1284 (95%)	0.08	54 (4%) 34 38	18, 34, 67, 107	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	LEU	8.9
1	B	558	TRP	4.9
1	B	579	LYS	4.3
1	A	580	GLU	4.3
1	B	549	ILE	4.2
1	B	521	SER	4.0
1	A	551	ILE	4.0
1	B	517	HIS	3.9
1	B	453	THR	3.8
1	A	553	LEU	3.8
1	B	598	LEU	3.7
1	A	633	VAL	3.7
1	B	548	THR	3.7
1	B	551	ILE	3.5
1	A	586	TYR	3.5
1	B	596	VAL	3.3
1	B	518	SER	3.3
1	B	580	GLU	3.2
1	B	586	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	543	VAL	3.1
1	B	554	LEU	3.1
2	D	221	CYS	3.0
1	B	522	LEU	3.0
1	B	574	TYR	3.0
1	A	578	GLY	2.9
1	B	553	LEU	2.8
1	A	579	LYS	2.8
1	B	430	VAL	2.8
1	B	452	SER	2.8
1	A	632	VAL	2.8
1	A	542	SER	2.7
1	A	589	TYR	2.7
1	B	547	ILE	2.7
1	B	595	SER	2.7
1	A	549	ILE	2.6
1	B	520	GLY	2.5
1	A	558	TRP	2.5
3	F	216	CYS	2.4
1	A	541	SER	2.4
1	B	599	PRO	2.4
1	A	582	GLN	2.4
1	B	578	GLY	2.4
1	B	530	LEU	2.4
1	A	630	TYR	2.3
1	B	473	CYS	2.3
1	B	515	ILE	2.3
1	B	581	VAL	2.2
1	A	451	THR	2.2
1	A	548	THR	2.2
1	B	559	GLU	2.1
1	B	508	GLY	2.1
3	E	9	SER	2.1
1	B	583	TRP	2.0
1	B	460	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
5	EDO	D	305	4/4	0.26	11.90	36,63,64,69	0
5	EDO	C	304	4/4	0.17	11.83	30,37,41,43	0
5	EDO	D	304	4/4	0.28	9.91	50,66,82,86	0
5	EDO	A	709	4/4	0.26	8.72	35,60,63,66	0
5	EDO	F	309	4/4	0.17	7.86	30,35,48,53	0
8	NAG	F	301	14/15	0.28	6.17	79,102,115,116	0
6	ACT	C	302	4/4	0.26	5.15	38,45,56,62	0
5	EDO	C	303	4/4	0.14	4.57	28,36,37,39	0
5	EDO	F	308	4/4	0.16	4.16	30,56,60,63	0
6	ACT	F	302	4/4	0.19	3.09	40,53,55,55	0
5	EDO	B	1002	4/4	0.20	2.63	49,50,51,52	0
5	EDO	D	303	4/4	0.18	2.44	28,33,45,56	0
5	EDO	F	306	4/4	0.15	2.36	28,35,51,59	0
5	EDO	F	304	4/4	0.19	2.30	37,48,71,72	0
5	EDO	F	305	4/4	0.20	2.25	49,51,63,70	0
5	EDO	A	704	4/4	0.21	1.78	25,48,50,52	0
5	EDO	D	308	4/4	0.15	1.75	39,40,41,45	0
5	EDO	D	307	4/4	0.12	1.61	30,40,41,51	0
5	EDO	A	702	4/4	0.12	1.48	42,43,44,49	0
5	EDO	E	303	4/4	0.13	1.47	37,41,45,46	0
5	EDO	A	703	4/4	0.17	1.44	39,39,60,68	0
5	EDO	B	1006	4/4	0.17	1.39	34,35,37,51	0
5	EDO	B	1005	4/4	0.20	1.39	26,46,48,57	0
5	EDO	E	302	4/4	0.11	0.74	39,47,48,61	0
5	EDO	A	705	4/4	0.08	0.68	33,37,38,39	0
6	ACT	C	301	4/4	0.15	0.35	37,39,40,49	0
5	EDO	F	307	4/4	0.13	0.24	34,44,44,45	0
5	EDO	A	707	4/4	0.09	-0.03	39,49,54,54	0
5	EDO	B	1004	4/4	0.14	-0.14	42,43,48,61	0
5	EDO	D	306	4/4	0.12	-0.22	51,63,65,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	708	4/4	0.09	-0.24	47,58,58,62	0
4	CYS	B	1001	7/7	0.08	-0.33	32,35,40,44	0
5	EDO	D	302	4/4	0.08	-0.34	25,40,40,42	0
4	CYS	A	701	7/7	0.06	-0.75	26,32,35,37	0
6	ACT	D	301	4/4	0.13	-0.75	26,28,29,31	0
6	ACT	E	301	4/4	0.13	-0.80	26,27,32,35	0
5	EDO	B	1003	4/4	0.13	-0.91	46,76,76,84	0
6	ACT	F	303	4/4	0.12	-1.01	21,25,27,29	0
5	EDO	A	706	4/4	0.08	-1.12	37,38,41,44	0
5	EDO	E	304	4/4	0.12	-1.31	40,43,50,58	0
7	NA	C	305	1/1	0.06	-1.41	32,32,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.