



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:31 AM BST

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

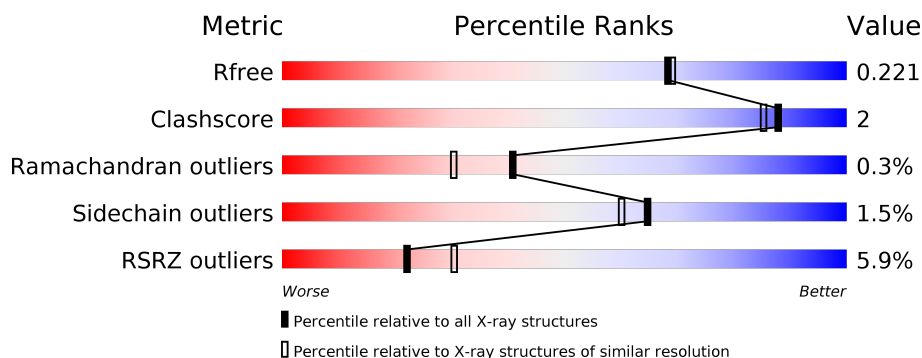
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	206	<div> <div>12%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>12%</div> </div> </div>
1	B	206	<div> <div>19%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>11%</div> </div> </div>
2	C	221	<div> <div></div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
2	D	221	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
3	E	215	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
3	F	215	<div> <div></div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>

2 Entry composition

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

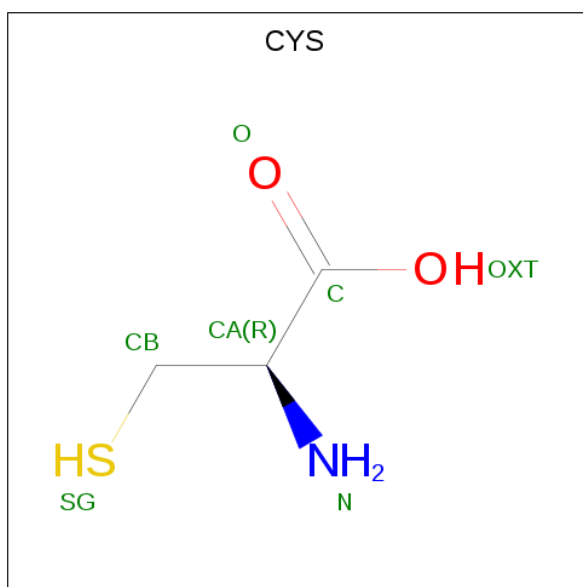
- Molecule 2 is a protein called Monoclonal antibody 9F8 fab fragment Heavy chain.

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: C₃H₇NO₂S).



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: C₂H₆O₂).



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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

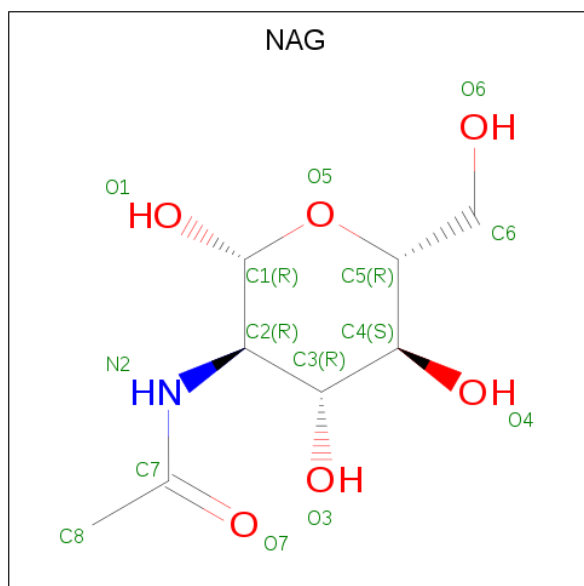
Continued from previous page...

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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		

Continued on next page...

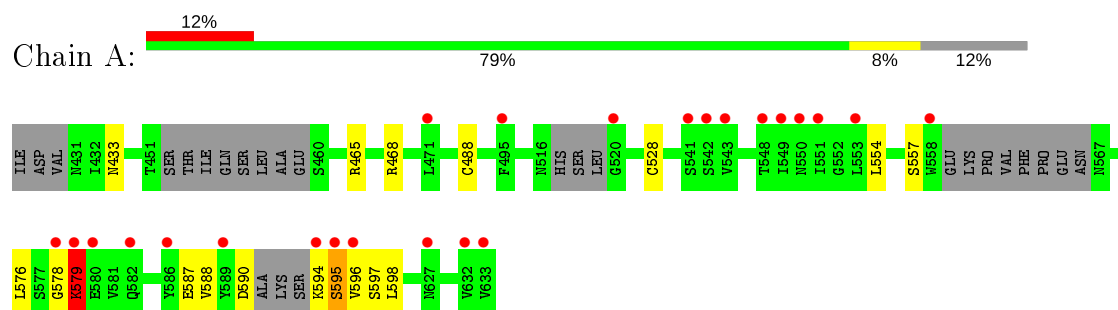
Continued from previous page...

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

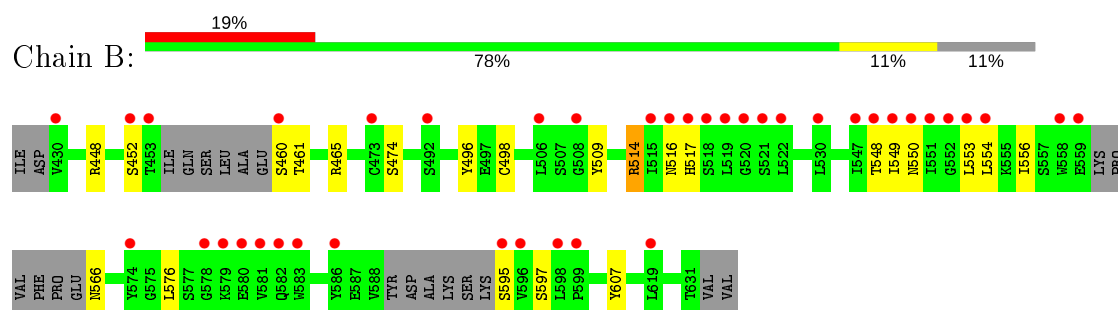
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

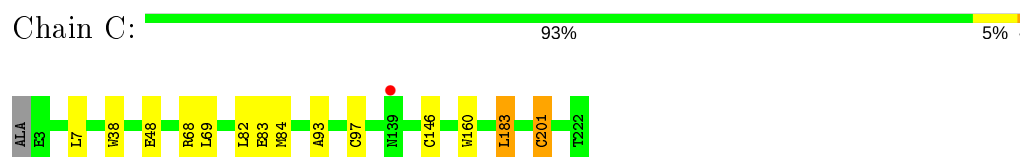
- Molecule 1: Leptin receptor



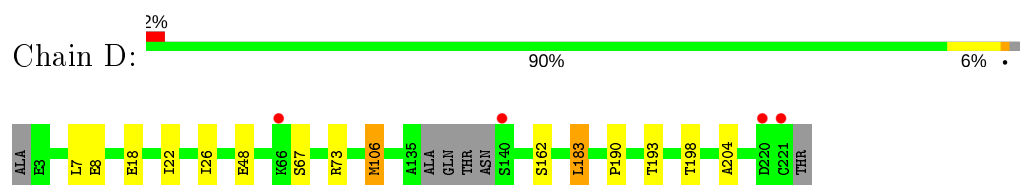
- Molecule 1: Leptin receptor



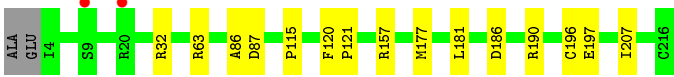
- Molecule 2: Monoclonal antibody 9F8 fab fragment Heavy chain



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.171 , 0.213 0.179 , 0.221	Depositor DCC
R_{free} test set	6724 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10514	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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

Continued on next page...

Continued from previous page...

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 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	1450	0	1426	11	0
1	B	1466	0	1432	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1640	0	1587	4	0
2	D	1610	0	1560	7	0
3	E	1663	0	1600	4	0
3	F	1657	0	1594	6	0
4	A	7	0	3	0	0
4	B	7	0	3	0	0
5	A	32	0	48	1	0
5	B	20	0	30	0	0
5	C	8	0	12	0	0
5	D	28	0	42	1	0
5	E	12	0	18	0	0
5	F	24	0	36	2	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	0	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	0	0
9	F	174	0	0	0	0
All	All	10514	0	9422	38	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 2.

All (38) 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:B:461:THR:CG2	1:B:516:ASN:HB2	2.19	0.73
1:B:461:THR:HG22	1:B:516:ASN:HB2	1.70	0.72
1:A:588:VAL:HG21	1:A:596:VAL:HG21	1.84	0.59
2:D:106:MET:HE1	3:F:100:PHE:HZ	1.71	0.56
2:D:7:LEU:HD12	2:D:8:GLU:N	2.21	0.55
1:A:528:CYS:H	5:F:306:EDO:C1	2.21	0.52
1:A:528:CYS:H	5:F:306:EDO:H11	1.77	0.49
3:E:157:ARG:HD3	3:E:181:LEU:HD11	1.95	0.48
3:F:191:HIS:O	3:F:213:ARG:HD3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ILE:O	1:B:595:SER:HA	2.16	0.46
1:A:554:LEU:O	1:A:597:SER:HA	2.16	0.46
1:A:588:VAL:CG2	1:A:596:VAL:HG21	2.45	0.45
1:A:557:SER:HB3	1:A:595:SER:HB2	1.99	0.45
2:D:26:ILE:HD12	2:D:26:ILE:C	2.37	0.45
1:A:597:SER:O	1:A:598:LEU:HD23	2.18	0.44
3:E:186:ASP:HB3	3:E:190:ARG:NH1	2.33	0.43
1:B:448:ARG:HA	1:B:496:TYR:O	2.19	0.43
1:B:548:THR:HG22	1:B:550:ASN:OD1	2.19	0.43
2:C:69:LEU:HD11	2:C:82:LEU:HD11	2.00	0.43
3:E:115:PRO:HG2	3:E:207:ILE:HD12	2.01	0.43
1:B:465:ARG:HG3	1:B:514:ARG:HH11	1.83	0.42
3:F:157:ARG:NH2	3:F:183:LEU:HD22	2.34	0.42
1:A:597:SER:C	1:A:598:LEU:HD23	2.39	0.42
2:D:190:PRO:HB2	2:D:193:THR:HG23	2.01	0.42
2:D:67:SER:N	5:D:306:EDO:O2	2.52	0.42
2:C:38:TRP:CE2	2:C:82:LEU:HB2	2.55	0.42
1:B:576:LEU:HD23	1:B:607:TYR:CE2	2.55	0.42
1:A:587:GLU:N	1:A:587:GLU:CD	2.73	0.41
3:F:35:VAL:HA	3:F:91:LEU:O	2.20	0.41
2:D:22:ILE:HG21	2:D:22:ILE:HD13	1.77	0.41
2:C:183:LEU:HD12	2:C:183:LEU:C	2.41	0.41
1:B:553:LEU:HD13	1:B:597:SER:HB3	2.01	0.41
1:B:554:LEU:O	1:B:597:SER:HA	2.21	0.41
1:A:433:ASN:OD1	3:F:56:ARG:NH2	2.52	0.41
2:D:106:MET:HE1	3:F:100:PHE:CZ	2.54	0.41
2:C:160:TRP:CZ3	2:C:201:CYS:HB3	2.56	0.40
1:A:488:CYS:O	5:A:707:EDO:H12	2.22	0.40
3:E:120:PHE:HA	3:E:121:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	13	4
1	B	176/206 (85%)	167 (95%)	8 (4%)	1 (1%)	25	14
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%)	41	30

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%)	41	30
1	B	170/191 (89%)	165 (97%)	5 (3%)	42	31
2	C	191/193 (99%)	189 (99%)	2 (1%)	76	74
2	D	188/193 (97%)	184 (98%)	4 (2%)	53	46
3	E	190/191 (100%)	190 (100%)	0	100	100
3	F	189/191 (99%)	188 (100%)	1 (0%)	88	88
All	All	1096/1150 (95%)	1079 (98%)	17 (2%)	65	58

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

Mol	Chain	Res	Type
1	A	576	LEU
1	A	579	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	EDO	A	702	-	3,3,3	0.44	0	2,2,2	0.31	0
5	EDO	E	303	-	3,3,3	0.63	0	2,2,2	0.25	0
8	NAG	F	301	3	14,14,15	0.84	0	17,19,21	2.30	4 (23%)
5	EDO	D	303	-	3,3,3	0.48	0	2,2,2	1.01	0
5	EDO	B	1006	-	3,3,3	0.31	0	2,2,2	0.40	0
5	EDO	C	304	-	3,3,3	0.47	0	2,2,2	0.52	0
5	EDO	F	304	-	3,3,3	0.49	0	2,2,2	0.63	0
6	ACT	F	303	-	1,3,3	1.29	0	0,3,3	0.00	-
5	EDO	D	302	-	3,3,3	0.70	0	2,2,2	0.18	0
5	EDO	E	302	-	3,3,3	0.40	0	2,2,2	0.38	0
6	ACT	C	301	-	1,3,3	2.94	1 (100%)	0,3,3	0.00	-
5	EDO	A	706	-	3,3,3	0.47	0	2,2,2	0.32	0
6	ACT	D	301	-	1,3,3	3.83	1 (100%)	0,3,3	0.00	-
5	EDO	D	304	-	3,3,3	0.56	0	2,2,2	0.74	0
5	EDO	A	703	-	3,3,3	0.77	0	2,2,2	0.30	0
5	EDO	B	1004	-	3,3,3	0.66	0	2,2,2	0.48	0
5	EDO	A	707	-	3,3,3	0.33	0	2,2,2	0.72	0
6	ACT	E	301	-	1,3,3	0.77	0	0,3,3	0.00	-
5	EDO	D	306	-	3,3,3	0.38	0	2,2,2	0.48	0
5	EDO	A	708	-	3,3,3	0.31	0	2,2,2	0.73	0
5	EDO	F	306	-	3,3,3	1.03	0	2,2,2	0.33	0
5	EDO	F	307	-	3,3,3	0.67	0	2,2,2	0.31	0
5	EDO	B	1002	-	3,3,3	0.39	0	2,2,2	0.84	0
5	EDO	A	705	-	3,3,3	0.49	0	2,2,2	0.28	0
5	EDO	D	307	-	3,3,3	0.55	0	2,2,2	0.43	0
5	EDO	A	704	-	3,3,3	0.23	0	2,2,2	0.42	0
5	EDO	F	308	-	3,3,3	0.59	0	2,2,2	0.87	0
5	EDO	D	308	-	3,3,3	0.48	0	2,2,2	0.80	0
6	ACT	C	302	-	1,3,3	0.11	0	0,3,3	0.00	-
5	EDO	C	303	-	3,3,3	0.79	0	2,2,2	0.10	0
5	EDO	F	305	-	3,3,3	0.65	0	2,2,2	0.26	0
5	EDO	B	1003	-	3,3,3	0.45	0	2,2,2	0.65	0
5	EDO	A	709	-	3,3,3	0.91	0	2,2,2	0.70	0
6	ACT	F	302	-	1,3,3	1.47	0	0,3,3	0.00	-
5	EDO	F	309	-	3,3,3	0.32	0	2,2,2	0.14	0
5	EDO	E	304	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	B	1005	-	3,3,3	0.44	0	2,2,2	0.73	0
5	EDO	D	305	-	3,3,3	0.37	0	2,2,2	0.86	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
5	EDO	A	702	-	-	1/1/1/1	-
5	EDO	E	303	-	-	0/1/1/1	-
8	NAG	F	301	3	-	3/6/23/26	0/1/1/1
5	EDO	D	303	-	-	0/1/1/1	-
5	EDO	B	1006	-	-	0/1/1/1	-
5	EDO	C	304	-	-	0/1/1/1	-
5	EDO	F	304	-	-	1/1/1/1	-
5	EDO	D	302	-	-	1/1/1/1	-
5	EDO	E	302	-	-	0/1/1/1	-
5	EDO	A	706	-	-	0/1/1/1	-
5	EDO	D	304	-	-	1/1/1/1	-
5	EDO	A	703	-	-	1/1/1/1	-
5	EDO	B	1004	-	-	1/1/1/1	-
5	EDO	A	707	-	-	0/1/1/1	-
5	EDO	D	306	-	-	0/1/1/1	-
5	EDO	A	708	-	-	0/1/1/1	-
5	EDO	F	306	-	-	0/1/1/1	-
5	EDO	F	307	-	-	0/1/1/1	-
5	EDO	B	1002	-	-	0/1/1/1	-
5	EDO	A	705	-	-	0/1/1/1	-
5	EDO	D	307	-	-	0/1/1/1	-
5	EDO	A	704	-	-	1/1/1/1	-
5	EDO	F	308	-	-	0/1/1/1	-
5	EDO	D	308	-	-	0/1/1/1	-
5	EDO	C	303	-	-	0/1/1/1	-
5	EDO	F	305	-	-	0/1/1/1	-
5	EDO	B	1003	-	-	0/1/1/1	-
5	EDO	A	709	-	-	1/1/1/1	-
5	EDO	F	309	-	-	0/1/1/1	-
5	EDO	E	304	-	-	0/1/1/1	-
5	EDO	B	1005	-	-	1/1/1/1	-
5	EDO	D	305	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	ACT	CH3-C	3.83	1.53	1.48
6	C	301	ACT	CH3-C	2.94	1.52	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	301	NAG	C2-N2-C7	5.65	130.94	122.90
8	F	301	NAG	C1-C2-N2	4.70	118.52	110.49
8	F	301	NAG	C1-O5-C5	3.58	117.04	112.19
8	F	301	NAG	O7-C7-N2	2.35	126.28	121.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	301	NAG	C1-C2-N2-C7
5	F	304	EDO	O1-C1-C2-O2
5	D	304	EDO	O1-C1-C2-O2
5	A	704	EDO	O1-C1-C2-O2
5	A	709	EDO	O1-C1-C2-O2
5	A	703	EDO	O1-C1-C2-O2
8	F	301	NAG	O5-C5-C6-O6
5	B	1004	EDO	O1-C1-C2-O2
5	B	1005	EDO	O1-C1-C2-O2
8	F	301	NAG	C4-C5-C6-O6
5	A	702	EDO	O1-C1-C2-O2
5	D	302	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	707	EDO	1	0
5	D	306	EDO	1	0
5	F	306	EDO	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	181/206 (87%)	0.66	24 (13%)	3 5	20, 38, 77, 107	0
1	B	184/206 (89%)	1.12	40 (21%)	0 1	19, 43, 88, 107	0
2	C	220/221 (99%)	-0.23	1 (0%)	91 94	18, 30, 48, 63	0
2	D	215/221 (97%)	-0.03	4 (1%)	66 74	19, 32, 63, 94	0
3	E	213/215 (99%)	-0.15	2 (0%)	84 89	21, 35, 54, 65	0
3	F	212/215 (98%)	-0.24	1 (0%)	91 94	19, 32, 48, 79	0
All	All	1225/1284 (95%)	0.15	72 (5%)	22 30	18, 34, 67, 107	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	LEU	11.3
1	B	558	TRP	5.2
1	A	580	GLU	5.1
1	A	551	ILE	5.0
1	B	579	LYS	4.9
2	D	221	CYS	4.9
1	B	549	ILE	4.7
3	F	216	CYS	4.6
1	B	551	ILE	4.5
1	B	518	SER	4.4
1	A	586	TYR	4.2
1	B	517	HIS	4.2
1	A	553	LEU	4.2
1	B	548	THR	4.1
1	B	596	VAL	4.1
1	B	521	SER	4.0
1	B	581	VAL	4.0
1	B	580	GLU	3.9
1	B	553	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	453	THR	3.8
1	A	542	SER	3.7
1	B	452	SER	3.7
1	B	598	LEU	3.6
1	B	520	GLY	3.6
1	A	633	VAL	3.6
1	A	632	VAL	3.4
1	A	582	GLN	3.3
1	A	543	VAL	3.2
1	A	548	THR	3.2
2	D	220	ASP	3.2
1	B	554	LEU	3.1
1	A	549	ILE	3.0
1	B	578	GLY	3.0
1	A	541	SER	3.0
1	B	547	ILE	3.0
1	B	574	TYR	2.9
1	A	578	GLY	2.9
1	B	586	TYR	2.8
1	B	473	CYS	2.8
1	B	559	GLU	2.8
1	B	530	LEU	2.8
1	A	520	GLY	2.8
1	B	583	TRP	2.8
1	A	579	LYS	2.7
1	B	515	ILE	2.7
1	B	516	ASN	2.7
3	E	9	SER	2.7
1	B	430	VAL	2.6
1	A	627	ASN	2.6
1	B	595	SER	2.5
1	A	595	SER	2.5
1	B	522	LEU	2.5
2	D	66	LYS	2.5
1	A	589	TYR	2.4
1	A	495	PHE	2.4
1	B	550	ASN	2.4
1	A	550	ASN	2.3
1	B	508	GLY	2.3
1	A	596	VAL	2.3
1	A	471	LEU	2.3
1	B	460	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	599	PRO	2.3
1	A	594	LYS	2.2
1	B	492	SER	2.2
1	B	506	LEU	2.2
1	A	558	TRP	2.2
1	B	552	GLY	2.2
1	B	582	GLN	2.2
3	E	20	ARG	2.1
2	D	140	SER	2.1
2	C	139	ASN	2.0
1	B	619	LEU	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 monosaccharides 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(Å ²)	Q<0.9
8	NAG	F	301	14/15	0.71	0.34	79,102,115,116	0
5	EDO	A	709	4/4	0.73	0.28	35,60,63,66	0
5	EDO	D	304	4/4	0.82	0.28	50,66,82,86	0
6	ACT	C	302	4/4	0.85	0.29	38,45,56,62	0
5	EDO	D	306	4/4	0.86	0.15	51,63,65,77	0
5	EDO	F	306	4/4	0.87	0.17	28,35,51,59	0
5	EDO	B	1002	4/4	0.90	0.22	49,50,51,52	0
5	EDO	E	302	4/4	0.90	0.11	39,47,48,61	0
5	EDO	A	703	4/4	0.90	0.14	39,39,60,68	0
5	EDO	F	308	4/4	0.90	0.17	30,56,60,63	0
5	EDO	F	305	4/4	0.91	0.19	49,51,63,70	0
5	EDO	B	1003	4/4	0.92	0.14	46,76,76,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	1004	4/4	0.92	0.14	42,43,48,61	0
6	ACT	F	302	4/4	0.92	0.17	40,53,55,55	0
5	EDO	D	305	4/4	0.92	0.28	36,63,64,69	0
5	EDO	D	308	4/4	0.92	0.15	39,40,41,45	0
5	EDO	E	303	4/4	0.93	0.14	37,41,45,46	0
5	EDO	B	1006	4/4	0.93	0.18	34,35,37,51	0
5	EDO	D	303	4/4	0.93	0.17	28,33,45,56	0
6	ACT	F	303	4/4	0.94	0.12	21,25,27,29	0
5	EDO	F	304	4/4	0.94	0.20	37,48,71,72	0
6	ACT	C	301	4/4	0.94	0.17	37,39,40,49	0
5	EDO	A	707	4/4	0.94	0.09	39,49,54,54	0
5	EDO	A	702	4/4	0.95	0.12	42,43,44,49	0
5	EDO	C	303	4/4	0.95	0.11	28,36,37,39	0
5	EDO	F	307	4/4	0.96	0.15	34,44,44,45	0
5	EDO	D	307	4/4	0.96	0.18	30,40,41,51	0
5	EDO	C	304	4/4	0.96	0.15	30,37,41,43	0
6	ACT	E	301	4/4	0.96	0.12	26,27,32,35	0
5	EDO	A	704	4/4	0.97	0.20	25,48,50,52	0
5	EDO	F	309	4/4	0.97	0.18	30,35,48,53	0
5	EDO	E	304	4/4	0.97	0.13	40,43,50,58	0
5	EDO	B	1005	4/4	0.97	0.20	26,46,48,57	0
5	EDO	A	708	4/4	0.97	0.08	47,58,58,62	0
7	NA	C	305	1/1	0.97	0.07	32,32,32,32	0
5	EDO	D	302	4/4	0.98	0.09	25,40,40,42	0
5	EDO	A	706	4/4	0.98	0.08	37,38,41,44	0
6	ACT	D	301	4/4	0.98	0.14	26,28,29,31	0
4	CYS	B	1001	7/7	0.98	0.08	32,35,40,44	0
4	CYS	A	701	7/7	0.99	0.07	26,32,35,37	0
5	EDO	A	705	4/4	0.99	0.09	33,37,38,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.