



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:25 PM UTC

PDB ID : 1E02 / pdb_00001e02
Title : Porcine Odorant Binding Protein Complexed with undecanal
Authors : Vincent, F.; Spinelli, S.; Cambillau, C.; Tegoni, M.
Deposited on : 2000-03-09
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

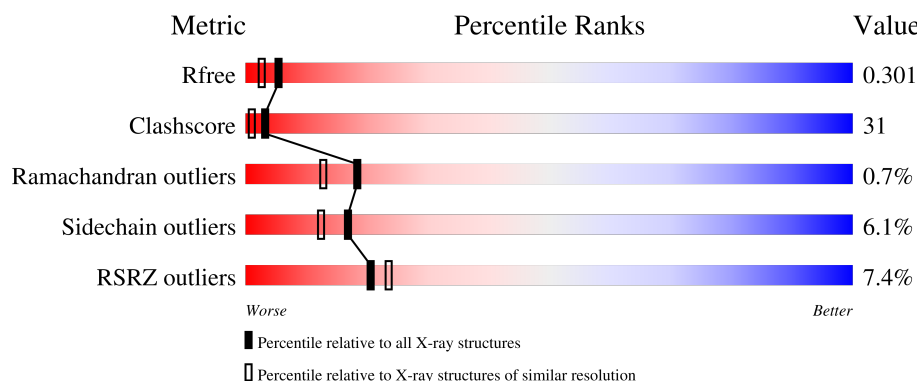
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	5% 61% 29% 5% • 5%
1	B	157	9% 27% 52% 12% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNA	A	600	-	-	X	-
2	UNA	B	600	-	-	X	-

2 Entry composition [i](#)

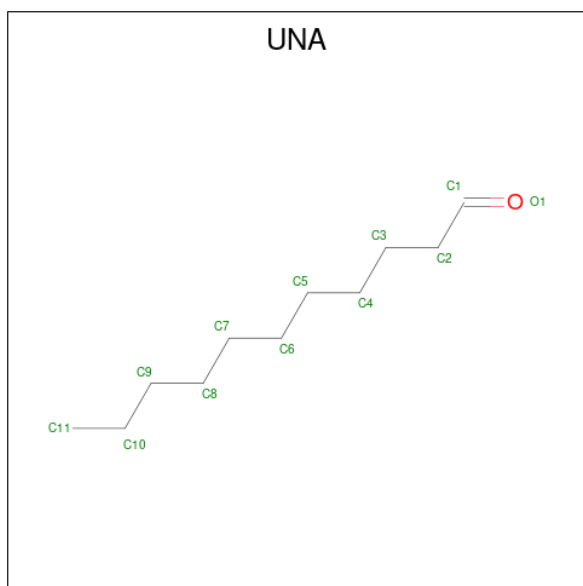
There are 3 unique types of molecules in this entry. The entry contains 2573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ODORANT-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	16	3	0
			1186	745	185	250	6			
1	B	147	Total	C	N	O	S	29	0	0
			1161	727	183	247	4			

- Molecule 2 is UNDECANAL (CCD ID: UNA) (formula: $C_{11}H_{22}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	11	1		
2	B	1	Total	C	O	0	0
			12	11	1		

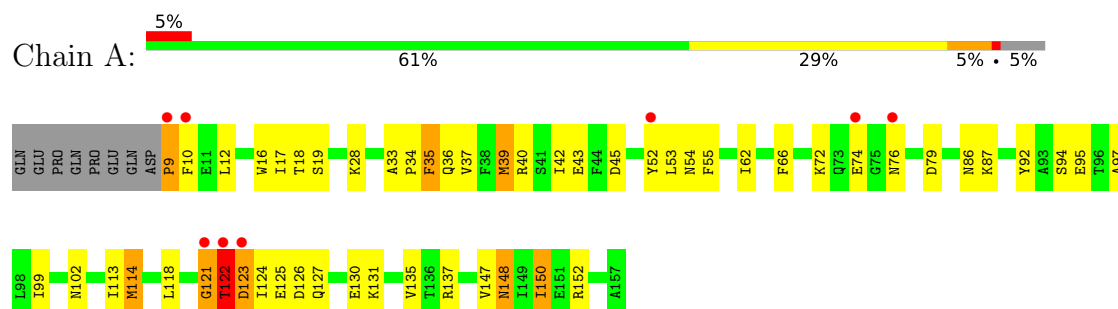
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total 114	O 114	0	0
3	B	88	Total 88	O 88	0	0

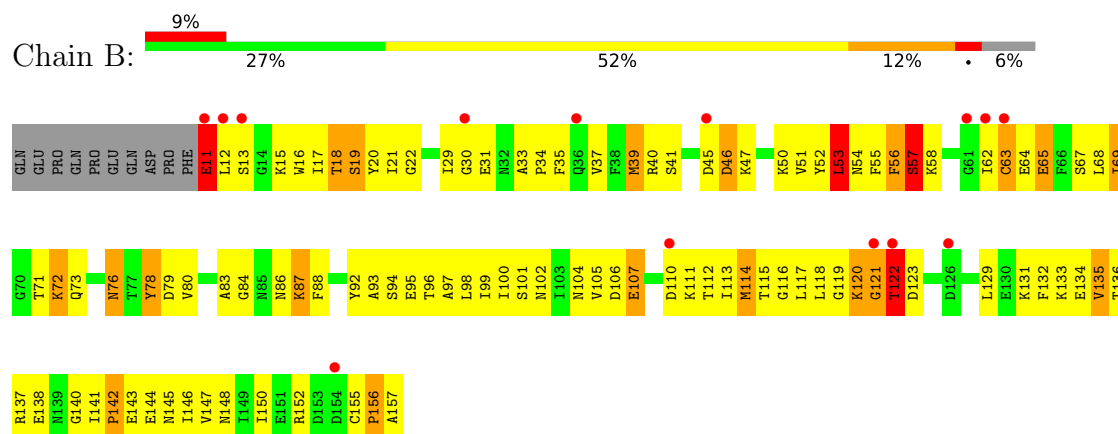
3 Residue-property plots

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: ODORANT-BINDING PROTEIN



• Molecule 1: ODORANT-BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.78Å 87.91Å 92.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.15 18.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	90.7 (18.00-2.15) 90.6 (18.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.35 (at 2.15Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.192 , 0.256 0.243 , 0.301	Depositor DCC
R_{free} test set	828 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2573	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNA

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	1.03	3/1220 (0.2%)	1.01	11/1641 (0.7%)
1	B	3.12	120/1178 (10.2%)	1.75	19/1586 (1.2%)
All	All	2.31	123/2398 (5.1%)	1.42	30/3227 (0.9%)

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	B	0	1

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLY	C-N	-30.38	0.99	1.33
1	B	143	GLU	N-CA	-13.74	1.27	1.46
1	B	64	GLU	C-O	13.19	1.38	1.23
1	B	121	GLY	C-N	-13.05	1.15	1.33
1	B	20	TYR	N-CA	-11.24	1.31	1.45
1	B	147	VAL	CA-C	-11.23	1.38	1.52
1	B	98	LEU	C-O	-10.83	1.11	1.24
1	B	137	ARG	CA-C	-10.66	1.38	1.52
1	B	79	ASP	C-N	-10.50	1.20	1.33
1	B	11	GLU	C-N	-10.30	1.19	1.33
1	B	105	VAL	CA-C	-9.85	1.44	1.53
1	B	113	ILE	C-O	-9.84	1.10	1.24
1	B	84	GLY	C-O	-9.83	1.11	1.23
1	B	116	GLY	C-O	-9.83	1.10	1.23
1	B	21	ILE	C-O	-9.63	1.13	1.23
1	B	20	TYR	C-O	-9.59	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	LYS	N-CA	9.58	1.57	1.46
1	B	22	GLY	CA-C	-9.55	1.44	1.52
1	B	93	ALA	C-O	-9.43	1.12	1.23
1	B	122	THR	C-N	-9.43	1.20	1.33
1	B	138	GLU	N-CA	9.36	1.58	1.46
1	B	51	VAL	CA-C	-9.15	1.41	1.52
1	B	142	PRO	CA-C	8.74	1.63	1.52
1	B	78	TYR	C-O	-8.63	1.12	1.24
1	B	136	THR	C-O	-8.60	1.14	1.24
1	B	100	ILE	C-O	-8.60	1.15	1.24
1	B	142	PRO	N-CD	8.54	1.59	1.47
1	B	99	ILE	C-O	-8.44	1.14	1.24
1	B	136	THR	CB-OG1	-8.25	1.30	1.43
1	B	147	VAL	C-N	-8.20	1.21	1.33
1	B	37	VAL	CA-C	-8.12	1.42	1.52
1	B	99	ILE	C-N	8.10	1.43	1.33
1	B	155	CYS	N-CA	7.99	1.57	1.45
1	B	40	ARG	CZ-NH2	-7.86	1.23	1.33
1	B	137	ARG	C-O	7.86	1.33	1.24
1	B	21	ILE	N-CA	-7.83	1.36	1.46
1	B	15	LYS	CA-CB	-7.83	1.41	1.53
1	B	100	ILE	CA-C	-7.82	1.43	1.52
1	B	92	TYR	N-CA	7.79	1.55	1.45
1	B	145	ASN	C-O	-7.74	1.11	1.24
1	B	46	ASP	C-N	-7.71	1.24	1.33
1	B	96	THR	CB-OG1	-7.63	1.31	1.43
1	B	155	CYS	CA-C	-7.50	1.43	1.53
1	B	80	VAL	N-CA	7.45	1.55	1.46
1	B	120	LYS	C-N	-7.36	1.22	1.33
1	B	94	SER	C-O	-7.21	1.14	1.24
1	B	87	LYS	N-CA	-7.11	1.38	1.46
1	B	144	GLU	N-CA	7.09	1.55	1.46
1	B	16	TRP	C-N	7.05	1.44	1.33
1	B	156	PRO	CA-C	-7.05	1.44	1.52
1	B	16	TRP	CD2-CE2	-7.03	1.29	1.41
1	B	94	SER	CA-CB	-7.02	1.41	1.53
1	B	56	PHE	C-O	-6.99	1.15	1.23
1	B	148	ASN	N-CA	6.98	1.54	1.46
1	B	29	ILE	CA-C	-6.87	1.43	1.52
1	B	135	VAL	N-CA	-6.78	1.37	1.46
1	B	140	GLY	C-N	6.75	1.38	1.32
1	B	80	VAL	CA-CB	-6.73	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	THR	CA-C	-6.63	1.44	1.52
1	B	114	MET	C-O	-6.62	1.15	1.23
1	B	37	VAL	N-CA	6.61	1.54	1.46
1	B	53	LEU	N-CA	-6.61	1.38	1.46
1	B	15	LYS	N-CA	-6.56	1.37	1.46
1	B	68	LEU	CA-CB	-6.51	1.42	1.53
1	B	68	LEU	C-N	6.50	1.42	1.33
1	B	57	SER	N-CA	-6.49	1.37	1.46
1	B	83	ALA	CA-C	-6.45	1.45	1.53
1	B	52	TYR	C-O	-6.38	1.16	1.24
1	B	117	LEU	N-CA	-6.36	1.38	1.46
1	B	54	ASN	C-O	-6.34	1.16	1.24
1	B	141	ILE	CA-C	6.33	1.58	1.52
1	B	141	ILE	C-O	-6.33	1.17	1.24
1	B	97	ALA	CA-C	-6.29	1.44	1.52
1	B	21	ILE	CA-CB	6.27	1.63	1.54
1	B	71	THR	C-O	-6.26	1.16	1.24
1	B	62	ILE	CA-C	6.07	1.59	1.52
1	B	29	ILE	CA-CB	6.04	1.62	1.54
1	B	115	THR	C-O	-5.95	1.16	1.23
1	B	54	ASN	N-CA	5.94	1.53	1.46
1	B	118	LEU	C-O	-5.93	1.16	1.23
1	B	54	ASN	CG-OD1	5.92	1.34	1.23
1	B	134	GLU	N-CA	-5.91	1.39	1.46
1	B	41	SER	CB-OG	-5.89	1.30	1.42
1	B	112	THR	C-O	5.83	1.30	1.24
1	B	65	GLU	CG-CD	-5.82	1.37	1.52
1	B	107	GLU	CD-OE2	5.80	1.36	1.25
1	B	146	ILE	CA-C	-5.79	1.45	1.52
1	B	137	ARG	N-CA	-5.78	1.39	1.46
1	A	122	THR	C-N	-5.76	1.25	1.33
1	B	118	LEU	CA-CB	5.69	1.62	1.53
1	B	92	TYR	CG-CD1	5.67	1.51	1.39
1	B	34	PRO	N-CA	5.59	1.54	1.47
1	B	45	ASP	C-O	-5.58	1.16	1.23
1	B	145	ASN	CA-CB	-5.55	1.45	1.53
1	B	72	LYS	N-CA	-5.54	1.39	1.46
1	B	67	SER	CA-C	-5.54	1.46	1.52
1	B	52	TYR	N-CA	5.53	1.52	1.46
1	B	69	ILE	N-CA	-5.53	1.39	1.46
1	B	111	LYS	CA-CB	-5.53	1.45	1.53
1	B	51	VAL	C-O	5.45	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	GLU	C-N	-5.42	1.26	1.33
1	B	67	SER	CA-CB	-5.41	1.45	1.53
1	B	106	ASP	CA-C	5.41	1.60	1.52
1	B	137	ARG	CA-CB	5.40	1.62	1.53
1	B	106	ASP	CB-CG	5.40	1.65	1.52
1	B	147	VAL	CA-CB	5.34	1.61	1.54
1	B	41	SER	CA-C	-5.31	1.45	1.52
1	B	19	SER	C-O	-5.31	1.17	1.23
1	B	95	GLU	C-N	5.30	1.41	1.33
1	B	40	ARG	CA-CB	5.29	1.62	1.53
1	B	80	VAL	C-N	-5.29	1.25	1.33
1	B	143	GLU	CA-C	-5.29	1.45	1.52
1	B	21	ILE	CA-C	-5.26	1.46	1.52
1	B	17	ILE	C-N	-5.26	1.26	1.33
1	B	31	GLU	C-O	-5.23	1.17	1.23
1	B	63	CYS	N-CA	-5.15	1.39	1.45
1	B	39	MET	N-CA	5.14	1.52	1.46
1	A	9	PRO	N-CD	5.13	1.54	1.47
1	B	51	VAL	CA-CB	5.08	1.63	1.55
1	B	115	THR	C-N	-5.07	1.26	1.33
1	B	17	ILE	CA-CB	-5.05	1.47	1.54
1	B	119	GLY	C-N	5.02	1.41	1.33
1	B	148	ASN	CA-CB	5.01	1.60	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	GLY	CA-C-N	12.27	144.97	121.54
1	B	121	GLY	C-N-CA	12.27	144.97	121.54
1	B	122	THR	O-C-N	10.61	136.70	122.59
1	B	20	TYR	O-C-N	-8.95	112.34	123.17
1	B	141	ILE	CA-C-N	7.63	127.64	119.78
1	B	141	ILE	C-N-CA	7.63	127.64	119.78
1	B	21	ILE	CA-C-N	7.41	127.74	122.33
1	B	21	ILE	C-N-CA	7.41	127.74	122.33
1	A	123	ASP	N-CA-CB	-7.17	98.69	110.52
1	B	147	VAL	N-CA-C	7.10	118.04	108.11
1	A	122	THR	CA-C-N	7.04	133.13	122.65
1	A	122	THR	C-N-CA	7.04	133.13	122.65
1	A	122	THR	O-C-N	6.43	135.55	122.05
1	A	35	PHE	N-CA-C	6.42	120.43	112.59
1	B	68	LEU	O-C-N	-6.11	115.46	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	GLN	N-CA-C	-5.77	98.53	108.56
1	B	121	GLY	O-C-N	5.75	130.17	122.70
1	A	97	ALA	N-CA-C	5.53	117.20	108.96
1	B	122	THR	CA-C-N	5.53	133.28	121.45
1	B	122	THR	C-N-CA	5.53	133.28	121.45
1	A	87	LYS	CA-C-N	-5.47	113.62	122.81
1	A	87	LYS	C-N-CA	-5.47	113.62	122.81
1	B	87	LYS	CA-C-N	-5.39	113.39	123.03
1	B	87	LYS	C-N-CA	-5.39	113.39	123.03
1	B	97	ALA	N-CA-C	5.37	117.35	109.24
1	B	132	PHE	O-C-N	-5.37	116.29	122.09
1	A	122	THR	CB-CA-C	-5.33	108.86	115.89
1	B	101	SER	N-CA-C	-5.28	100.58	109.07
1	A	125	GLU	N-CA-C	-5.03	100.54	108.73
1	B	37	VAL	N-CA-C	5.01	115.79	108.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	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	1186	0	1133	76	0
1	B	1161	0	1104	55	0
2	A	12	0	22	32	0
2	B	12	0	22	15	0
3	A	114	0	0	3	0
3	B	88	0	0	15	0
All	All	2573	0	2281	140	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 31.

All (140) 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:39[B]:MET:CE	2:A:600:UNA:H62	1.32	1.52
1:A:39[B]:MET:HE2	2:A:600:UNA:C6	1.57	1.32
1:B:122:THR:CG2	1:B:123:ASP:N	1.81	1.30
1:B:122:THR:HG23	1:B:123:ASP:CA	1.66	1.25
1:A:122:THR:CG2	1:A:123:ASP:H	1.43	1.17
1:A:122:THR:CG2	1:A:123:ASP:N	2.05	1.11
1:A:39[A]:MET:HE2	1:A:55:PHE:HB3	1.31	1.10
1:B:122:THR:HG23	1:B:123:ASP:CB	1.82	1.09
1:A:72:LYS:HE2	3:A:2051:HOH:O	1.51	1.08
1:A:122:THR:HG23	1:A:123:ASP:N	1.52	1.07
1:A:39[B]:MET:CG	2:A:600:UNA:H72	1.83	1.06
1:A:39[B]:MET:HG3	2:A:600:UNA:H72	1.36	1.06
1:A:122:THR:HG23	1:A:123:ASP:H	0.88	1.02
2:B:600:UNA:H61	2:B:600:UNA:O1	1.58	1.02
2:B:600:UNA:C1	2:B:600:UNA:H91	1.90	1.01
1:A:39[B]:MET:CE	2:A:600:UNA:C6	2.28	0.99
1:B:110:ASP:O	3:B:2060:HOH:O	1.84	0.94
1:A:12:LEU:HD21	3:B:2018:HOH:O	1.70	0.90
1:B:122:THR:HG23	1:B:123:ASP:N	1.19	0.88
1:A:122:THR:HG23	1:A:123:ASP:CA	2.02	0.88
1:A:122:THR:HG23	1:A:123:ASP:CB	2.04	0.86
1:B:157:ALA:HB2	3:B:2088:HOH:O	1.76	0.86
1:A:39[B]:MET:SD	2:A:600:UNA:H62	2.16	0.85
2:B:600:UNA:H61	2:B:600:UNA:C1	2.06	0.84
1:A:53:LEU:HD22	2:A:600:UNA:H41	1.59	0.83
1:A:39[B]:MET:HE1	2:A:600:UNA:H42	1.64	0.79
1:A:39[B]:MET:HE1	2:A:600:UNA:H62	1.63	0.78
1:A:39[A]:MET:CG	2:A:600:UNA:H72	2.12	0.77
1:B:55:PHE:CZ	2:B:600:UNA:H113	2.19	0.77
1:B:55:PHE:CE2	2:B:600:UNA:C11	2.68	0.76
1:A:39[A]:MET:HG2	2:A:600:UNA:H72	1.66	0.76
1:B:122:THR:CG2	1:B:123:ASP:CB	2.63	0.75
1:A:39[A]:MET:HE3	2:A:600:UNA:H42	1.70	0.72
1:A:39[B]:MET:HE2	2:A:600:UNA:H62	0.74	0.71
1:A:39[B]:MET:CE	2:A:600:UNA:H42	2.20	0.71
1:B:55:PHE:CE2	2:B:600:UNA:H112	2.27	0.70
1:A:122:THR:CG2	1:A:123:ASP:O	2.40	0.69
1:A:39[A]:MET:HE2	1:A:55:PHE:CB	2.18	0.68
1:B:157:ALA:CB	3:B:2088:HOH:O	2.34	0.68
1:A:39[B]:MET:SD	2:A:600:UNA:C6	2.80	0.68
1:A:10:PHE:HE2	1:A:94:SER:HA	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:UNA:O1	2:B:600:UNA:H91	1.95	0.67
1:A:39[B]:MET:SD	2:A:600:UNA:H72	2.33	0.67
1:A:39[B]:MET:SD	2:A:600:UNA:H42	2.35	0.66
1:A:122:THR:HG23	1:A:123:ASP:HB3	1.77	0.66
1:B:55:PHE:CZ	2:B:600:UNA:C11	2.78	0.65
1:A:122:THR:HG22	1:A:123:ASP:O	1.96	0.65
1:B:69:ILE:HG13	3:B:2041:HOH:O	1.95	0.65
1:A:86:ASN:HB3	1:A:102:ASN:HD21	1.60	0.64
1:A:53:LEU:HD13	2:A:600:UNA:C3	2.27	0.64
1:B:46:ASP:HB3	3:B:2023:HOH:O	1.98	0.64
2:B:600:UNA:C1	2:B:600:UNA:C9	2.71	0.64
1:A:39[A]:MET:CE	1:A:55:PHE:HB3	2.20	0.63
1:A:39[B]:MET:SD	2:A:600:UNA:C7	2.87	0.63
1:B:12:LEU:H	1:B:12:LEU:HD23	1.64	0.62
1:B:122:THR:HG23	1:B:123:ASP:HB2	1.78	0.62
1:A:39[A]:MET:CE	2:A:600:UNA:H42	2.30	0.62
1:B:122:THR:HG23	1:B:123:ASP:CG	2.25	0.61
1:A:39[A]:MET:HG3	2:A:600:UNA:H72	1.81	0.61
1:B:122:THR:CG2	1:B:123:ASP:HB2	2.32	0.60
1:A:53:LEU:HD13	2:A:600:UNA:H31	1.85	0.59
1:A:19[B]:SER:HB3	1:A:124:ILE:HD11	1.86	0.58
1:A:43:GLU:HB2	1:A:52:TYR:HB2	1.86	0.58
1:A:131:LYS:O	1:A:135:VAL:HG23	2.05	0.56
1:A:53:LEU:HD13	2:A:600:UNA:H41	1.89	0.55
1:A:147:VAL:CG2	1:A:152:ARG:HE	2.20	0.55
1:B:11:GLU:C	1:B:13:SER:H	2.14	0.55
2:B:600:UNA:C9	2:B:600:UNA:H1	2.37	0.54
1:A:39[B]:MET:HE1	2:A:600:UNA:C4	2.37	0.54
1:B:86:ASN:HD22	1:B:102:ASN:HD21	1.54	0.54
1:A:39[A]:MET:SD	2:A:600:UNA:H62	2.48	0.54
1:A:37:VAL:HG13	1:A:55:PHE:CD2	2.43	0.53
1:B:56:PHE:CZ	1:B:156:PRO:HG2	2.42	0.53
2:B:600:UNA:O1	2:B:600:UNA:C6	2.47	0.52
2:B:600:UNA:H91	2:B:600:UNA:H1	1.85	0.51
1:B:122:THR:CG2	1:B:123:ASP:CG	2.83	0.50
1:A:148:ASN:C	1:A:148:ASN:HD22	2.18	0.50
1:A:35:PHE:CG	1:A:114[B]:MET:HE1	2.48	0.49
1:B:50:LYS:HE2	3:B:2014:HOH:O	2.13	0.48
1:B:72:LYS:HG2	1:B:78:TYR:CE2	2.47	0.48
1:B:152:ARG:NH1	3:B:2084:HOH:O	2.38	0.48
1:B:102:ASN:CB	2:B:600:UNA:H51	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HD21	2:A:600:UNA:H71	1.95	0.48
1:A:53:LEU:HD13	2:A:600:UNA:C4	2.44	0.47
1:A:53:LEU:CD2	2:A:600:UNA:H41	2.38	0.47
1:A:39[B]:MET:HE2	1:A:42:ILE:HD11	1.96	0.47
1:B:76:ASN:ND2	3:B:2045:HOH:O	2.47	0.47
1:A:35:PHE:CD1	1:A:114[A]:MET:HE1	2.50	0.47
1:B:35:PHE:CD2	1:B:114:MET:SD	3.08	0.46
1:B:142:PRO:CD	3:B:2008:HOH:O	2.63	0.46
1:A:102:ASN:HB3	1:A:114[B]:MET:HG3	1.98	0.45
1:A:150:ILE:H	1:A:150:ILE:HG13	1.52	0.45
1:B:35:PHE:CD2	2:B:600:UNA:H41	2.52	0.45
1:B:131:LYS:O	1:B:135:VAL:HG23	2.17	0.45
1:A:127:GLN:NE2	3:A:2091:HOH:O	2.45	0.45
1:A:33:ALA:HB1	1:A:34:PRO:HD2	2.00	0.44
1:B:104:ASN:HB2	1:B:114:MET:HE1	1.99	0.44
1:B:86:ASN:ND2	1:B:102:ASN:HD21	2.15	0.44
2:A:600:UNA:H111	2:A:600:UNA:H82	1.79	0.44
1:B:35:PHE:HD2	2:B:600:UNA:H41	1.81	0.44
1:A:126:ASP:O	1:A:130:GLU:HG2	2.17	0.44
2:A:600:UNA:H82	2:A:600:UNA:H51	1.68	0.44
1:B:39:MET:HE1	1:B:53:LEU:HB3	1.99	0.44
1:A:122:THR:HG23	1:A:123:ASP:C	2.43	0.44
1:A:45:ASP:HB2	1:A:52:TYR:HE2	1.83	0.43
1:B:11:GLU:C	1:B:13:SER:N	2.76	0.43
1:B:57:SER:HB3	3:B:2031:HOH:O	2.18	0.43
1:B:39:MET:HA	1:B:55:PHE:HB3	2.01	0.43
1:A:17:ILE:HG13	1:A:121:GLY:HA2	1.99	0.43
1:B:58:LYS:HE2	1:B:63:CYS:SG	2.59	0.43
1:A:28:LYS:O	1:A:35:PHE:HB2	2.18	0.43
1:B:12:LEU:H	1:B:12:LEU:CD2	2.31	0.43
1:A:18:THR:OG1	1:A:39[B]:MET:HG2	2.18	0.43
1:A:39[B]:MET:HG3	2:A:600:UNA:C7	2.27	0.43
1:A:54:ASN:HA	1:A:66:PHE:O	2.19	0.43
1:B:86:ASN:HD21	1:B:104:ASN:HD22	1.67	0.42
1:B:35:PHE:HZ	1:B:86:ASN:HD21	1.67	0.42
1:B:87:LYS:HD3	3:B:2043:HOH:O	2.20	0.42
1:B:107:GLU:HG3	3:B:2059:HOH:O	2.18	0.42
1:B:30:GLY:O	1:B:33:ALA:HB3	2.20	0.42
1:B:18:THR:O	1:B:150:ILE:HG23	2.19	0.42
1:B:56:PHE:CE1	1:B:65:GLU:HB2	2.55	0.42
1:A:39[A]:MET:CE	1:A:55:PHE:CD1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HD21	2:A:600:UNA:C7	2.50	0.41
1:B:122:THR:CG2	1:B:123:ASP:CA	2.61	0.41
1:A:40:ARG:HD3	1:A:40:ARG:HA	1.92	0.41
1:A:137:ARG:NH1	1:B:107:GLU:HG2	2.36	0.41
1:A:16:TRP:O	1:A:39[A]:MET:HB3	2.20	0.41
1:A:42:ILE:HG23	1:A:53:LEU:HD23	2.02	0.41
1:A:102:ASN:O	1:A:113:ILE:HD12	2.21	0.41
1:B:129:LEU:HD22	1:B:133:LYS:HE3	2.03	0.41
1:B:19:SER:HA	1:B:150:ILE:HG23	2.03	0.40
1:B:142:PRO:HD3	3:B:2008:HOH:O	2.21	0.40
1:B:88:PHE:HB3	1:B:102:ASN:OD1	2.20	0.40
1:B:133:LYS:NZ	3:B:2070:HOH:O	2.52	0.40
1:B:152:ARG:HD2	1:B:152:ARG:H	1.85	0.40
1:A:102:ASN:HB3	1:A:114[B]:MET:CG	2.51	0.40
1:A:9:PRO:N	3:A:2001:HOH:O	2.55	0.40
1:A:92:TYR:HB3	1:A:99:ILE:HB	2.03	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	150/157 (96%)	145 (97%)	5 (3%)	0	100	100
1	B	145/157 (92%)	129 (89%)	14 (10%)	2 (1%)	9	4
All	All	295/314 (94%)	274 (93%)	19 (6%)	2 (1%)	18	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	THR
1	B	121	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	135/140 (96%)	123 (91%)	12 (9%)	9	5
1	B	130/140 (93%)	124 (95%)	6 (5%)	24	22
All	All	265/280 (95%)	247 (93%)	18 (7%)	17	10

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39[A]	MET
1	A	39[B]	MET
1	A	62	ILE
1	A	74	GLU
1	A	76	ASN
1	A	79	ASP
1	A	95	GLU
1	A	114[A]	MET
1	A	114[B]	MET
1	A	122	THR
1	A	148	ASN
1	A	150	ILE
1	B	11	GLU
1	B	53	LEU
1	B	57	SER
1	B	73	GLN
1	B	76	ASN
1	B	122	THR

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

Mol	Chain	Res	Type
1	A	81	ASN
1	A	85	ASN
1	A	102	ASN
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	148	ASN
1	B	73	GLN
1	B	86	ASN
1	B	139	ASN
1	B	145	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UNA	B	600	-	10,11,11	1.84	1 (10%)	9,10,10	0.66	0
2	UNA	A	600	-	10,11,11	1.28	2 (20%)	9,10,10	1.20	1 (11%)

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	UNA	B	600	-	-	8/9/9/9	-
2	UNA	A	600	-	-	7/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	UNA	O1-C1	5.22	1.49	1.20
2	A	600	UNA	C7-C8	2.61	1.64	1.51
2	A	600	UNA	C3-C2	2.13	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	UNA	O1-C1-C2	-2.85	102.48	126.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	UNA	O1-C1-C2-C3
2	A	600	UNA	C5-C6-C7-C8
2	B	600	UNA	C6-C7-C8-C9
2	A	600	UNA	C11-C10-C9-C8
2	B	600	UNA	C7-C8-C9-C10
2	B	600	UNA	C2-C3-C4-C5
2	A	600	UNA	C4-C5-C6-C7
2	A	600	UNA	C6-C7-C8-C9
2	A	600	UNA	C2-C3-C4-C5
2	B	600	UNA	C4-C5-C6-C7
2	B	600	UNA	C5-C6-C7-C8
2	B	600	UNA	C11-C10-C9-C8
2	A	600	UNA	C3-C4-C5-C6
2	B	600	UNA	C1-C2-C3-C4
2	A	600	UNA	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	UNA	15	0
2	A	600	UNA	32	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	122:THR	C	123:ASP	N	1.20
1	B	11:GLU	C	12:LEU	N	1.19
1	B	121:GLY	C	122:THR	N	1.15
1	A	121:GLY	C	122:THR	N	0.99

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	149/157 (94%)	0.32	8 (5%) 31 35	13, 24, 48, 65	12 (8%)
1	B	147/157 (93%)	0.70	14 (9%) 14 15	12, 31, 52, 65	27 (18%)
All	All	296/314 (94%)	0.51	22 (7%) 20 23	12, 28, 50, 65	39 (13%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	THR	4.2
1	B	11	GLU	3.9
1	A	121	GLY	3.8
1	A	76	ASN	3.6
1	B	126	ASP	3.4
1	A	122	THR	3.4
1	B	45	ASP	3.2
1	B	121	GLY	3.1
1	A	9	PRO	3.1
1	B	110	ASP	3.0
1	A	74	GLU	2.7
1	B	61	GLY	2.7
1	B	13	SER	2.7
1	B	36	GLN	2.6
1	B	63	CYS	2.6
1	B	62	ILE	2.5
1	B	12	LEU	2.5
1	A	52	TYR	2.3
1	A	123	ASP	2.3
1	B	154	ASP	2.2
1	B	30	GLY	2.1
1	A	10	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UNA	A	600	12/12	0.63	0.26	41,78,86,87	0
2	UNA	B	600	12/12	0.73	0.15	55,62,68,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.