



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:55 PM UTC

PDB ID : 5ORF / pdb_00005orf
Title : Structure of ovine serum albumin in P1 space group
Authors : Talaj, J.A.; Bujacz, A.; Bujacz, G.; Pietrzyk-Brzezinska, A.J.
Deposited on : 2017-08-16
Resolution : 2.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

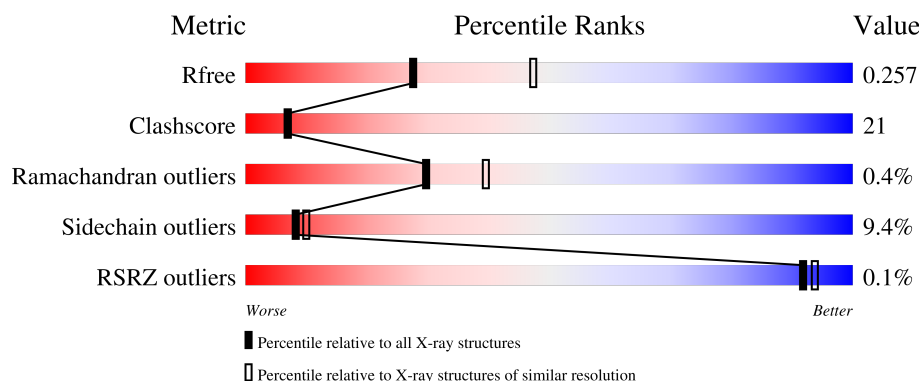
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	583	 51% 40% 9%
1	B	583	 57% 37% 6% •
1	C	583	 57% 37% 5% •
1	D	583	 51% 39% 9% •

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
4	PRO	C	605	-	-	X	-
4	PRO	D	603	-	-	X	-

2 Entry composition [i](#)

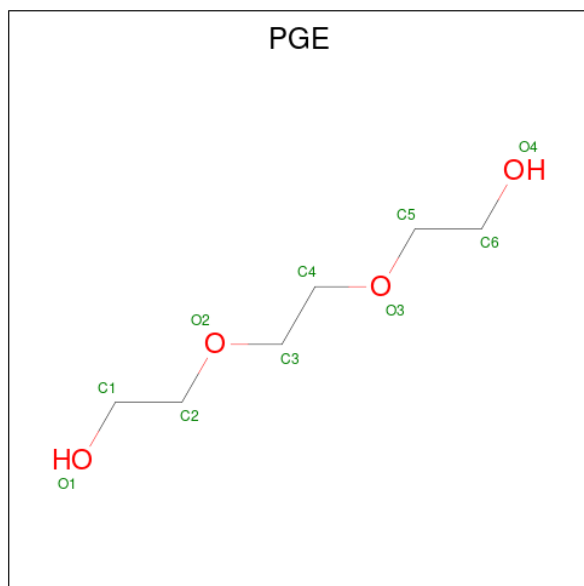
There are 5 unique types of molecules in this entry. The entry contains 19129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4645	2933	780	893	39			
1	B	583	Total	C	N	O	S	0	0	0
			4645	2933	780	893	39			
1	C	583	Total	C	N	O	S	0	0	0
			4645	2933	780	893	39			
1	D	583	Total	C	N	O	S	0	0	0
			4645	2933	780	893	39			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



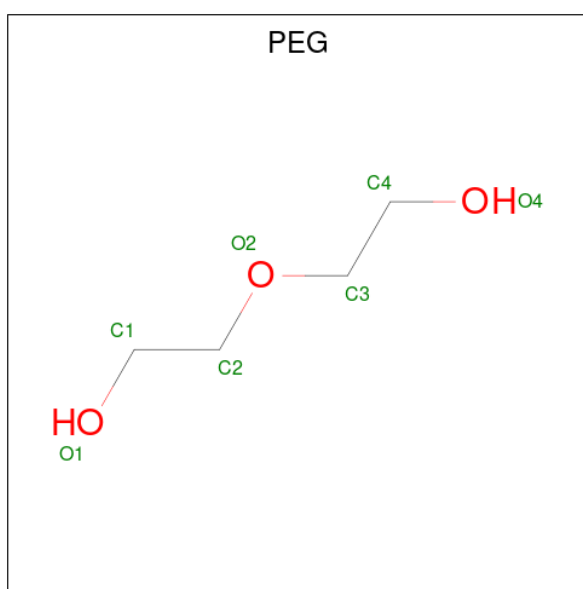
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		

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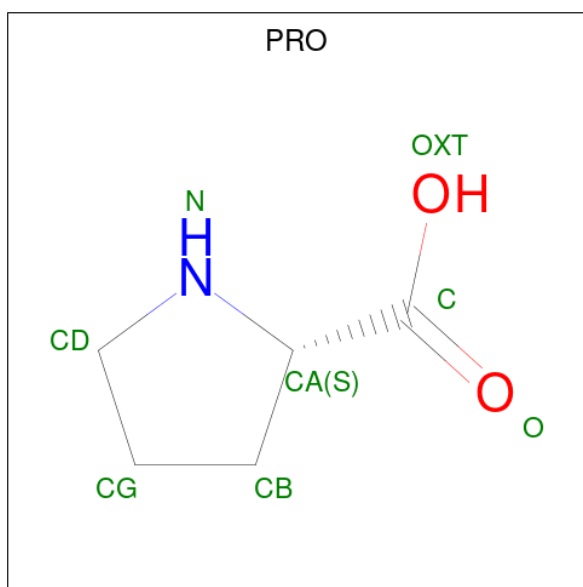
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	5	1	2		
4	A	1	Total	C	N	O	0	0
			8	5	1	2		
4	A	1	Total	C	N	O	0	0
			8	5	1	2		
4	B	1	Total	C	N	O	0	0
			8	5	1	2		
4	B	1	Total	C	N	O	0	0
			8	5	1	2		
4	B	1	Total	C	N	O	0	0
			8	5	1	2		
4	C	1	Total	C	N	O	0	0
			8	5	1	2		
4	C	1	Total	C	N	O	0	0
			8	5	1	2		
4	C	1	Total	C	N	O	0	0
			8	5	1	2		
4	D	1	Total	C	N	O	0	0
			8	5	1	2		
4	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		

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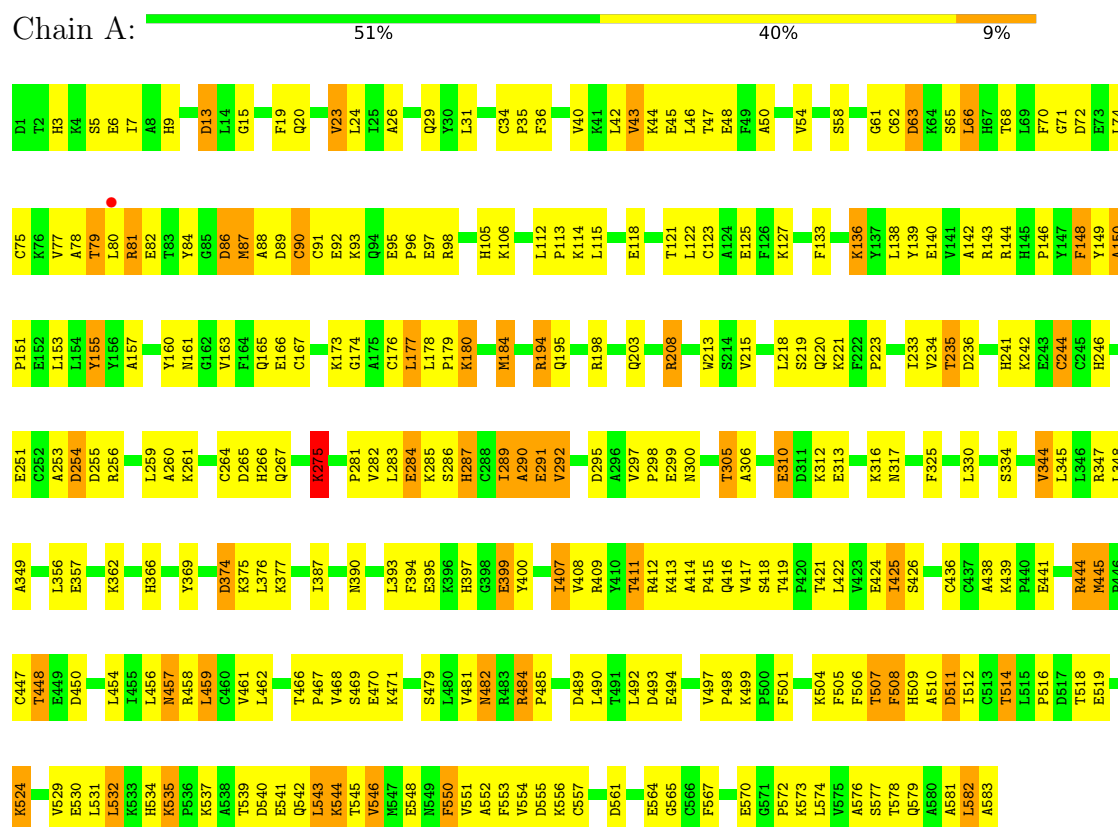
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	112	Total 112	O 112	0	0
5	C	87	Total 87	O 87	0	0
5	D	97	Total 97	O 97	0	0

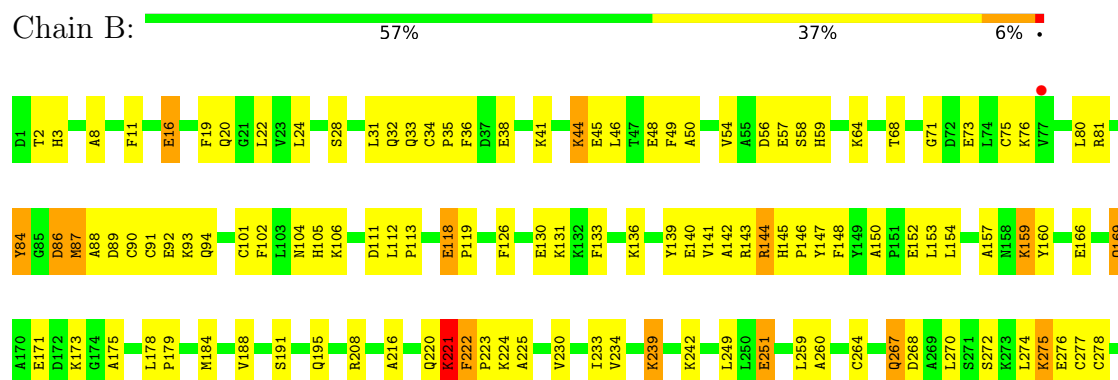
3 Residue-property plots [i](#)

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: Serum albumin



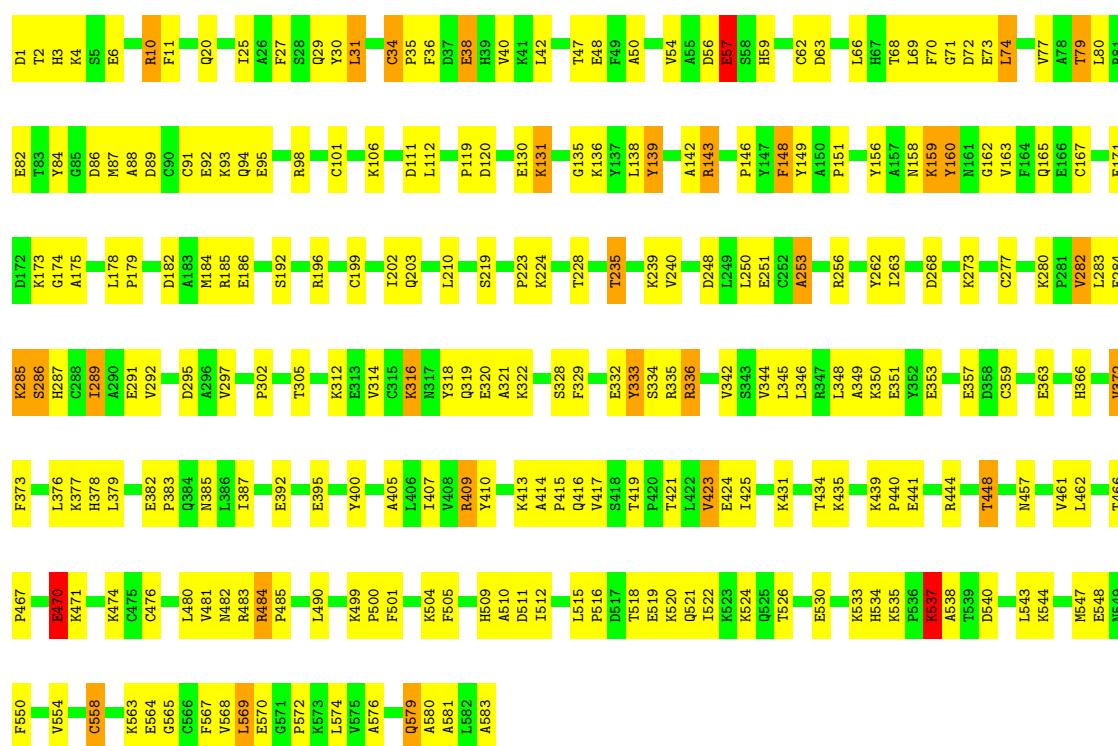
• Molecule 1: Serum albumin





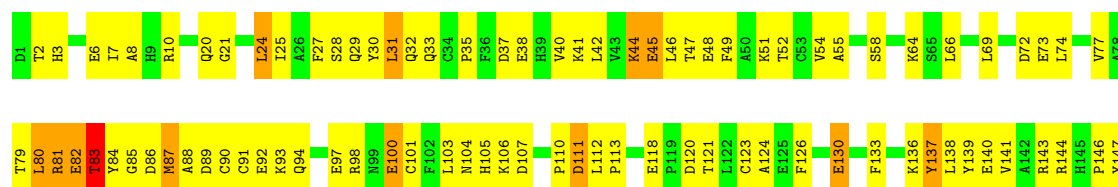
• Molecule 1: Serum albumin

Chain C: 57% 37% 5% •



• Molecule 1: Serum albumin

Chain D: 51% 39% 9% •



H509	A510	D511	I512	C513	T514	L515	P516	E519	S520	K524	Q525	L528	V529	E530	L531	L532	K533	P536	T539	D540	E541	L543	K544	T545	V546	M547	E548	N549	F550	F553	V554	D555	K556	C557	C558	D561	D562	K563	E564	G565	C566	L569	E570	G571	P572	K573	L574	A583			
R409	Y410	T411	R412	T419	E424	I425	S426	R427	A438	E441	R444	M445	P446	D450	L454	I455	L456	C460	E464	K465	T466	P467	V468	S469	E470	K471	V472	S479	L480	R484	P485	L490	T491	D493	E494	V497	P498	K499	D502	E503	K504	F505	F508								
Y318	D323	V324	F325	L326	F329	S334	A341	K342	S343	V344	L346	R347	L348	A349	K350	C359	K362	E363	D364	F365	H366	A367	C368	F373	L376	K377	H378	E382	P383	Q384	N385	L386	I387	C391	E392	L393	F394	E395	Y400	G401	F402	Q403	L406	I407	V408						
Q220	P223	K224	T228	D229	V230	T231	T235	D236	K239	K242	E243	C244	C245	H246	G247	D248	L249	L250	E251	R256	L259	A260	Q267	K275	E276	C277	K280	P281	V282	K285	S286	H287	D293	K294	D295	L301	P302	L303	T305	A306	D307	F308	V314	C315							
F148	P151	E152	L153	L154	Y155	Y156	K159	Y160	Q165	E166	C167	G168	Q169	K173	G174	A175	C176	L177	L178	P179	K180	M184	K187	V188	L189	A190	S191	A193	R194	Q195	R196	L197	R198	C199	A200	S201	I202	Q203	K204	F205	G206	E207	K211	A212	W213	S214	V215	A216	R217	L218	S219

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.82Å 78.05Å 109.71Å 89.81° 74.54° 73.15°	Depositor
Resolution (Å)	49.00 – 2.54 49.00 – 2.54	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.00-2.54) 90.2 (49.00-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.196 , 0.258 0.194 , 0.257	Depositor DCC
R_{free} test set	1414 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19129	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.15% 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: PEG, PGE

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	1.27	14/4742 (0.3%)	1.39	45/6402 (0.7%)
1	B	1.26	10/4742 (0.2%)	1.40	41/6402 (0.6%)
1	C	1.30	12/4742 (0.3%)	1.39	43/6402 (0.7%)
1	D	1.33	20/4742 (0.4%)	1.44	48/6402 (0.7%)
All	All	1.29	56/18968 (0.3%)	1.41	177/25608 (0.7%)

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	250	LEU	N-CA	7.98	1.55	1.46
1	B	406	LEU	C-O	-7.61	1.15	1.24
1	D	219	SER	CA-C	-7.33	1.42	1.52
1	D	342	VAL	C-O	-7.08	1.15	1.24
1	C	31	LEU	CA-C	-7.02	1.42	1.53

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	GLU	N-CA-C	-10.81	97.83	111.02
1	D	497	VAL	CA-C-N	-10.49	108.70	119.92
1	D	497	VAL	C-N-CA	-10.49	108.70	119.92
1	A	118	GLU	CA-C-N	9.86	129.49	119.24
1	A	118	GLU	C-N-CA	9.86	129.49	119.24

There are no chirality outliers.

There are no planarity outliers.

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	4645	0	4548	217	0
1	B	4645	0	4548	169	0
1	C	4645	0	4548	180	0
1	D	4645	0	4552	223	0
2	A	20	0	28	1	0
2	B	10	0	14	3	0
2	C	20	0	28	9	0
2	D	10	0	14	3	0
3	A	7	0	10	0	0
3	C	7	0	10	0	0
4	A	24	0	21	4	0
4	B	24	0	21	1	0
4	C	24	0	21	9	0
4	D	16	0	14	6	0
5	A	91	0	0	8	0
5	B	112	0	0	14	0
5	C	87	0	0	5	0
5	D	97	0	0	4	0
All	All	19129	0	18377	782	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 21.

The worst 5 of 782 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:D:33:GLN:N	1:D:84:TYR:OH	1.66	1.25
1:C:174:GLY:H	4:C:605:PRO:HB3	1.12	1.12
1:C:409:ARG:HH21	2:C:601:PGE:H22	1.11	1.10
1:D:79:THR:HB	1:D:83:THR:CG2	1.82	1.10
1:D:79:THR:HB	1:D:83:THR:HG23	1.17	1.08

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	581/583 (100%)	502 (86%)	76 (13%)	3 (0%)	24	34
1	B	581/583 (100%)	524 (90%)	55 (10%)	2 (0%)	36	45
1	C	581/583 (100%)	527 (91%)	51 (9%)	3 (0%)	24	34
1	D	581/583 (100%)	529 (91%)	51 (9%)	1 (0%)	43	56
All	All	2324/2332 (100%)	2082 (90%)	233 (10%)	9 (0%)	30	39

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	74	LEU
1	A	415	PRO
1	A	290	ALA
1	D	494	GLU
1	B	282	VAL

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	516/516 (100%)	465 (90%)	51 (10%)	7	9
1	B	516/516 (100%)	461 (89%)	55 (11%)	6	7
1	C	516/516 (100%)	481 (93%)	35 (7%)	14	20
1	D	516/516 (100%)	461 (89%)	55 (11%)	6	7
All	All	2064/2064 (100%)	1868 (90%)	196 (10%)	8	9

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	239	LYS
1	D	20	GLN
1	C	286	SER
1	C	424	GLU
1	D	64	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	300	ASN
1	D	579	GLN
1	D	482	ASN
1	C	67	HIS
1	D	105	HIS

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](#)

19 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
4	PRO	B	604	-	8,8,8	0.69	0	10,10,10	1.41	2 (20%)
4	PRO	C	605	-	8,8,8	1.00	1 (12%)	10,10,10	1.35	1 (10%)
4	PRO	B	602	-	8,8,8	0.98	1 (12%)	10,10,10	2.13	3 (30%)
4	PRO	A	606	-	8,8,8	0.81	0	10,10,10	1.29	1 (10%)
2	PGE	A	602	-	9,9,9	0.63	0	8,8,8	0.46	0
2	PGE	D	601	-	9,9,9	0.67	0	8,8,8	1.59	2 (25%)
2	PGE	A	601	-	9,9,9	0.74	0	8,8,8	0.63	0
4	PRO	D	603	-	8,8,8	1.14	1 (12%)	10,10,10	1.66	1 (10%)
2	PGE	B	601	-	9,9,9	0.49	0	8,8,8	0.91	0
3	PEG	A	603	-	6,6,6	0.64	0	5,5,5	0.49	0
4	PRO	D	602	-	8,8,8	0.90	0	10,10,10	1.25	1 (10%)
4	PRO	B	603	-	8,8,8	0.84	0	10,10,10	1.27	1 (10%)
4	PRO	A	605	-	8,8,8	0.92	1 (12%)	10,10,10	1.45	2 (20%)
3	PEG	C	603	-	6,6,6	1.91	1 (16%)	5,5,5	1.10	0
2	PGE	C	601	-	9,9,9	0.46	0	8,8,8	1.05	1 (12%)
4	PRO	C	604	-	8,8,8	0.85	1 (12%)	10,10,10	1.41	2 (20%)
4	PRO	C	606	-	8,8,8	0.97	1 (12%)	10,10,10	1.17	1 (10%)
2	PGE	C	602	-	9,9,9	0.81	0	8,8,8	0.71	0
4	PRO	A	604	-	8,8,8	0.81	0	10,10,10	1.64	2 (20%)

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	PRO	B	604	-	-	2/4/11/11	0/1/1/1
4	PRO	C	605	-	-	0/4/11/11	0/1/1/1
4	PRO	B	602	-	-	0/4/11/11	0/1/1/1
4	PRO	A	606	-	-	0/4/11/11	0/1/1/1
2	PGE	A	602	-	-	7/7/7/7	-
2	PGE	D	601	-	-	5/7/7/7	-
2	PGE	A	601	-	-	3/7/7/7	-
4	PRO	D	603	-	-	4/4/11/11	0/1/1/1
2	PGE	B	601	-	-	4/7/7/7	-
3	PEG	A	603	-	-	2/4/4/4	-
4	PRO	D	602	-	-	4/4/11/11	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PRO	B	603	-	-	4/4/11/11	0/1/1/1
4	PRO	A	605	-	-	4/4/11/11	0/1/1/1
3	PEG	C	603	-	-	3/4/4/4	-
2	PGE	C	601	-	-	4/7/7/7	-
4	PRO	C	604	-	-	2/4/11/11	0/1/1/1
4	PRO	C	606	-	-	4/4/11/11	0/1/1/1
2	PGE	C	602	-	-	4/7/7/7	-
4	PRO	A	604	-	-	0/4/11/11	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	PEG	O2-C3	3.26	1.56	1.42
4	B	602	PRO	OXT-C	-2.36	1.23	1.30
4	A	605	PRO	OXT-C	-2.30	1.23	1.30
4	C	606	PRO	OXT-C	-2.10	1.23	1.30
4	C	604	PRO	OXT-C	-2.09	1.24	1.30

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	PRO	OXT-C-O	-4.97	112.81	124.08
4	D	603	PRO	OXT-C-O	-3.58	115.97	124.08
4	B	602	PRO	C-CA-N	3.08	118.88	106.84
2	D	601	PGE	O4-C6-C5	-3.04	93.90	111.82
2	D	601	PGE	O3-C5-C6	-3.03	96.76	110.11

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	PRO	O-C-CA-N
4	A	605	PRO	OXT-C-CA-N
4	A	605	PRO	O-C-CA-CB
4	A	605	PRO	OXT-C-CA-CB
4	B	603	PRO	O-C-CA-N

There are no ring outliers.

11 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	PRO	1	0
4	C	605	PRO	9	0
4	A	606	PRO	2	0
2	D	601	PGE	3	0
2	A	601	PGE	1	0
4	D	603	PRO	6	0
2	B	601	PGE	3	0
4	A	605	PRO	1	0
2	C	601	PGE	4	0
2	C	602	PGE	5	0
4	A	604	PRO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	583/583 (100%)	-0.33	1 (0%) 91 93	31, 54, 87, 140	0
1	B	583/583 (100%)	-0.42	1 (0%) 91 93	28, 50, 83, 110	0
1	C	583/583 (100%)	-0.43	0 100 100	27, 50, 79, 129	0
1	D	583/583 (100%)	-0.38	0 100 100	31, 50, 84, 121	0
All	All	2332/2332 (100%)	-0.39	2 (0%) 92 94	27, 51, 84, 140	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	VAL	2.7
1	A	80	LEU	2.3

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
4	PRO	C	605	8/8	0.80	0.11	70,71,77,80	0
4	PRO	B	602	8/8	0.82	0.09	48,62,72,79	0
4	PRO	D	603	8/8	0.82	0.12	59,68,72,74	0
4	PRO	A	606	8/8	0.84	0.10	58,81,91,91	0
4	PRO	B	604	8/8	0.84	0.08	58,69,74,75	0
4	PRO	D	602	8/8	0.85	0.07	71,78,87,91	0
3	PEG	C	603	7/7	0.86	0.10	32,34,37,37	0
4	PRO	C	606	8/8	0.86	0.08	56,61,66,70	0
4	PRO	A	605	8/8	0.87	0.08	71,79,81,82	0
4	PRO	B	603	8/8	0.88	0.08	61,67,70,73	0
2	PGE	C	602	10/10	0.88	0.09	46,59,67,67	0
3	PEG	A	603	7/7	0.89	0.09	52,58,65,68	0
2	PGE	A	602	10/10	0.90	0.07	55,65,71,72	0
4	PRO	A	604	8/8	0.92	0.08	63,74,81,83	0
4	PRO	C	604	8/8	0.92	0.09	69,73,80,88	0
2	PGE	D	601	10/10	0.93	0.09	50,60,76,78	0
2	PGE	B	601	10/10	0.94	0.12	44,60,68,72	0
2	PGE	A	601	10/10	0.94	0.10	52,60,67,72	0
2	PGE	C	601	10/10	0.95	0.10	48,62,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.