



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 PM UTC

PDB ID : 4ZIQ / pdb_00004ziq
Title : Crystal structure of trypsin activated alpha-2-macroglobulin from Escherichia coli.
Authors : Garcia-Ferrer, I.; Arede, P.; Gomez-Blanco, J.; Luque, D.; Duquerroy, S.; Caston, J.R.; Goulas, T.; Gomis-Ruth, X.F.
Deposited on : 2015-04-28
Resolution : 2.55 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

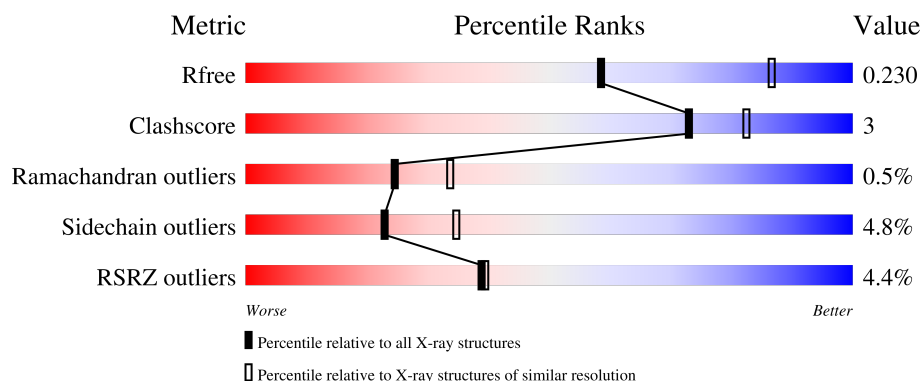
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1617	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11338 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 Uncharacterized lipoprotein YfhM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1450	11224	7092	1951	2157	24	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	expression tag	UNP P76578
A	38	PRO	-	expression tag	UNP P76578
A	39	MET	-	expression tag	UNP P76578

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Cl 3	0	0

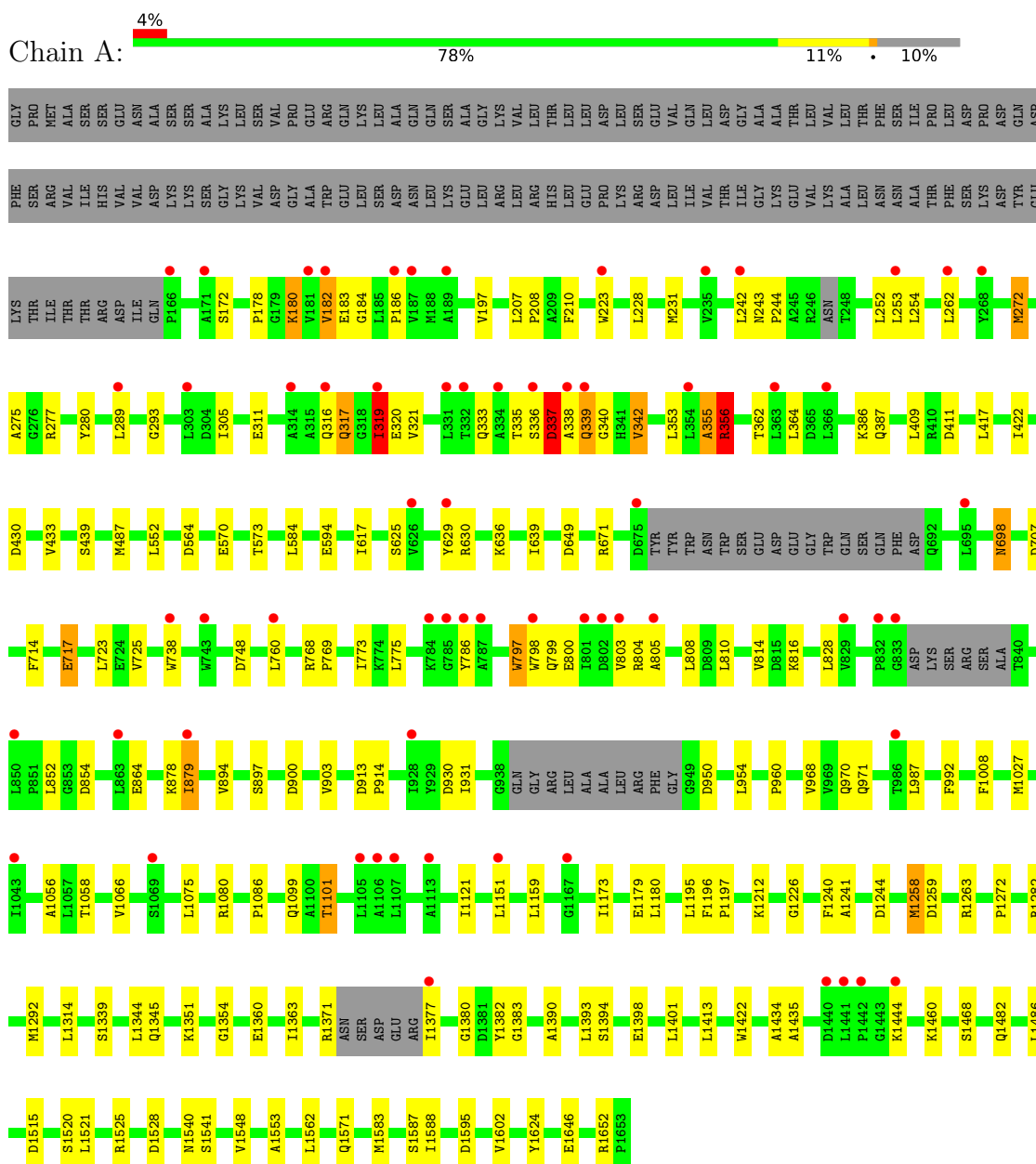
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total 105	O 105	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: Uncharacterized lipoprotein YfhM



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	274.28Å 95.36Å 81.09Å 90.00° 104.77° 90.00°	Depositor
Resolution (Å)	47.68 – 2.55 47.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.68-2.55) 98.9 (47.68-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.221 0.199 , 0.230	Depositor DCC
R_{free} test set	1083 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11338	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: CL, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	2/11456 (0.0%)	1.16	31/15582 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1583	MET	SD-CE	-5.52	1.65	1.79
1	A	1258	MET	SD-CE	-5.07	1.66	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ILE	N-CA-C	-7.72	105.64	111.90
1	A	799	GLN	CA-C-N	6.54	134.03	121.54
1	A	799	GLN	C-N-CA	6.54	134.03	121.54
1	A	1595	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	336	SER	CA-C-N	6.25	133.48	121.54
1	A	336	SER	C-N-CA	6.25	133.48	121.54
1	A	1272	PRO	CA-C-N	6.17	128.55	120.28
1	A	1272	PRO	C-N-CA	6.17	128.55	120.28
1	A	1515	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	930	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	430	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	564	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	1528	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	355	ALA	CA-C-N	5.55	132.15	121.54
1	A	355	ALA	C-N-CA	5.55	132.15	121.54
1	A	411	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	1562	LEU	CA-C-N	5.43	127.56	120.28
1	A	1562	LEU	C-N-CA	5.43	127.56	120.28
1	A	913	ASP	CA-CB-CG	5.39	117.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	797	TRP	CA-C-N	5.38	131.82	121.54
1	A	797	TRP	C-N-CA	5.38	131.82	121.54
1	A	1548	VAL	N-CA-CB	5.29	118.57	111.90
1	A	900	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	1383	GLY	N-CA-C	5.26	120.65	112.60
1	A	903	VAL	N-CA-C	-5.26	106.56	111.45
1	A	649	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	337	ASP	CA-C-N	5.17	128.68	121.02
1	A	337	ASP	C-N-CA	5.17	128.68	121.02
1	A	1354	GLY	N-CA-C	5.15	121.80	114.85
1	A	386	LYS	CA-C-N	5.04	128.00	120.95
1	A	386	LYS	C-N-CA	5.04	128.00	120.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	11224	0	11146	71	0
2	A	6	0	8	3	0
3	A	3	0	0	0	0
4	A	105	0	0	0	0
All	All	11338	0	11154	71	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 3.

All (71) 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:321:VAL:HG21	1:A:342:VAL:HG21	1.70	0.71
1:A:786:TYR:HA	1:A:800:GLU:O	1.95	0.67
1:A:769:PRO:HB3	1:A:816:LYS:HA	1.79	0.64
1:A:1380:GLY:H	2:A:1701:GOL:H31	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:HD12	1:A:931:ILE:HG23	1.80	0.63
1:A:914:PRO:HB2	1:A:1008:PHE:HB3	1.82	0.60
1:A:197:VAL:HG22	1:A:272:MET:HB2	1.83	0.60
1:A:617:ILE:HD11	1:A:725:VAL:HG12	1.88	0.55
1:A:182:VAL:HG22	1:A:184:GLY:H	1.73	0.53
1:A:639:ILE:HG22	1:A:738:TRP:HB3	1.90	0.53
1:A:305:ILE:HB	1:A:342:VAL:HG13	1.90	0.53
1:A:321:VAL:HG11	1:A:342:VAL:HG11	1.91	0.53
1:A:1195:LEU:HD11	1:A:1226:GLY:HA3	1.91	0.52
1:A:1027:MET:HE2	1:A:1121:ILE:HB	1.90	0.52
1:A:1259:ASP:OD1	1:A:1263:ARG:HD2	2.10	0.52
1:A:1393:LEU:HD23	1:A:1434:ALA:HB1	1.91	0.52
1:A:409:LEU:HD22	1:A:422:ILE:HD11	1.92	0.51
1:A:180:LYS:HD2	1:A:311:GLU:CD	2.35	0.51
1:A:968:VAL:HG21	1:A:992:PHE:CD1	2.45	0.50
1:A:172:SER:HB2	1:A:186:PRO:HG2	1.92	0.50
1:A:800:GLU:HG2	1:A:810:LEU:HD21	1.92	0.50
1:A:1173:ILE:HD13	1:A:1435:ALA:HB3	1.93	0.50
1:A:1240:PHE:HE1	1:A:1258:MET:HE3	1.76	0.50
1:A:1380:GLY:HA2	2:A:1701:GOL:H11	1.93	0.50
1:A:1241:ALA:HB3	1:A:1244:ASP:O	2.12	0.49
1:A:864:GLU:HB3	1:A:878:LYS:HB2	1.94	0.49
1:A:1056:ALA:HB3	1:A:1101:THR:HG23	1.93	0.49
1:A:1394:SER:O	1:A:1398:GLU:HB2	2.12	0.49
1:A:897:SER:HB3	1:A:971:GLN:HG3	1.93	0.48
1:A:1314:LEU:HD22	1:A:1345:GLN:HG2	1.95	0.48
1:A:1390:ALA:HA	1:A:1413:LEU:HD11	1.95	0.48
1:A:1382:TYR:H	2:A:1701:GOL:H32	1.78	0.48
1:A:803:VAL:HA	1:A:808:LEU:HD13	1.96	0.48
1:A:1344:LEU:HD12	1:A:1363:ILE:HG12	1.96	0.48
1:A:768:ARG:HD3	1:A:854:ASP:HB2	1.95	0.47
1:A:293:GLY:HA2	1:A:931:ILE:HD11	1.97	0.47
1:A:317:GLN:HA	1:A:340:GLY:HA3	1.95	0.47
1:A:1159:LEU:HB3	1:A:1468:SER:HB3	1.96	0.47
1:A:210:PHE:HD2	1:A:231:MET:HG3	1.79	0.46
1:A:207:LEU:N	1:A:208:PRO:HD2	2.30	0.46
1:A:954:LEU:HD22	1:A:960:PRO:HG3	1.97	0.46
1:A:316:GLN:HB2	1:A:339:GLN:HB3	1.97	0.46
1:A:321:VAL:HG23	1:A:333:GLN:HA	1.97	0.45
1:A:320:GLU:HB2	1:A:356:ARG:H	1.81	0.45
1:A:671:ARG:HH21	1:A:717:GLU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ALA:C	1:A:340:GLY:H	2.25	0.44
1:A:698:ASN:HD22	1:A:714:PHE:HE1	1.66	0.44
1:A:760:LEU:HB3	1:A:775:LEU:HD11	2.00	0.44
1:A:552:LEU:HD22	1:A:584:LEU:HD21	2.01	0.43
1:A:178:PRO:HB2	1:A:180:LYS:O	2.18	0.43
1:A:1282:ARG:HH22	1:A:1292:MET:HE1	1.84	0.43
1:A:321:VAL:H	1:A:333:GLN:HG3	1.82	0.43
1:A:184:GLY:HA3	1:A:254:LEU:O	2.19	0.42
1:A:487:MET:HE2	1:A:594:GLU:HG3	2.00	0.42
1:A:625:SER:HA	1:A:636:LYS:HA	2.01	0.42
1:A:1066:VAL:HB	1:A:1086:PRO:HB2	2.01	0.42
1:A:1180:LEU:HD11	1:A:1197:PRO:HB2	2.02	0.42
1:A:182:VAL:HG13	1:A:183:GLU:H	1.85	0.42
1:A:355:ALA:HB3	1:A:362:THR:HB	2.02	0.42
1:A:1588:ILE:HG12	1:A:1602:VAL:HG12	2.02	0.41
1:A:970:GLN:HB3	1:A:987:LEU:HD22	2.02	0.41
1:A:1151:LEU:HD22	1:A:1159:LEU:HD21	2.02	0.41
1:A:319:ILE:HB	1:A:335:THR:HB	2.02	0.41
1:A:1525:ARG:HG2	1:A:1652:ARG:HB2	2.02	0.41
1:A:1339:SER:HB2	1:A:1371:ARG:HG3	2.02	0.41
1:A:1344:LEU:CD1	1:A:1363:ILE:HG12	2.50	0.41
1:A:243:ASN:N	1:A:244:PRO:HD3	2.36	0.41
1:A:879:ILE:HG21	1:A:894:VAL:HG21	2.02	0.41
1:A:1553:ALA:HB3	1:A:1624:TYR:CD1	2.56	0.40
1:A:804:ARG:HD3	1:A:805:ALA:H	1.86	0.40
1:A:1179:GLU:HG3	1:A:1212:LYS:HB2	2.03	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	1438/1617 (89%)	1364 (95%)	67 (5%)	7 (0%)	24 34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ASP
1	A	275	ALA
1	A	798	TRP
1	A	1521	LEU
1	A	748	ASP
1	A	182	VAL
1	A	356	ARG

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	1199/1344 (89%)	1141 (95%)	58 (5%)	23 35

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	223	TRP
1	A	228	LEU
1	A	242	LEU
1	A	252	LEU
1	A	253	LEU
1	A	262	LEU
1	A	272	MET
1	A	277	ARG
1	A	280	TYR
1	A	289	LEU
1	A	317	GLN
1	A	319	ILE
1	A	337	ASP

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Mol	Chain	Res	Type
1	A	339	GLN
1	A	342	VAL
1	A	353	LEU
1	A	356	ARG
1	A	387	GLN
1	A	417	LEU
1	A	433	VAL
1	A	439	SER
1	A	570	GLU
1	A	573	THR
1	A	629	TYR
1	A	630	ARG
1	A	698	ASN
1	A	707	ASP
1	A	717	GLU
1	A	723	LEU
1	A	773	ILE
1	A	797	TRP
1	A	814	VAL
1	A	828	LEU
1	A	852	LEU
1	A	879	ILE
1	A	950	ASP
1	A	1058	THR
1	A	1075	LEU
1	A	1080	ARG
1	A	1099	GLN
1	A	1101	THR
1	A	1196	PHE
1	A	1351	LYS
1	A	1360	GLU
1	A	1377	ILE
1	A	1401	LEU
1	A	1422	TRP
1	A	1444	LYS
1	A	1460	LYS
1	A	1482	GLN
1	A	1486	LEU
1	A	1520	SER
1	A	1540	ASN
1	A	1541	SER
1	A	1571	GLN

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Mol	Chain	Res	Type
1	A	1587	SER
1	A	1646	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	349	ASN
1	A	387	GLN
1	A	406	ASN
1	A	471	GLN
1	A	581	HIS
1	A	698	ASN
1	A	821	HIS
1	A	872	ASN
1	A	916	GLN
1	A	971	GLN
1	A	1099	GLN
1	A	1116	HIS
1	A	1139	GLN
1	A	1153	ASN
1	A	1162	GLN
1	A	1172	ASN
1	A	1300	ASN
1	A	1389	ASN
1	A	1416	GLN
1	A	1448	GLN
1	A	1463	ASN
1	A	1465	ASN
1	A	1495	GLN
1	A	1577	GLN
1	A	1590	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
2	GOL	A	1701	-	5,5,5	0.09	0	5,5,5	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1701	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1701	GOL	3	0

5.7 Other polymers [i](#)

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, 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	1450/1617 (89%)	0.27	64 (4%) 39 39	52, 105, 179, 274	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	5.9
1	A	833	GLY	4.3
1	A	338	ALA	4.1
1	A	786	TYR	3.7
1	A	253	LEU	3.6
1	A	1377	ILE	3.5
1	A	1106	ALA	3.5
1	A	1441	LEU	3.4
1	A	1442	PRO	3.3
1	A	787	ALA	3.3
1	A	675	ASP	3.3
1	A	785	GLY	3.3
1	A	1107	LEU	3.2
1	A	339	GLN	3.1
1	A	171	ALA	3.1
1	A	331	LEU	3.0
1	A	801	ILE	3.0
1	A	314	ALA	3.0
1	A	166	PRO	2.8
1	A	186	PRO	2.8
1	A	803	VAL	2.7
1	A	332	THR	2.7
1	A	319	ILE	2.7
1	A	334	ALA	2.7
1	A	1043	ILE	2.7
1	A	798	TRP	2.6
1	A	743	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	928	ILE	2.6
1	A	268	TYR	2.6
1	A	182	VAL	2.6
1	A	235	VAL	2.6
1	A	316	GLN	2.5
1	A	850	LEU	2.5
1	A	1151	LEU	2.5
1	A	181	VAL	2.4
1	A	1105	LEU	2.3
1	A	303	LEU	2.3
1	A	784	LYS	2.3
1	A	189	ALA	2.3
1	A	223	TRP	2.3
1	A	1444	LYS	2.3
1	A	289	LEU	2.2
1	A	1069	SER	2.2
1	A	629	TYR	2.2
1	A	863	LEU	2.2
1	A	336	SER	2.2
1	A	879	ILE	2.2
1	A	187	VAL	2.1
1	A	829	VAL	2.1
1	A	242	LEU	2.1
1	A	1113	ALA	2.1
1	A	354	LEU	2.1
1	A	363	LEU	2.1
1	A	695	LEU	2.1
1	A	626	VAL	2.1
1	A	1167	GLY	2.1
1	A	1440	ASP	2.1
1	A	760	LEU	2.0
1	A	802	ASP	2.0
1	A	832	PRO	2.0
1	A	366	LEU	2.0
1	A	805	ALA	2.0
1	A	986	THR	2.0
1	A	738	TRP	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 [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	GOL	A	1701	6/6	0.73	0.18	105,111,113,113	0
3	CL	A	1703	1/1	0.84	0.29	87,87,87,87	1
3	CL	A	1702	1/1	0.91	0.28	74,74,74,74	1
3	CL	A	1704	1/1	0.91	0.50	84,84,84,84	1

6.5 Other polymers [i](#)

There are no such residues in this entry.