Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:59 PM GMT

PDB ID	:	4ZIQ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

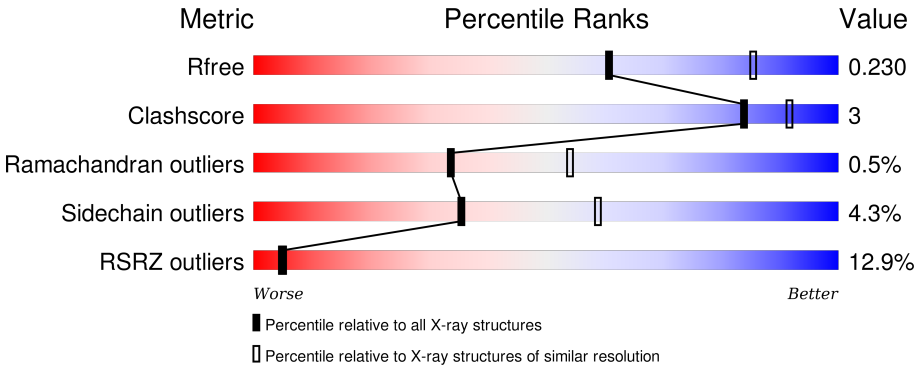
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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. 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 <=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	12% 80% 9% • 10%

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
3	CL	A	1703	-	-	-	X

2 Entry composition

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.

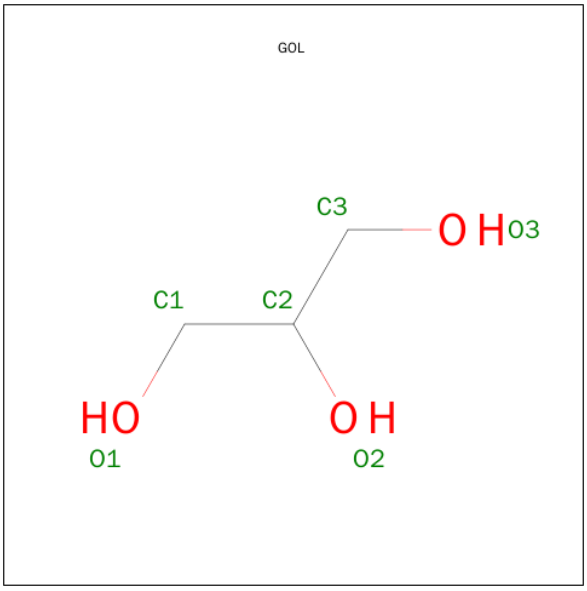
- Molecule 1 is a protein called Uncharacterized lipoprotein YfhM.

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 (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

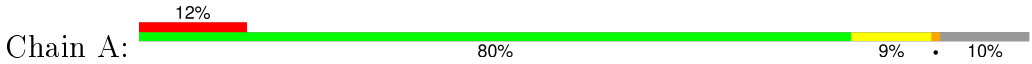
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0

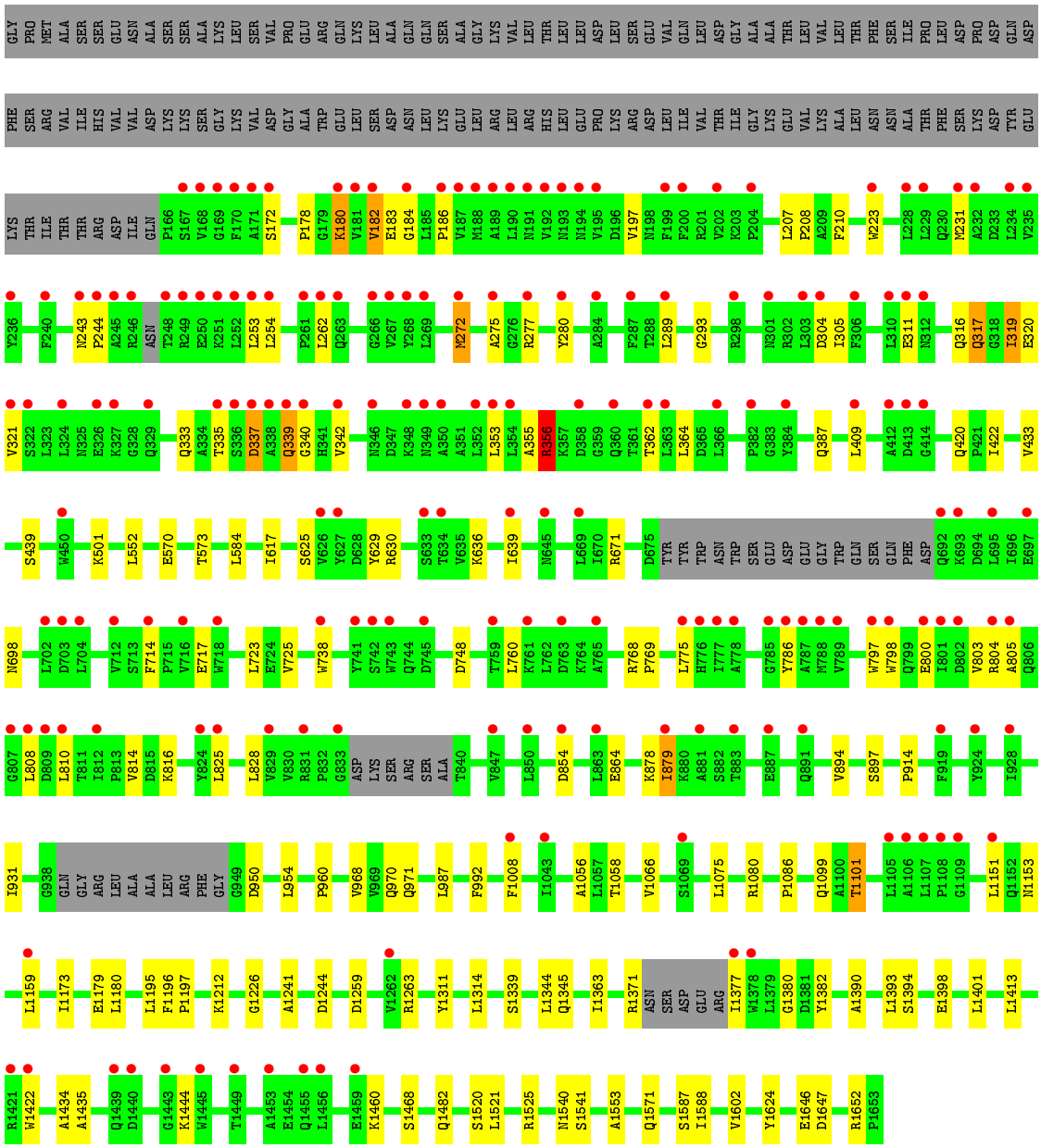
3 Residue-property plots (i)

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

- Molecule 1: Uncharacterized lipoprotein YfhM

Chain A:





4 Data and refinement statistics (i)

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) 98.8 (47.68-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (1.68%)	DCC
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 74.7	EDS
Estimated twinning fraction	0.029 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 65409 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL

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	0.44	0/11456	0.63	0/15582

There are no bond length outliers.

There are no bond angle outliers.

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	11224	0	11146	66	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	66	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 (66) 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
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:1393:LEU:HD23	1:A:1434:ALA:HB1	1.91	0.52
1:A:1259:ASP:OD1	1:A:1263:ARG:HD2	2.10	0.52
1:A:409:LEU:HD22	1:A:422:ILE:HD11	1.92	0.51
1:A:968:VAL:HG21	1:A:992:PHE:CD1	2.45	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:172:SER:HB2	1:A:186:PRO:HG2	1.92	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:1390:ALA:HA	1:A:1413:LEU:HD11	1.95	0.48
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: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:180:LYS:HD2	1:A:311:GLU:CD	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ARG:HH21	1:A:717:GLU:HB2	1.82	0.45
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: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: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:879:ILE:HG21	1:A:894:VAL:HG21	2.02	0.41
1:A:243:ASN:N	1:A:244:PRO:HD3	2.36	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%)	34 54

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 (i)

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%)	1147 (96%)	52 (4%)	35 59

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	223	TRP
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	304	ASP
1	A	317	GLN
1	A	319	ILE
1	A	337	ASP
1	A	339	GLN
1	A	353	LEU
1	A	356	ARG
1	A	387	GLN
1	A	420	GLN
1	A	433	VAL

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Mol	Chain	Res	Type
1	A	439	SER
1	A	501	LYS
1	A	570	GLU
1	A	573	THR
1	A	629	TYR
1	A	630	ARG
1	A	723	LEU
1	A	797	TRP
1	A	814	VAL
1	A	825	LEU
1	A	828	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	1153	ASN
1	A	1196	PHE
1	A	1311	TYR
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	1520	SER
1	A	1540	ASN
1	A	1541	SER
1	A	1571	GLN
1	A	1587	SER
1	A	1646	GLU
1	A	1647	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
1	A	419	ASN
1	A	698	ASN
1	A	980	GLN

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Mol	Chain	Res	Type
1	A	1153	ASN
1	A	1446	GLN
1	A	1540	ASN
1	A	1582	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	0.11	0	5,5,5	0.32	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	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.82	187 (12%)	5	5	52, 105, 179, 274	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	14.3
1	A	245	ALA	11.1
1	A	189	ALA	9.2
1	A	248	THR	9.1
1	A	190	LEU	9.0
1	A	223	TRP	8.4
1	A	786	TYR	7.8
1	A	188	MET	7.4
1	A	187	VAL	6.9
1	A	833	GLY	6.8
1	A	244	PRO	6.8
1	A	228	LEU	6.4
1	A	743	TRP	6.4
1	A	1106	ALA	6.3
1	A	235	VAL	6.2
1	A	249	ARG	6.2
1	A	191	ASN	6.0
1	A	192	VAL	5.8
1	A	321	VAL	5.8
1	A	246	ARG	5.8
1	A	741	TYR	5.7
1	A	825	LEU	5.6
1	A	268	TYR	5.5
1	A	280	TYR	5.5
1	A	289	LEU	5.4
1	A	366	LEU	5.3
1	A	718	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	778	ALA	5.0
1	A	252	LEU	5.0
1	A	745	ASP	5.0
1	A	807	GLY	4.9
1	A	346	ASN	4.8
1	A	303	LEU	4.8
1	A	850	LEU	4.7
1	A	1105	LEU	4.7
1	A	627	TYR	4.5
1	A	312	ASN	4.5
1	A	306	PHE	4.4
1	A	171	ALA	4.3
1	A	787	ALA	4.3
1	A	863	LEU	4.3
1	A	231	MET	4.3
1	A	253	LEU	4.2
1	A	337	ASP	4.2
1	A	928	ILE	4.2
1	A	338	ALA	4.2
1	A	716	VAL	4.2
1	A	200	PHE	4.1
1	A	266	GLY	4.1
1	A	1422	TRP	4.0
1	A	335	THR	4.0
1	A	785	GLY	4.0
1	A	1377	ILE	4.0
1	A	352	LEU	3.9
1	A	883	THR	3.9
1	A	1109	GLY	3.9
1	A	336	SER	3.9
1	A	348	LYS	3.8
1	A	634	THR	3.8
1	A	1453	ALA	3.8
1	A	358	ASP	3.8
1	A	194	ASN	3.8
1	A	626	VAL	3.8
1	A	798	TRP	3.7
1	A	186	PRO	3.7
1	A	805	ALA	3.6
1	A	891	GLN	3.6
1	A	362	THR	3.6
1	A	363	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	168	VAL	3.6
1	A	181	VAL	3.6
1	A	384	TYR	3.6
1	A	777	ILE	3.5
1	A	193	ASN	3.5
1	A	812	ILE	3.5
1	A	738	TRP	3.4
1	A	1421	ARG	3.4
1	A	879	ILE	3.4
1	A	322	SER	3.3
1	A	232	ALA	3.3
1	A	1107	LEU	3.3
1	A	326	GLU	3.3
1	A	250	GLU	3.2
1	A	802	ASP	3.2
1	A	310	LEU	3.1
1	A	1449	THR	3.1
1	A	409	LEU	3.1
1	A	702	LEU	3.1
1	A	243	ASN	3.0
1	A	765	ALA	3.0
1	A	776	HIS	3.0
1	A	229	LEU	3.0
1	A	697	GLU	3.0
1	A	1456	LEU	3.0
1	A	182	VAL	3.0
1	A	180	LYS	3.0
1	A	349	ASN	2.9
1	A	887	GLU	2.9
1	A	327	LYS	2.9
1	A	350	ALA	2.9
1	A	797	TRP	2.9
1	A	881	ALA	2.9
1	A	645	ASN	2.8
1	A	195	VAL	2.8
1	A	789	VAL	2.8
1	A	269	LEU	2.8
1	A	692	GLN	2.8
1	A	329	GLN	2.8
1	A	1043	ILE	2.8
1	A	263	GLN	2.8
1	A	808	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	170	PHE	2.7
1	A	1378	TRP	2.7
1	A	1439	GLN	2.7
1	A	1440	ASP	2.7
1	A	1069	SER	2.7
1	A	202	VAL	2.7
1	A	354	LEU	2.7
1	A	847	VAL	2.6
1	A	169	GLY	2.6
1	A	763	ASP	2.6
1	A	382	PRO	2.6
1	A	714	PHE	2.6
1	A	761	LYS	2.6
1	A	267	VAL	2.5
1	A	234	LEU	2.5
1	A	800	GLU	2.5
1	A	829	VAL	2.5
1	A	1159	LEU	2.5
1	A	339	GLN	2.5
1	A	1445	TRP	2.5
1	A	184	GLY	2.5
1	A	199	PHE	2.5
1	A	287	PHE	2.5
1	A	924	TYR	2.5
1	A	254	LEU	2.4
1	A	353	LEU	2.4
1	A	669	LEU	2.4
1	A	831	ARG	2.4
1	A	693	LYS	2.4
1	A	703	ASP	2.4
1	A	204	PRO	2.4
1	A	788	MET	2.4
1	A	298	ARG	2.4
1	A	1443	GLY	2.3
1	A	742	SER	2.3
1	A	759	THR	2.3
1	A	695	LEU	2.3
1	A	704	LEU	2.3
1	A	775	LEU	2.3
1	A	712	VAL	2.3
1	A	167	SER	2.3
1	A	414	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	804	ARG	2.3
1	A	275	ALA	2.3
1	A	1459	GLU	2.3
1	A	639	ILE	2.2
1	A	251	LYS	2.2
1	A	277	ARG	2.2
1	A	1151	LEU	2.2
1	A	1455	GLN	2.2
1	A	284	ALA	2.2
1	A	301	ASN	2.2
1	A	342	VAL	2.2
1	A	236	TYR	2.2
1	A	1262	VAL	2.2
1	A	809	ASP	2.2
1	A	1008	PHE	2.2
1	A	261	PRO	2.2
1	A	304	ASP	2.1
1	A	450	TRP	2.1
1	A	824	TYR	2.1
1	A	801	ILE	2.1
1	A	1108	PRO	2.1
1	A	360	GLN	2.1
1	A	919	PHE	2.1
1	A	633	SER	2.1
1	A	324	LEU	2.1
1	A	854	ASP	2.1
1	A	172	SER	2.1
1	A	412	ALA	2.0
1	A	413	ASP	2.0
1	A	272	MET	2.0
1	A	340	GLY	2.0
1	A	311	GLU	2.0
1	A	810	LEU	2.0
1	A	240	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	CL	A	1703	1/1	0.83	0.37	10.82	87,87,87,87	1
2	GOL	A	1701	6/6	0.58	0.36	1.53	105,111,113,113	0
3	CL	A	1702	1/1	0.82	0.42	-	74,74,74,74	1
3	CL	A	1704	1/1	0.70	1.34	-	84,84,84,84	1

6.5 Other polymers (i)

There are no such residues in this entry.