



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:35 PM UTC

PDB ID : 5CD7 / pdb_00005cd7
Title : Crystal structure of the NTD L199M of Drosophila Oskar protein
Authors : Yang, N.; Hu, M.; Yu, Z.; Wang, M.; Lehmann, R.; Xu, R.M.
Deposited on : 2015-07-03
Resolution : 2.50 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

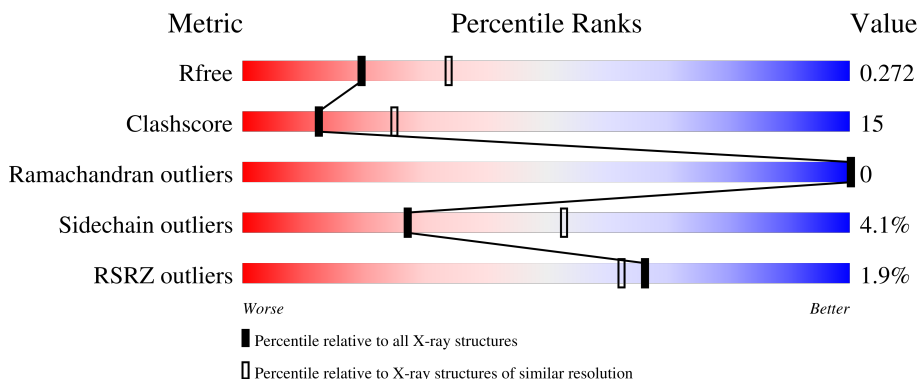
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 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	77	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; background: linear-gradient(to right, red 0%, orange 10%, yellow 25%, green 75%);"></div> <div style="margin-left: 10px;"> <p>75% 25%</p> </div> </div>
1	B	77	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; background: linear-gradient(to right, red 0%, orange 3%, yellow 56%, green 56%, yellow 87%, orange 93%, grey 99%);"></div> <div style="margin-left: 10px;"> <p>3% 56% 31% 6% 6%</p> </div> </div>
1	C	77	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; background: linear-gradient(to right, red 0%, orange 1%, yellow 69%, green 69%, yellow 96%, grey 99%);"></div> <div style="margin-left: 10px;"> <p>69% 27% ..</p> </div> </div>
1	D	77	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 20px; background: linear-gradient(to right, green 68%, yellow 94%, grey 99%);"></div> <div style="margin-left: 10px;"> <p>68% 26% . 5%</p> </div> </div>
1	E	77	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; background: linear-gradient(to right, red 0%, orange 4%, yellow 55%, green 55%, yellow 84%, orange 89%, grey 99%);"></div> <div style="margin-left: 10px;"> <p>4% 55% 29% 5% 12%</p> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	77	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a green segment on the left labeled '55%', a yellow segment in the middle labeled '32%', and a grey segment on the right labeled '12%'. A small red square is at the beginning of the bar, and a small black dot is at the end of the grey segment. A '%' symbol is positioned above the start of the bar.</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3452 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 Maternal effect protein oskar.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	77	602	376	104	120	1	1	0	0	0
1	B	72	568	356	98	112	1	1	0	0	0
1	C	75	590	368	101	119	1	1	0	1	0
1	D	73	574	359	99	114	1	1	0	0	0
1	E	68	527	331	91	103	1	1	0	0	0
1	F	68	526	329	91	104	1	1	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

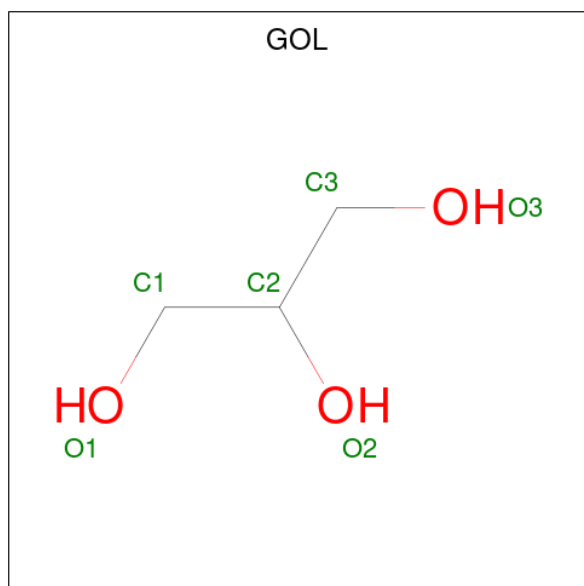
Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLY	-	expression tag	UNP P25158
A	149	SER	-	expression tag	UNP P25158
A	199	MSE	LEU	engineered mutation	UNP P25158
B	148	GLY	-	expression tag	UNP P25158
B	149	SER	-	expression tag	UNP P25158
B	199	MSE	LEU	engineered mutation	UNP P25158
C	148	GLY	-	expression tag	UNP P25158
C	149	SER	-	expression tag	UNP P25158
C	199	MSE	LEU	engineered mutation	UNP P25158
D	148	GLY	-	expression tag	UNP P25158
D	149	SER	-	expression tag	UNP P25158
D	199	MSE	LEU	engineered mutation	UNP P25158
E	148	GLY	-	expression tag	UNP P25158
E	149	SER	-	expression tag	UNP P25158
E	199	MSE	LEU	engineered mutation	UNP P25158
F	148	GLY	-	expression tag	UNP P25158
F	149	SER	-	expression tag	UNP P25158

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	199	MSE	LEU	engineered mutation	UNP P25158

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

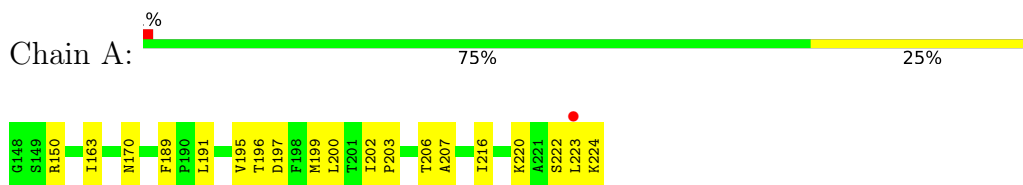
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	7	Total O 7 7	0	0
3	C	5	Total O 5 5	0	0
3	D	6	Total O 6 6	0	0
3	E	2	Total O 2 2	0	0

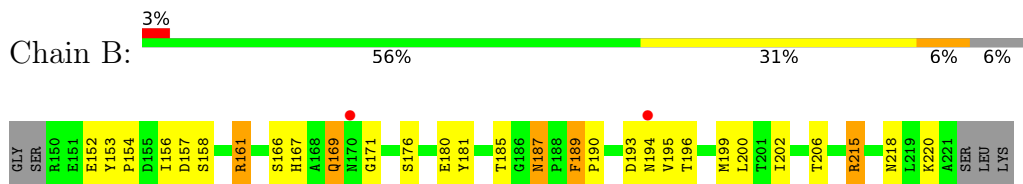
3 Residue-property plots [i](#)

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.

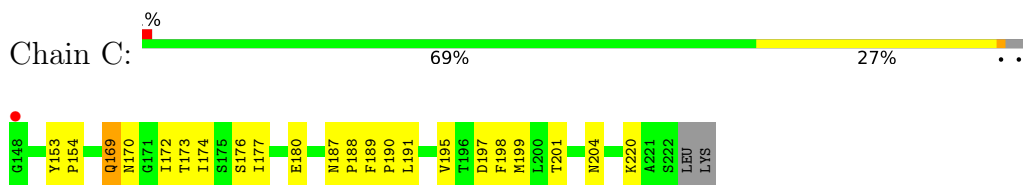
- Molecule 1: Maternal effect protein oskar



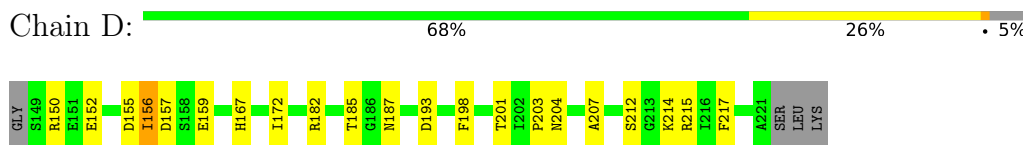
- Molecule 1: Maternal effect protein oskar



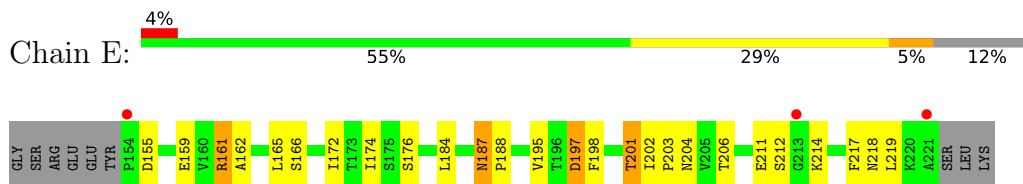
- Molecule 1: Maternal effect protein oskar



- Molecule 1: Maternal effect protein oskar

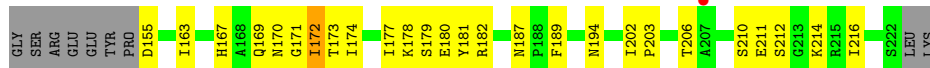


- Molecule 1: Maternal effect protein oskar



- Molecule 1: Maternal effect protein oskar

Chain F:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.96Å 38.31Å 102.13Å 90.00° 95.54° 90.00°	Depositor
Resolution (Å)	37.73 – 2.50 37.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.73-2.50) 99.0 (37.73-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.214 , 0.270 0.216 , 0.272	Depositor DCC
R_{free} test set	859 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtrriage
Anisotropy	0.573	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3452	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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: 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	0.44	0/611	0.84	1/822 (0.1%)
1	B	0.39	0/577	0.87	3/779 (0.4%)
1	C	0.38	0/602	0.87	0/812
1	D	0.38	0/583	0.95	1/787 (0.1%)
1	E	0.35	0/535	0.95	2/722 (0.3%)
1	F	0.31	0/533	0.89	3/719 (0.4%)
All	All	0.38	0/3441	0.90	10/4641 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	187	ASN	CA-C-N	7.38	127.42	119.89
1	E	187	ASN	C-N-CA	7.38	127.42	119.89
1	F	189	PHE	CA-C-N	6.23	125.45	118.97
1	F	189	PHE	C-N-CA	6.23	125.45	118.97
1	B	167	HIS	N-CA-C	5.80	120.48	113.17
1	A	170	ASN	N-CA-C	5.52	120.12	113.17
1	B	189	PHE	CA-C-N	5.41	124.86	119.24
1	B	189	PHE	C-N-CA	5.41	124.86	119.24
1	D	156	ILE	N-CA-C	5.38	116.00	110.36
1	F	172	ILE	N-CA-C	5.00	114.96	108.35

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	602	0	600	17	0
1	B	568	0	563	24	0
1	C	590	0	582	18	0
1	D	574	0	568	17	0
1	E	527	0	530	17	0
1	F	526	0	527	21	0
2	A	18	0	24	4	0
2	F	6	0	8	1	0
3	A	21	0	0	0	0
3	B	7	0	0	0	0
3	C	5	0	0	0	0
3	D	6	0	0	2	0
3	E	2	0	0	0	0
All	All	3452	0	3402	104	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 15.

All (104) 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:150:ARG:NH1	1:D:157:ASP:OD2	2.00	0.95
1:B:153:TYR:CZ	1:B:190:PRO:HB3	2.10	0.87
1:F:210:SER:HB3	1:F:214:LYS:HB2	1.57	0.86
1:A:163:ILE:HA	2:A:302:GOL:H32	1.58	0.85
1:A:222:SER:HB3	1:D:182:ARG:HE	1.47	0.79
1:F:173:THR:O	1:F:177:ILE:HG13	1.85	0.75
1:A:223:LEU:H	1:A:223:LEU:HD23	1.50	0.75
1:D:155:ASP:HA	3:D:305:HOH:O	1.90	0.70
1:F:169:GLN:HG3	1:F:170:ASN:OD1	1.93	0.69
1:D:150:ARG:HG2	1:D:156:ILE:HG21	1.75	0.69
1:C:189:PHE:CE2	1:C:191:LEU:HB2	2.27	0.69
1:C:189:PHE:HE2	1:C:191:LEU:HB2	1.61	0.65
1:D:167:HIS:CD2	1:D:172:ILE:HD12	2.30	0.65
1:A:224:LYS:HB3	1:D:182:ARG:HH22	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:HG3	1:E:184:LEU:HD11	1.80	0.63
1:A:189:PHE:CE2	1:A:191:LEU:HB2	2.33	0.63
1:A:206:THR:HG23	1:A:220:LYS:HG3	1.80	0.62
1:B:166:SER:O	1:B:169:GLN:NE2	2.32	0.60
1:A:197:ASP:OD2	1:B:215:ARG:NH1	2.35	0.60
1:F:172:ILE:HD13	1:F:177:ILE:HG12	1.82	0.60
1:C:197:ASP:O	1:C:201:THR:HG23	2.01	0.60
1:A:163:ILE:HA	2:A:302:GOL:C3	2.31	0.59
1:C:204:ASN:OD1	1:C:220:LYS:HB2	2.03	0.59
1:D:157:ASP:HB2	3:D:306:HOH:O	2.03	0.58
1:A:222:SER:HB3	1:D:182:ARG:NE	2.18	0.58
1:E:161:ARG:NH1	1:E:165:LEU:HD22	2.18	0.58
1:F:167:HIS:CE1	1:F:172:ILE:HD12	2.38	0.58
1:E:197:ASP:OD1	1:E:197:ASP:N	2.37	0.57
1:F:174:ILE:HG22	1:F:178:LYS:HE3	1.88	0.56
1:D:207:ALA:HB2	1:D:217:PHE:CE2	2.41	0.55
1:B:206:THR:HG23	1:B:220:LYS:HG2	1.89	0.54
1:E:211:GLU:H	1:E:211:GLU:CD	2.16	0.54
1:D:198:PHE:O	1:D:201:THR:OG1	2.26	0.53
1:F:210:SER:OG	1:F:211:GLU:N	2.39	0.53
1:D:155:ASP:O	1:D:159:GLU:HG3	2.08	0.53
1:F:210:SER:CB	1:F:214:LYS:HB2	2.36	0.53
1:B:193:ASP:OD1	1:B:194:ASN:N	2.43	0.52
1:B:161:ARG:HB3	1:E:162:ALA:HB1	1.92	0.52
1:F:179:SER:OG	1:F:180:GLU:N	2.43	0.52
1:F:182:ARG:HA	1:F:187:ASN:O	2.10	0.51
1:E:174:ILE:HD13	1:E:195:VAL:HB	1.93	0.50
1:A:223:LEU:HD23	1:A:223:LEU:N	2.25	0.50
1:D:156:ILE:HG23	1:D:157:ASP:N	2.27	0.50
1:B:195:VAL:O	1:B:199:MSE:HG2	2.12	0.50
1:E:206:THR:O	1:E:217:PHE:HA	2.12	0.49
1:B:153:TYR:CE2	1:B:190:PRO:HB3	2.46	0.48
1:B:206:THR:CG2	1:B:220:LYS:HG2	2.44	0.48
1:C:153:TYR:CZ	1:C:190:PRO:HB2	2.48	0.47
1:C:172:ILE:HG12	1:C:176:SER:HB3	1.94	0.47
1:F:171:GLY:HA3	1:F:216:ILE:CG2	2.45	0.47
1:E:218:ASN:CG	1:E:219:LEU:H	2.23	0.46
1:E:203:PRO:O	1:E:204:ASN:HB2	2.16	0.46
1:D:212:SER:HB3	1:D:214:LYS:HE3	1.96	0.46
1:E:161:ARG:O	1:E:165:LEU:HB2	2.15	0.46
1:E:172:ILE:HD11	1:E:176:SER:C	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:ILE:HD11	1:F:181:TYR:HA	1.98	0.46
1:F:171:GLY:HA3	1:F:216:ILE:HG23	1.98	0.46
1:C:195:VAL:O	1:C:199:MSE:HG2	2.16	0.45
1:F:211:GLU:CD	1:F:214:LYS:HZ2	2.20	0.45
1:C:169:GLN:HG3	1:C:170:ASN:OD1	2.16	0.45
1:F:173:THR:HG22	1:F:174:ILE:N	2.32	0.45
1:D:203:PRO:O	1:D:204:ASN:HB2	2.16	0.45
1:B:152:GLU:O	1:B:154:PRO:HD3	2.17	0.44
1:A:195:VAL:O	1:A:199:MSE:HG2	2.17	0.44
1:F:194:ASN:O	1:F:194:ASN:ND2	2.51	0.44
1:F:194:ASN:HA	2:F:301:GOL:H11	1.98	0.44
1:D:212:SER:HB2	1:D:214:LYS:HG3	1.99	0.44
1:F:212:SER:HB3	1:F:214:LYS:HE3	2.00	0.44
1:B:176:SER:O	1:B:180:GLU:HG2	2.18	0.44
1:E:198:PHE:O	1:E:201:THR:HB	2.18	0.44
1:C:173:THR:HG22	1:C:174:ILE:N	2.31	0.44
1:C:153:TYR:HA	1:C:154:PRO:HD3	1.84	0.44
1:C:198:PHE:O	1:C:201:THR:OG1	2.23	0.43
1:B:161:ARG:HD2	1:B:202:ILE:CG2	2.48	0.43
1:C:187:ASN:HB2	1:C:188:PRO:HD2	2.01	0.43
1:B:169:GLN:HE21	1:B:169:GLN:HB3	1.61	0.43
1:A:207:ALA:HA	1:A:216:ILE:O	2.18	0.43
1:B:181:TYR:CG	1:B:189:PHE:HD1	2.37	0.43
1:C:169:GLN:HE21	1:C:169:GLN:C	2.25	0.43
1:C:189:PHE:CZ	1:C:191:LEU:HD13	2.54	0.43
1:A:202:ILE:HA	1:A:203:PRO:HD3	1.90	0.43
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.84	0.42
1:B:181:TYR:CZ	1:B:185:THR:HG21	2.54	0.42
1:B:161:ARG:NH2	1:E:159:GLU:HG2	2.34	0.42
1:E:212:SER:HB3	1:E:214:LYS:HE3	2.01	0.42
1:C:153:TYR:CE2	1:C:190:PRO:HB2	2.54	0.42
1:A:196:THR:HG21	1:B:200:LEU:HD12	2.01	0.42
1:B:185:THR:OG1	1:B:187:ASN:ND2	2.52	0.42
1:C:187:ASN:HB2	1:C:188:PRO:CD	2.50	0.41
1:F:174:ILE:CG2	1:F:178:LYS:HE3	2.49	0.41
1:B:171:GLY:HA2	1:B:218:ASN:OD1	2.20	0.41
1:F:167:HIS:NE2	1:F:180:GLU:HG3	2.35	0.41
1:C:174:ILE:O	1:C:177:ILE:HB	2.21	0.41
1:C:176:SER:O	1:C:180:GLU:HG2	2.19	0.41
1:A:200:LEU:HD13	1:B:196:THR:HG21	2.03	0.41
1:B:158:SER:HB3	1:E:161:ARG:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:THR:C	1:D:187:ASN:H	2.29	0.41
1:A:195:VAL:HG23	2:A:301:GOL:H11	2.03	0.41
1:B:156:ILE:HG23	1:B:157:ASP:N	2.35	0.40
1:D:182:ARG:HA	1:D:187:ASN:O	2.20	0.40
1:E:202:ILE:HA	1:E:203:PRO:HD3	1.95	0.40
1:F:202:ILE:HA	1:F:203:PRO:HD3	1.93	0.40
1:E:187:ASN:HA	1:E:188:PRO:HD3	1.82	0.40
1:A:195:VAL:CG2	2:A:301:GOL:H11	2.51	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	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
1	B	70/77 (91%)	66 (94%)	4 (6%)	0	100	100
1	C	74/77 (96%)	74 (100%)	0	0	100	100
1	D	71/77 (92%)	69 (97%)	2 (3%)	0	100	100
1	E	66/77 (86%)	63 (96%)	3 (4%)	0	100	100
1	F	66/77 (86%)	61 (92%)	5 (8%)	0	100	100
All	All	422/462 (91%)	406 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	69/68 (102%)	68 (99%)	1 (1%)	59	81
1	B	65/68 (96%)	61 (94%)	4 (6%)	16	34
1	C	68/68 (100%)	67 (98%)	1 (2%)	57	80
1	D	66/68 (97%)	63 (96%)	3 (4%)	24	49
1	E	61/68 (90%)	56 (92%)	5 (8%)	10	23
1	F	61/68 (90%)	59 (97%)	2 (3%)	33	61
All	All	390/408 (96%)	374 (96%)	16 (4%)	27	53

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	B	161	ARG
1	B	169	GLN
1	B	187	ASN
1	B	215	ARG
1	C	169	GLN
1	D	152	GLU
1	D	193	ASP
1	D	215	ARG
1	E	155	ASP
1	E	161	ARG
1	E	166	SER
1	E	197	ASP
1	E	201	THR
1	F	155	ASP
1	F	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	B	187	ASN
1	C	169	GLN
1	D	167	HIS
1	E	194	ASN
1	F	194	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](#)

4 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	GOL	F	301	-	5,5,5	0.36	0	5,5,5	0.32	0
2	GOL	A	302	-	5,5,5	0.39	0	5,5,5	0.31	0
2	GOL	A	303	-	5,5,5	0.32	0	5,5,5	0.34	0
2	GOL	A	301	-	5,5,5	0.37	0	5,5,5	0.24	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	F	301	-	-	4/4/4/4	-
2	GOL	A	302	-	-	2/4/4/4	-
2	GOL	A	303	-	-	2/4/4/4	-
2	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-C3
2	A	301	GOL	C1-C2-C3-O3
2	A	302	GOL	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-C3
2	A	303	GOL	C1-C2-C3-O3
2	F	301	GOL	O1-C1-C2-C3
2	F	301	GOL	C1-C2-C3-O3
2	A	301	GOL	O1-C1-C2-O2
2	A	301	GOL	O2-C2-C3-O3
2	A	303	GOL	O2-C2-C3-O3
2	F	301	GOL	O2-C2-C3-O3
2	F	301	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	GOL	1	0
2	A	302	GOL	2	0
2	A	301	GOL	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 [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	76/77 (98%)	-0.17	1 (1%) 75 71	36, 54, 112, 130	0
1	B	71/77 (92%)	0.28	2 (2%) 55 50	45, 77, 130, 150	0
1	C	74/77 (96%)	0.16	1 (1%) 73 70	39, 82, 121, 139	1 (1%)
1	D	72/77 (93%)	0.12	0 100 100	51, 83, 126, 138	0
1	E	67/77 (87%)	0.55	3 (4%) 38 33	70, 106, 167, 188	0
1	F	67/77 (87%)	0.52	1 (1%) 72 68	69, 112, 169, 190	0
All	All	427/462 (92%)	0.23	8 (1%) 66 62	36, 88, 139, 190	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	221	ALA	3.6
1	E	154	PRO	2.6
1	C	148	GLY	2.4
1	A	223	LEU	2.4
1	B	170	ASN	2.2
1	B	194	ASN	2.1
1	F	207	ALA	2.1
1	E	213	GLY	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 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(Å ²)	Q<0.9
2	GOL	F	301	6/6	0.70	0.12	113,115,116,117	0
2	GOL	A	303	6/6	0.76	0.14	74,78,81,82	0
2	GOL	A	301	6/6	0.77	0.20	67,74,75,75	0
2	GOL	A	302	6/6	0.90	0.23	34,39,42,45	6

6.5 Other polymers [i](#)

There are no such residues in this entry.