



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:18 AM EDT

PDB ID : 5UVE
Title : Crystal Structure of the ABC Transporter Substrate-binding protein BAB1_0226 from Brucella abortus
Authors : Kim, Y.; Chhor, G.; Endres, M.; Hero, J.; Babnigg, G.; Crosson, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2017-02-20
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

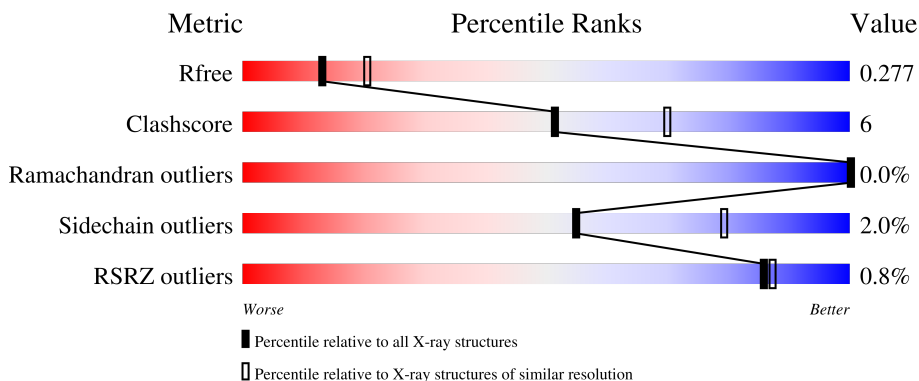
1 Overall quality at a glance i

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	282	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">87% 12%</p>
1	B	282	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">82% 17% .</p>
1	C	282	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">87% 11% ..</p>
1	D	282	<div style="display: flex; align-items: center;"> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">85% 14% .</p>
1	E	282	<div style="display: flex; align-items: center;"> <div style="width: 88%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">88% 12%</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	282	 85% 14%
1	G	282	 87% 11%
1	H	282	 82% 16%

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	GOL	B	401	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16923 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 Substrate-binding region of ABC-type glycine betaine transport system.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	Se	0	0	0
			2103	1343	350	409	1			
1	B	281	Total	C	N	O	Se	0	0	0
			2103	1343	350	409	1			
1	C	280	Total	C	N	O	Se	0	0	0
			2094	1337	348	408	1			
1	D	281	Total	C	N	O	Se	0	0	0
			2100	1340	349	410	1			
1	E	281	Total	C	N	O	Se	0	0	0
			2103	1343	350	409	1			
1	F	281	Total	C	N	O	Se	0	0	0
			2100	1340	349	410	1			
1	G	281	Total	C	N	O	Se	0	0	0
			2100	1340	349	410	1			
1	H	281	Total	C	N	O	Se	0	0	0
			2100	1340	349	410	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	SER	-	expression tag	UNP Q2YP76
A	24	ASN	-	expression tag	UNP Q2YP76
A	25	ALA	-	expression tag	UNP Q2YP76
B	23	SER	-	expression tag	UNP Q2YP76
B	24	ASN	-	expression tag	UNP Q2YP76
B	25	ALA	-	expression tag	UNP Q2YP76
C	23	SER	-	expression tag	UNP Q2YP76
C	24	ASN	-	expression tag	UNP Q2YP76
C	25	ALA	-	expression tag	UNP Q2YP76
D	23	SER	-	expression tag	UNP Q2YP76
D	24	ASN	-	expression tag	UNP Q2YP76
D	25	ALA	-	expression tag	UNP Q2YP76

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	23	SER	-	expression tag	UNP Q2YP76
E	24	ASN	-	expression tag	UNP Q2YP76
E	25	ALA	-	expression tag	UNP Q2YP76
F	23	SER	-	expression tag	UNP Q2YP76
F	24	ASN	-	expression tag	UNP Q2YP76
F	25	ALA	-	expression tag	UNP Q2YP76
G	23	SER	-	expression tag	UNP Q2YP76
G	24	ASN	-	expression tag	UNP Q2YP76
G	25	ALA	-	expression tag	UNP Q2YP76
H	23	SER	-	expression tag	UNP Q2YP76
H	24	ASN	-	expression tag	UNP Q2YP76
H	25	ALA	-	expression tag	UNP Q2YP76

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0

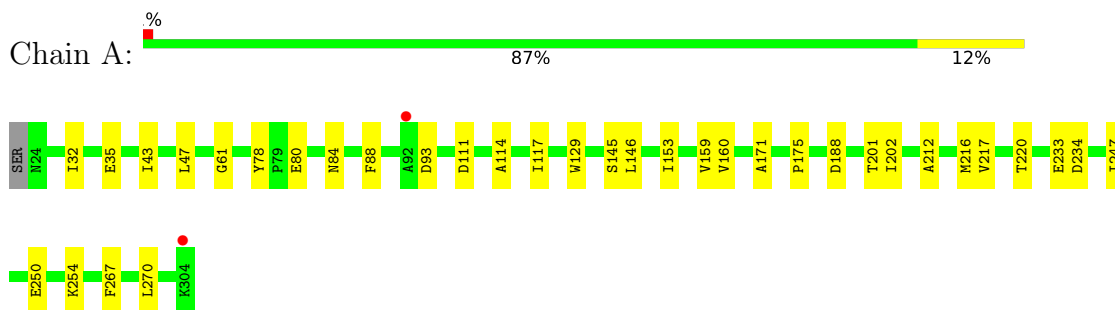
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	9	Total O 9 9	0	0
4	C	15	Total O 15 15	0	0
4	D	15	Total O 15 15	0	0
4	E	11	Total O 11 11	0	0
4	F	12	Total O 12 12	0	0
4	G	13	Total O 13 13	0	0
4	H	12	Total O 12 12	0	0

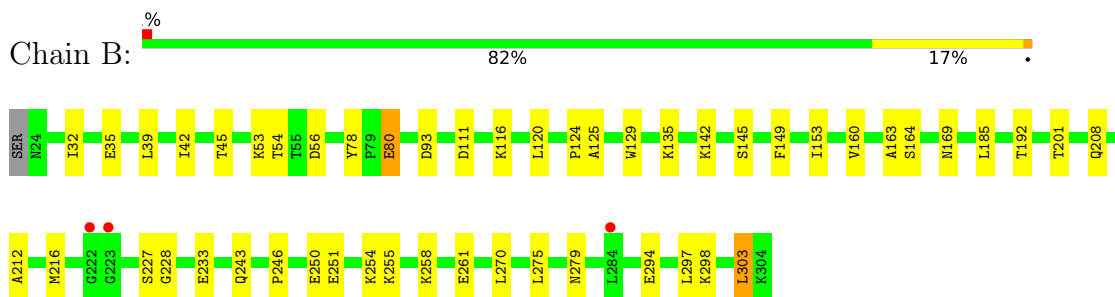
3 Residue-property plots

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.

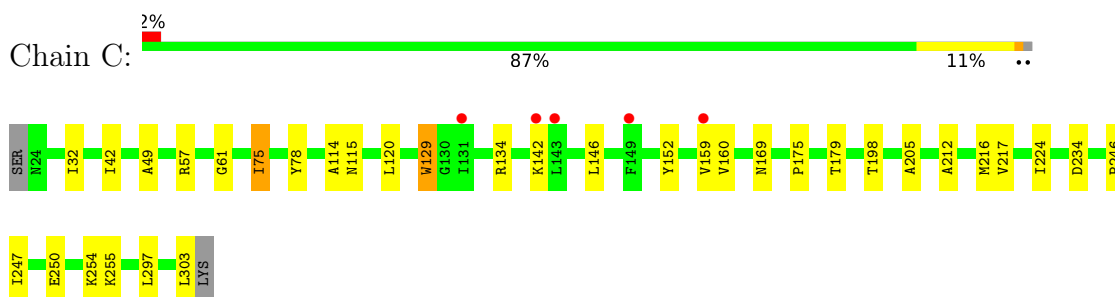
- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system



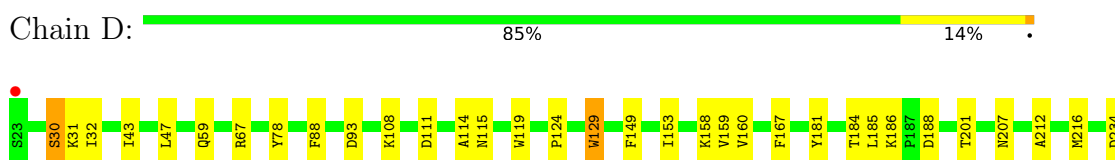
- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system

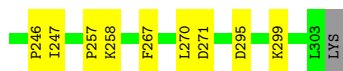


- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system



- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system





- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system

Chain E: 88% 12%



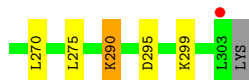
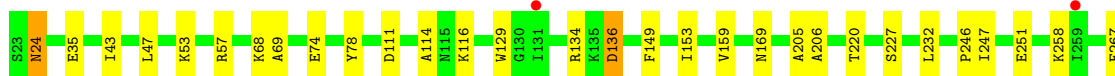
- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system

Chain F: 85% 14%



- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system

Chain G: 87% 11%



- Molecule 1: Substrate-binding region of ABC-type glycine betaine transport system

Chain H: 82% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.60Å 92.74Å 95.12Å 95.19° 110.87° 111.35°	Depositor
Resolution (Å)	41.78 – 2.50 49.58 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.4 (41.78-2.50) 96.6 (49.58-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.226 , 0.277 0.226 , 0.277	Depositor DCC
R_{free} test set	4001 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtrriage
Anisotropy	0.284	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 11.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.077 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16923	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: GOL, CA

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	0.29	0/2141	0.54	0/2912
1	B	0.34	0/2141	0.61	2/2912 (0.1%)
1	C	0.34	1/2132 (0.0%)	0.59	4/2901 (0.1%)
1	D	0.33	0/2138	0.55	0/2909
1	E	0.31	0/2141	0.52	0/2912
1	F	0.30	0/2138	0.55	0/2909
1	G	0.32	0/2138	0.57	1/2909 (0.0%)
1	H	0.35	0/2138	0.61	2/2909 (0.1%)
All	All	0.32	1/17107 (0.0%)	0.57	9/23273 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	LYS	CD-CE	5.00	1.63	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	96	LEU	CA-CB-CG	9.41	136.95	115.30
1	C	75	ILE	CG1-CB-CG2	-8.23	93.29	111.40
1	B	142	LYS	CG-CD-CE	-6.59	92.14	111.90
1	G	251	GLU	CA-CB-CG	6.47	127.64	113.40
1	C	255	LYS	CD-CE-NZ	-5.61	98.80	111.70
1	H	261	GLU	CG-CD-OE2	-5.58	107.13	118.30
1	C	255	LYS	CA-CB-CG	5.56	125.63	113.40
1	B	303	LEU	CB-CG-CD2	5.18	119.80	111.00
1	C	142	LYS	CB-CG-CD	5.08	124.80	111.60

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	2103	0	2126	20	0
1	B	2103	0	2126	36	0
1	C	2094	0	2113	20	0
1	D	2100	0	2118	26	0
1	E	2103	0	2126	21	0
1	F	2100	0	2118	29	0
1	G	2100	0	2118	22	0
1	H	2100	0	2118	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	B	6	0	8	0	0
3	E	6	0	8	0	0
4	A	13	0	0	0	0
4	B	9	0	0	0	0
4	C	15	0	0	1	0
4	D	15	0	0	0	0
4	E	11	0	0	1	0
4	F	12	0	0	0	0
4	G	13	0	0	0	0
4	H	12	0	0	3	0
All	All	16923	0	16979	189	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 6.

All (189) 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:H:99:ASP:HB3	1:H:102:LYS:HB2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:TYR:OH	1:E:234:ASP:OD1	2.11	0.68
1:H:298:LYS:HE3	1:H:299:LYS:HG2	1.76	0.68
1:H:256:ASP:OD1	4:H:501:HOH:O	2.13	0.67
1:C:160:VAL:HB	1:C:212:ALA:HA	1.75	0.66
1:F:24:ASN:HD22	1:F:24:ASN:N	1.93	0.65
1:A:114:ALA:HA	1:F:56:ASP:HB3	1.78	0.65
1:E:269:LYS:NZ	4:E:501:HOH:O	2.29	0.64
1:D:153:ILE:HG12	1:D:159:VAL:HG11	1.80	0.64
1:G:24:ASN:N	1:G:24:ASN:OD1	2.32	0.63
1:E:64:PRO:O	1:E:68:LYS:HG2	1.99	0.61
1:B:120:LEU:HB2	1:B:246:PRO:HG2	1.81	0.61
1:D:129:TRP:CE2	1:D:167:PHE:HD1	2.18	0.61
1:D:181:TYR:OH	1:D:234:ASP:OD1	2.14	0.61
1:F:120:LEU:HD12	1:F:246:PRO:HB2	1.83	0.61
1:D:295:ASP:O	1:D:299:LYS:HG2	2.01	0.60
1:F:277:ASP:O	1:F:281:ARG:HG3	2.00	0.60
1:B:125:ALA:O	1:B:243:GLN:HG2	2.02	0.60
1:B:45:THR:HG21	1:B:294:GLU:HG2	1.84	0.60
1:H:124:PRO:HG2	1:H:271:ASP:HA	1.84	0.59
1:B:53:LYS:HD2	1:G:116:LYS:HE2	1.85	0.58
1:C:175:PRO:O	1:C:179:THR:HG23	2.04	0.58
1:G:153:ILE:HG12	1:G:159:VAL:HG11	1.85	0.58
1:G:270:LEU:HD22	1:G:275:LEU:HD13	1.84	0.58
1:A:153:ILE:HG12	1:A:159:VAL:HG11	1.86	0.58
1:G:136:ASP:OD1	1:G:136:ASP:N	2.29	0.58
1:B:54:THR:O	1:G:116:LYS:NZ	2.38	0.57
1:B:124:PRO:HA	1:B:243:GLN:OE1	2.04	0.57
1:C:129:TRP:HE1	1:C:216:MSE:HG3	1.69	0.57
1:F:220:THR:HG22	1:F:272:LEU:HD12	1.86	0.57
1:A:35:GLU:OE2	1:A:220:THR:OG1	2.23	0.57
1:F:146:LEU:HD12	1:F:234:ASP:HA	1.86	0.57
1:B:78:TYR:CE1	1:B:80:GLU:HG2	2.40	0.56
1:A:43:ILE:O	1:A:47:LEU:HG	2.05	0.56
1:B:35:GLU:HG3	1:B:279:ASN:HD21	1.70	0.56
1:B:56:ASP:HB3	1:G:114:ALA:HA	1.87	0.56
1:A:160:VAL:CG2	1:A:212:ALA:HA	2.36	0.55
1:E:160:VAL:HB	1:E:212:ALA:HA	1.89	0.55
1:A:32:ILE:HD13	1:A:61:GLY:HA2	1.89	0.55
1:B:201:THR:HG21	1:B:216:MSE:HE2	1.87	0.55
1:B:135:LYS:HD3	1:B:228:GLY:HA2	1.88	0.54
1:A:160:VAL:HG22	1:A:212:ALA:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:TRP:CE2	1:E:167:PHE:HD1	2.25	0.54
1:C:152:TYR:HE2	1:C:159:VAL:HG23	1.73	0.54
1:B:169:ASN:HB3	1:H:93:ASP:O	2.08	0.53
1:H:220:THR:HG23	1:H:272:LEU:HD12	1.90	0.53
1:B:93:ASP:O	1:H:169:ASN:HB3	2.08	0.53
1:H:159:VAL:O	1:H:189:GLN:HB3	2.08	0.53
1:A:267:PHE:HA	1:A:270:LEU:HD12	1.91	0.53
1:A:145:SER:HA	1:A:233:GLU:N	2.24	0.53
1:B:145:SER:HA	1:B:233:GLU:H	1.74	0.53
1:D:201:THR:HG21	1:D:216:MSE:HE2	1.91	0.53
1:H:153:ILE:HD11	1:H:183:PHE:CD1	2.44	0.53
1:C:115:ASN:OD1	1:H:57:ARG:NH2	2.36	0.53
1:F:270:LEU:HD22	1:F:275:LEU:HD13	1.91	0.52
1:B:78:TYR:CZ	1:B:80:GLU:HG2	2.45	0.52
1:F:201:THR:HG21	1:F:216:MSE:HE2	1.91	0.52
1:D:32:ILE:HA	1:D:59:GLN:HG2	1.91	0.52
1:B:298:LYS:HB2	1:B:303:LEU:HD12	1.90	0.52
1:B:160:VAL:HB	1:B:212:ALA:HA	1.91	0.52
1:E:269:LYS:HD3	1:E:300:ASN:OD1	2.09	0.52
1:F:251:GLU:O	1:F:255:LYS:HD3	2.10	0.52
1:G:134:ARG:NH1	1:G:205:ALA:O	2.43	0.52
1:D:160:VAL:HB	1:D:212:ALA:HA	1.92	0.51
1:D:184:THR:HG23	1:D:186:LYS:HE3	1.93	0.51
1:E:191:ILE:HD12	1:E:212:ALA:HB2	1.93	0.51
1:B:227:SER:HA	1:D:207:ASN:OD1	2.10	0.50
1:H:27:ALA:HA	1:H:55:THR:HG22	1.93	0.50
1:E:31:LYS:NZ	1:E:80:GLU:OE1	2.37	0.50
1:D:257:PRO:HD2	1:D:258:LYS:NZ	2.27	0.50
1:B:93:ASP:OD2	1:H:170:SER:HB2	2.11	0.50
1:D:115:ASN:OD1	1:E:57:ARG:NH1	2.44	0.50
1:H:220:THR:HG21	1:H:275:LEU:HB3	1.94	0.50
1:A:117:ILE:HG21	1:A:247:ILE:HD12	1.93	0.50
1:G:78:TYR:CE1	1:G:247:ILE:HD11	2.47	0.50
1:F:31:LYS:NZ	1:F:80:GLU:OE1	2.40	0.49
1:H:219:GLY:O	1:H:276:GLN:NE2	2.45	0.49
1:D:108:LYS:HG3	1:D:119:TRP:HB2	1.95	0.49
1:C:32:ILE:HD12	1:C:61:GLY:HA2	1.95	0.49
1:F:24:ASN:O	1:F:25:ALA:HB2	2.13	0.49
1:B:42:ILE:HG23	1:B:297:LEU:HD21	1.95	0.49
1:D:267:PHE:HA	1:D:270:LEU:HD12	1.95	0.48
1:H:153:ILE:HD11	1:H:183:PHE:CG	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:SER:HB3	1:F:244:PRO:HG2	1.96	0.48
1:F:124:PRO:HG2	1:F:271:ASP:HA	1.95	0.48
1:H:160:VAL:HB	1:H:212:ALA:HA	1.95	0.48
1:C:146:LEU:HD12	1:C:234:ASP:HA	1.97	0.47
1:C:250:GLU:O	1:C:254:LYS:HG3	2.14	0.47
1:H:153:ILE:HG21	1:H:159:VAL:HG11	1.96	0.47
1:H:267:PHE:HA	1:H:270:LEU:HD12	1.95	0.47
1:E:283:GLN:HG2	1:E:284:LEU:HG	1.96	0.47
1:H:146:LEU:HD12	1:H:234:ASP:HA	1.96	0.47
1:A:93:ASP:O	1:C:169:ASN:HB3	2.14	0.47
1:G:57:ARG:HH22	1:G:74:GLU:HB3	1.79	0.47
1:B:53:LYS:HD2	1:G:116:LYS:CE	2.44	0.47
1:C:217:VAL:HG13	1:C:224:ILE:HD11	1.96	0.47
1:E:93:ASP:O	1:F:169:ASN:HB3	2.14	0.47
1:E:201:THR:HG21	1:E:216:MSE:HE2	1.96	0.47
1:H:140:GLU:OE1	4:H:502:HOH:O	2.20	0.47
1:C:42:ILE:HG23	1:C:297:LEU:HD21	1.96	0.46
1:E:135:LYS:HG3	1:E:136:ASP:N	2.30	0.46
1:A:145:SER:HA	1:A:233:GLU:H	1.79	0.46
1:D:30:SER:OG	1:D:31:LYS:N	2.48	0.46
1:F:78:TYR:CE2	1:F:247:ILE:HD11	2.51	0.46
1:B:149:PHE:O	1:B:153:ILE:HG13	2.15	0.46
1:E:129:TRP:HH2	1:E:166:GLU:HG2	1.79	0.46
1:G:149:PHE:HB2	1:G:232:LEU:HD13	1.98	0.46
1:F:267:PHE:HA	1:F:270:LEU:HD12	1.97	0.46
1:B:251:GLU:O	1:B:255:LYS:HD2	2.15	0.45
1:B:145:SER:HA	1:B:233:GLU:N	2.32	0.45
1:B:35:GLU:HG3	1:B:279:ASN:ND2	2.31	0.45
1:F:186:LYS:HB2	1:F:186:LYS:HE2	1.84	0.45
1:H:191:ILE:HD12	1:H:212:ALA:HB2	1.97	0.45
1:A:202:ILE:HD11	1:A:217:VAL:HG12	1.99	0.45
1:D:153:ILE:HD13	1:D:185:LEU:HD21	1.98	0.45
1:A:84:ASN:HB3	1:A:88:PHE:CZ	2.53	0.44
1:B:32:ILE:HG13	1:B:32:ILE:O	2.17	0.44
1:G:69:ALA:HA	1:G:74:GLU:HG3	1.99	0.44
1:A:78:TYR:CE1	1:A:247:ILE:HD11	2.53	0.44
1:H:159:VAL:HA	1:H:213:ASN:HD21	1.82	0.44
1:F:274:THR:O	1:F:278:LEU:HG	2.18	0.44
1:H:178:GLN:HG2	1:H:183:PHE:CE1	2.52	0.44
1:A:171:ALA:HA	1:A:175:PRO:HG2	2.00	0.44
1:D:43:ILE:O	1:D:47:LEU:HD13	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:TRP:CZ2	1:D:167:PHE:HD1	2.36	0.44
1:E:45:THR:HG21	1:E:294:GLU:HG2	1.99	0.44
1:D:124:PRO:HG2	1:D:271:ASP:HA	1.99	0.43
1:B:39:LEU:HD21	1:B:275:LEU:HD11	1.99	0.43
1:D:149:PHE:CZ	1:D:153:ILE:HD11	2.53	0.43
1:A:250:GLU:HG2	1:A:254:LYS:HE2	1.99	0.43
1:B:164:SER:HB3	1:B:216:MSE:HE1	2.00	0.43
1:B:258:LYS:O	1:B:261:GLU:HG2	2.18	0.43
1:B:270:LEU:HD22	1:B:275:LEU:HD13	2.00	0.43
1:G:35:GLU:OE1	1:G:220:THR:OG1	2.30	0.43
1:H:68:LYS:HD2	1:H:68:LYS:HA	1.85	0.43
1:F:206:ALA:HB2	1:F:227:SER:HB3	1.99	0.43
1:G:295:ASP:O	1:G:299:LYS:HG3	2.19	0.43
1:F:278:LEU:HD22	1:F:292:VAL:HG13	2.00	0.43
1:H:277:ASP:O	1:H:281:ARG:HG3	2.18	0.43
1:D:258:LYS:HD3	1:D:258:LYS:N	2.33	0.42
1:D:78:TYR:CE1	1:D:247:ILE:HD11	2.53	0.42
1:E:149:PHE:CE2	1:E:153:ILE:HD11	2.54	0.42
1:B:298:LYS:CB	1:B:303:LEU:HD12	2.49	0.42
1:C:120:LEU:HD12	1:C:246:PRO:HB2	2.00	0.42
1:E:267:PHE:HA	1:E:270:LEU:HD12	2.00	0.42
1:F:117:ILE:HG21	1:F:247:ILE:HD12	2.01	0.42
1:D:246:PRO:HG3	1:D:267:PHE:CE1	2.55	0.42
1:A:146:LEU:HD12	1:A:234:ASP:HA	2.01	0.42
1:G:57:ARG:NH2	1:G:74:GLU:HB3	2.34	0.42
1:C:198:THR:CG2	1:C:217:VAL:HA	2.50	0.42
1:G:258:LYS:HB2	1:G:258:LYS:HE2	1.78	0.42
1:H:246:PRO:HD3	1:H:267:PHE:CE2	2.54	0.42
1:D:257:PRO:HD2	1:D:258:LYS:HZ2	1.83	0.42
1:G:206:ALA:HB2	1:G:227:SER:HB3	2.01	0.42
1:C:114:ALA:HA	1:H:56:ASP:HB3	2.01	0.42
1:C:198:THR:HG21	1:C:217:VAL:HA	2.01	0.42
1:G:246:PRO:HG3	1:G:267:PHE:CE1	2.55	0.42
1:C:134:ARG:NH1	1:C:205:ALA:O	2.48	0.41
1:F:129:TRP:HE1	1:F:216:MSE:SE	2.52	0.41
1:F:149:PHE:CE2	1:F:153:ILE:HD11	2.55	0.41
1:F:224:ILE:HG23	1:F:229:LEU:HB2	2.02	0.41
1:F:275:LEU:HD12	1:F:275:LEU:HA	1.75	0.41
1:H:68:LYS:NZ	4:H:503:HOH:O	2.26	0.41
1:A:78:TYR:OH	1:A:80:GLU:OE1	2.31	0.41
1:A:201:THR:HG21	1:A:216:MSE:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ALA:O	1:B:192:THR:HA	2.20	0.41
1:D:93:ASP:O	1:G:169:ASN:HB3	2.20	0.41
1:E:149:PHE:HZ	1:E:159:VAL:HG21	1.85	0.41
1:C:75:ILE:HD13	1:C:75:ILE:HG21	1.84	0.41
1:C:78:TYR:CE1	1:C:247:ILE:HD11	2.56	0.41
1:C:49:ALA:HB2	1:C:303:LEU:HD13	2.01	0.41
1:F:133:VAL:HG12	1:F:134:ARG:O	2.21	0.41
1:G:290:LYS:HB3	1:G:290:LYS:HE2	1.73	0.41
1:H:67:ARG:HD2	1:H:88:PHE:CE1	2.56	0.41
1:C:57:ARG:NH2	4:C:503:HOH:O	2.48	0.41
1:D:114:ALA:HA	1:E:56:ASP:HB3	2.02	0.41
1:F:149:PHE:O	1:F:153:ILE:HG13	2.21	0.41
1:B:208:GLN:HA	1:B:212:ALA:O	2.21	0.40
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.87	0.40
1:E:33:ASP:N	1:E:33:ASP:OD1	2.54	0.40
1:F:35:GLU:OE1	1:F:275:LEU:HG	2.21	0.40
1:E:149:PHE:CZ	1:E:159:VAL:HG21	2.57	0.40
1:F:24:ASN:HD22	1:F:24:ASN:H	1.66	0.40
1:H:234:ASP:OD2	1:H:238:VAL:N	2.54	0.40
1:B:153:ILE:HD13	1:B:185:LEU:HD21	2.03	0.40
1:B:250:GLU:HG2	1:B:254:LYS:HE2	2.03	0.40
1:D:67:ARG:HD2	1:D:88:PHE:CE1	2.56	0.40
1:G:43:ILE:O	1:G:47:LEU:HD13	2.22	0.40
1:H:167:PHE:HB2	1:H:216:MSE:SE	2.72	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	279/282 (99%)	275 (99%)	4 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	279/282 (99%)	275 (99%)	4 (1%)	0	100	100
1	C	278/282 (99%)	274 (99%)	4 (1%)	0	100	100
1	D	279/282 (99%)	275 (99%)	4 (1%)	0	100	100
1	E	279/282 (99%)	275 (99%)	4 (1%)	0	100	100
1	F	279/282 (99%)	274 (98%)	4 (1%)	1 (0%)	34	54
1	G	279/282 (99%)	275 (99%)	4 (1%)	0	100	100
1	H	279/282 (99%)	276 (99%)	3 (1%)	0	100	100
All	All	2231/2256 (99%)	2199 (99%)	31 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	25	ALA

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	218/218 (100%)	215 (99%)	3 (1%)	67	86
1	B	218/218 (100%)	214 (98%)	4 (2%)	59	81
1	C	217/218 (100%)	216 (100%)	1 (0%)	88	96
1	D	218/218 (100%)	213 (98%)	5 (2%)	50	76
1	E	218/218 (100%)	214 (98%)	4 (2%)	59	81
1	F	218/218 (100%)	216 (99%)	2 (1%)	78	92
1	G	218/218 (100%)	211 (97%)	7 (3%)	39	65
1	H	218/218 (100%)	210 (96%)	8 (4%)	34	60
All	All	1743/1744 (100%)	1709 (98%)	34 (2%)	55	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASP
1	A	129	TRP
1	A	188	ASP
1	B	80	GLU
1	B	111	ASP
1	B	116	LYS
1	B	129	TRP
1	C	129	TRP
1	D	30	SER
1	D	111	ASP
1	D	129	TRP
1	D	158	LYS
1	D	188	ASP
1	E	55	THR
1	E	111	ASP
1	E	129	TRP
1	E	304	LYS
1	F	24	ASN
1	F	129	TRP
1	G	24	ASN
1	G	53	LYS
1	G	68	LYS
1	G	111	ASP
1	G	129	TRP
1	G	136	ASP
1	G	290	LYS
1	H	23	SER
1	H	33	ASP
1	H	53	LYS
1	H	96	LEU
1	H	111	ASP
1	H	129	TRP
1	H	276	GLN
1	H	298	LYS

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

Mol	Chain	Res	Type
1	C	50	ASN
1	C	239	GLN
1	E	48	ASN
1	E	115	ASN
1	E	178	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	24	ASN
1	G	239	GLN
1	H	178	GLN
1	H	243	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z > 2$
3	GOL	B	401	-	5,5,5	0.36	0	5,5,5	0.26	0
3	GOL	E	402	-	5,5,5	0.37	0	5,5,5	0.19	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
3	GOL	B	401	-	-	0/4/4/4	-
3	GOL	E	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	402	GOL	O1-C1-C2-C3
3	E	402	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

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	280/282 (99%)	-0.26	2 (0%) 87 89	30, 47, 62, 86	0
1	B	280/282 (99%)	-0.16	3 (1%) 80 82	27, 46, 64, 80	0
1	C	279/282 (98%)	-0.17	5 (1%) 68 71	33, 49, 72, 87	0
1	D	280/282 (99%)	-0.17	1 (0%) 92 93	28, 44, 61, 79	0
1	E	280/282 (99%)	-0.29	0 100 100	28, 44, 61, 83	0
1	F	280/282 (99%)	-0.29	1 (0%) 92 93	30, 42, 57, 88	0
1	G	280/282 (99%)	-0.07	3 (1%) 80 82	30, 46, 64, 75	0
1	H	280/282 (99%)	-0.15	2 (0%) 87 89	27, 46, 65, 95	0
All	All	2239/2256 (99%)	-0.19	17 (0%) 86 87	27, 46, 64, 95	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	143	LEU	5.1
1	A	304	LYS	3.4
1	D	23	SER	3.0
1	C	131	ILE	2.7
1	B	222	GLY	2.6
1	H	252	VAL	2.5
1	G	303	LEU	2.5
1	C	149	PHE	2.4
1	B	284	LEU	2.4
1	H	259	ILE	2.2
1	G	131	ILE	2.2
1	C	142	LYS	2.1
1	B	223	GLY	2.1
1	F	267	PHE	2.1
1	G	259	ILE	2.1
1	A	92	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	159	VAL	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 monosaccharides 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
3	GOL	E	402	6/6	0.62	0.33	97,99,101,102	0
3	GOL	B	401	6/6	0.80	0.45	61,70,72,76	0
2	CA	E	401	1/1	0.90	0.14	49,49,49,49	0
2	CA	C	401	1/1	0.95	0.17	52,52,52,52	0
2	CA	A	401	1/1	0.95	0.11	47,47,47,47	0
2	CA	H	401	1/1	0.97	0.14	46,46,46,46	0
2	CA	B	402	1/1	0.97	0.15	47,47,47,47	0
2	CA	G	401	1/1	0.97	0.14	57,57,57,57	0
2	CA	D	401	1/1	0.98	0.14	50,50,50,50	0
2	CA	F	401	1/1	0.99	0.17	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.