Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1L5X
Title	:	The 2.0-Angstrom resolution crystal structure of a survival protein E (SurE) homolog from Pyrobaculum aerophilum
Authors	:	Mura, C.; Katz, J.E.; Clarke, S.G.; Eisenberg, D.
Deposited on	:	2002-03-08
Resolution	:	2.00 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:

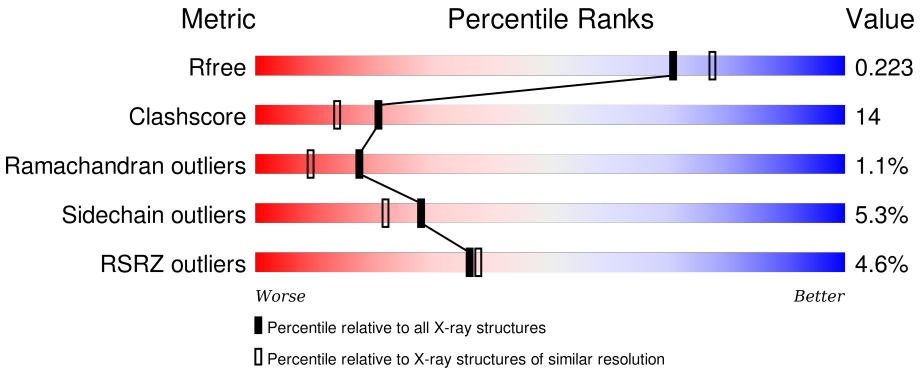
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	280	4% 74% 20%
1	B	280	5% 74% 22%

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
2	GOL	A	301	-	X	-	X
2	GOL	A	302	-	X	-	X
2	GOL	A	303	-	X	-	-
2	GOL	A	304	-	X	-	X
2	GOL	A	305	-	X	-	X
2	GOL	A	306	-	X	-	X
2	GOL	A	307	-	X	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4567 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 Survival protein E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	Se	0	0	0
			2105	1340	363	395	1	6			
1	B	278	Total	C	N	O	S	Se	0	0	0
			2125	1352	369	397	1	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
A	53	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
A	145	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
A	161	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
A	252	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
A	258	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
A	267	SER	-	SEE REMARK 999	UNP Q8ZU79
A	268	LYS	-	SEE REMARK 999	UNP Q8ZU79
A	269	LEU	-	SEE REMARK 999	UNP Q8ZU79
A	270	ALA	-	SEE REMARK 999	UNP Q8ZU79
A	271	ALA	-	SEE REMARK 999	UNP Q8ZU79
A	272	ALA	-	SEE REMARK 999	UNP Q8ZU79
A	273	LEU	-	SEE REMARK 999	UNP Q8ZU79
A	274	GLU	-	SEE REMARK 999	UNP Q8ZU79
A	275	HIS	-	SEE REMARK 999	UNP Q8ZU79
A	276	HIS	-	SEE REMARK 999	UNP Q8ZU79
A	277	HIS	-	SEE REMARK 999	UNP Q8ZU79
A	278	HIS	-	SEE REMARK 999	UNP Q8ZU79
A	279	HIS	-	SEE REMARK 999	UNP Q8ZU79
A	280	HIS	-	SEE REMARK 999	UNP Q8ZU79
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
B	53	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
B	145	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
B	161	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
B	252	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79

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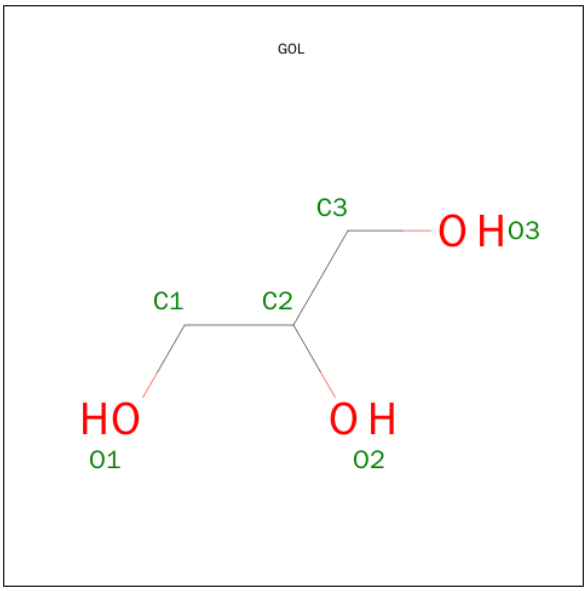
Chain	Residue	Modelled	Actual	Comment	Reference
B	258	MSE	MET	MODIFIED RESIDUE	UNP Q8ZU79
B	267	SER	-	SEE REMARK 999	UNP Q8ZU79
B	268	LYS	-	SEE REMARK 999	UNP Q8ZU79
B	269	LEU	-	SEE REMARK 999	UNP Q8ZU79
B	270	ALA	-	SEE REMARK 999	UNP Q8ZU79
B	271	ALA	-	SEE REMARK 999	UNP Q8ZU79
B	272	ALA	-	SEE REMARK 999	UNP Q8ZU79
B	273	LEU	-	SEE REMARK 999	UNP Q8ZU79
B	274	GLU	-	SEE REMARK 999	UNP Q8ZU79
B	275	HIS	-	SEE REMARK 999	UNP Q8ZU79
B	276	HIS	-	SEE REMARK 999	UNP Q8ZU79
B	277	HIS	-	SEE REMARK 999	UNP Q8ZU79
B	278	HIS	-	SEE REMARK 999	UNP Q8ZU79
B	279	HIS	-	SEE REMARK 999	UNP Q8ZU79
B	280	HIS	-	SEE REMARK 999	UNP Q8ZU79

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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	A	1	Total C O 6 3 3	0	0

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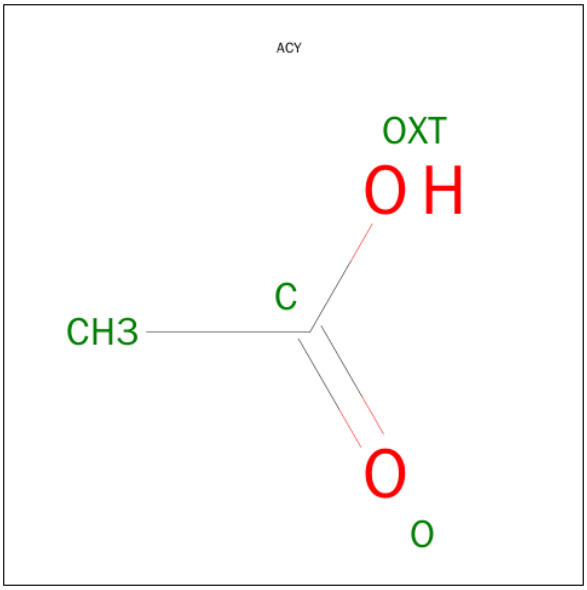
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 4 is water.

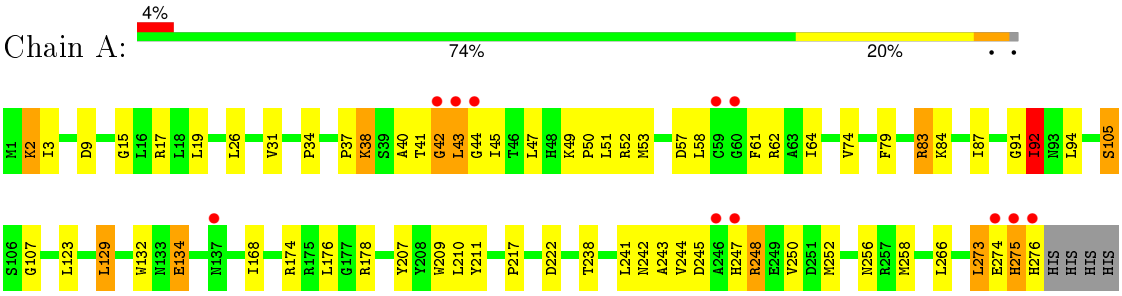
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	150	Total O 150 150	0	0
4	B	137	Total O 137 137	0	0

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.

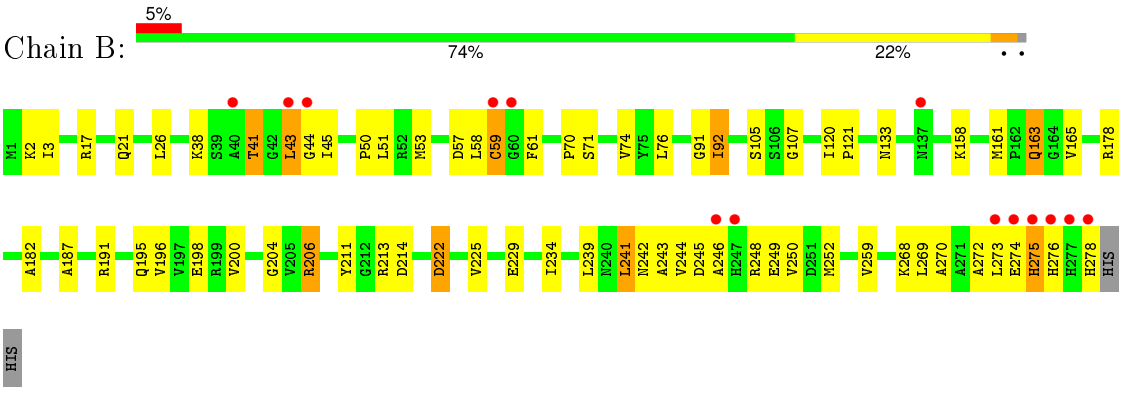
- Molecule 1: Survival protein E

Chain A:



- Molecule 1: Survival protein E

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.50Å 90.50Å 129.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.59 – 2.00 42.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.59-2.00) 96.0 (42.73-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.223 0.185 , 0.223	Depositor DCC
R_{free} test set	2033 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.7	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 42100 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4567	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, ACY

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	0.68	0/2138	0.85	7/2900 (0.2%)
1	B	0.66	0/2160	0.88	6/2930 (0.2%)
All	All	0.67	0/4298	0.86	13/5830 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	GLY	C-N-CA	11.28	149.89	121.70
1	A	92	ILE	N-CA-C	-9.35	85.75	111.00
1	B	91	GLY	CA-C-N	-9.19	96.99	117.20
1	A	91	GLY	C-N-CA	7.59	140.68	121.70
1	B	91	GLY	O-C-N	7.22	134.26	122.70
1	B	92	ILE	N-CA-C	-7.11	91.80	111.00
1	B	92	ILE	N-CA-CB	6.86	126.59	110.80
1	A	91	GLY	CA-C-N	-6.76	102.32	117.20
1	A	129	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	222	ASP	CB-CG-OD1	5.38	123.15	118.30
1	A	91	GLY	O-C-N	5.37	131.29	122.70
1	B	222	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	91	GLY	N-CA-C	5.11	125.87	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain

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	2105	0	2145	68	0
1	B	2125	0	2158	77	0
2	A	42	0	28	1	0
3	A	8	0	6	0	0
4	A	150	0	0	12	0
4	B	137	0	0	6	0
All	All	4567	0	4337	124	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 14.

All (124) 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:134:GLU:HG3	4:A:550:HOH:O	1.57	1.05
1:A:53:MSE:HE2	1:A:64:ILE:HG21	1.50	0.93
1:A:248:ARG:O	1:B:246:ALA:HB1	1.77	0.84
1:B:182:ALA:HB1	1:B:234:ILE:HD11	1.62	0.82
1:A:74:VAL:HG23	4:A:546:HOH:O	1.80	0.81
1:B:121:PRO:HB3	1:B:161:MSE:HE1	1.60	0.81
1:B:17:ARG:NH2	1:B:59:CYS:O	2.16	0.78
1:B:74:VAL:HG23	4:B:306:HOH:O	1.83	0.78
1:A:2:LYS:HG3	1:A:83:ARG:NH2	2.00	0.77
1:A:43:LEU:HD21	1:A:107:GLY:HA2	1.67	0.76
1:A:19:LEU:HB2	1:A:92:ILE:HG12	1.70	0.72
1:A:45:ILE:HG13	1:B:211:TYR:CZ	2.25	0.72
1:B:158:LYS:HE2	4:B:401:HOH:O	1.88	0.71
1:B:272:ALA:HA	1:B:275:HIS:CD2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:H	2:A:301:GOL:H11	1.53	0.71
1:A:244:VAL:HG23	1:A:245:ASP:N	2.05	0.70
1:A:211:TYR:CE2	1:B:45:ILE:HG23	2.26	0.70
1:A:244:VAL:HG23	1:A:245:ASP:H	1.57	0.69
1:A:43:LEU:HD22	4:A:544:HOH:O	1.91	0.68
1:B:121:PRO:HA	1:B:161:MSE:HE3	1.75	0.68
1:B:38:LYS:HD2	1:B:43:LEU:HD23	1.77	0.67
1:B:43:LEU:HD13	1:B:44:GLY:H	1.59	0.67
1:A:105:SER:HB3	1:B:44:GLY:CA	2.25	0.66
1:B:121:PRO:HB3	1:B:161:MSE:CE	2.24	0.66
1:B:182:ALA:HB1	1:B:234:ILE:CD1	2.25	0.66
1:A:43:LEU:HD13	4:A:543:HOH:O	1.95	0.66
1:B:43:LEU:HD21	1:B:107:GLY:HA2	1.76	0.66
1:A:252:MSE:HE1	1:B:244:VAL:HA	1.77	0.65
1:A:43:LEU:HB3	1:B:43:LEU:HB3	1.79	0.64
1:A:42:GLY:HA3	4:A:517:HOH:O	1.97	0.64
1:B:195:GLN:OE1	1:B:213:ARG:HB2	1.97	0.64
1:B:121:PRO:CB	1:B:161:MSE:HE1	2.29	0.63
1:B:276:HIS:C	1:B:278:HIS:H	2.02	0.63
1:A:243:ALA:O	1:B:250:VAL:HG21	1.99	0.63
1:A:15:GLY:O	1:A:92:ILE:HB	1.99	0.62
1:A:242:ASN:HB3	1:A:244:VAL:HG22	1.82	0.62
1:B:121:PRO:HA	1:B:161:MSE:CE	2.30	0.61
1:A:247:HIS:HB2	4:A:532:HOH:O	2.01	0.61
1:A:210:LEU:HD13	1:B:51:LEU:HD23	1.83	0.61
1:A:211:TYR:CZ	1:B:45:ILE:HG13	2.36	0.60
1:A:2:LYS:HG3	1:A:83:ARG:HH21	1.65	0.60
1:B:178:ARG:HG2	1:B:270:ALA:HB1	1.82	0.60
1:A:209:TRP:CH2	1:B:50:PRO:HD3	2.37	0.59
1:B:17:ARG:O	1:B:21:GLN:HG3	2.03	0.59
1:B:270:ALA:O	1:B:274:GLU:HG3	2.03	0.59
1:B:43:LEU:HD13	1:B:44:GLY:N	2.19	0.58
1:A:241:LEU:HD11	1:B:241:LEU:HD11	1.86	0.58
1:B:191:ARG:NH1	1:B:214:ASP:OD1	2.37	0.57
1:A:244:VAL:CG2	1:A:245:ASP:H	2.18	0.56
1:A:105:SER:HB3	1:B:44:GLY:HA2	1.87	0.56
1:A:17:ARG:NH2	1:A:58:LEU:O	2.38	0.56
1:A:178:ARG:NH1	1:A:274:GLU:HG2	2.21	0.55
1:A:47:LEU:HD22	4:B:417:HOH:O	2.05	0.55
1:A:44:GLY:HA2	4:A:543:HOH:O	2.06	0.54
1:A:274:GLU:C	1:A:276:HIS:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:OE1	1:B:206:ARG:HD3	2.07	0.53
1:A:105:SER:HB3	1:B:44:GLY:HA3	1.90	0.53
1:A:44:GLY:CA	1:B:105:SER:HB2	2.39	0.52
1:A:92:ILE:HG22	1:A:132:TRP:CH2	2.45	0.52
1:B:244:VAL:HG23	1:B:245:ASP:N	2.25	0.52
1:B:206:ARG:HH11	1:B:206:ARG:HB2	1.74	0.52
1:A:178:ARG:HG2	4:A:548:HOH:O	2.09	0.51
1:A:129:LEU:HD13	4:A:550:HOH:O	2.10	0.51
1:B:198:GLU:OE1	1:B:206:ARG:CD	2.58	0.51
1:A:275:HIS:O	1:A:276:HIS:C	2.47	0.51
1:A:250:VAL:HG21	1:B:243:ALA:O	2.10	0.51
1:B:43:LEU:CD2	1:B:107:GLY:HA2	2.41	0.51
1:A:244:VAL:CG2	1:A:245:ASP:N	2.71	0.51
1:B:268:LYS:NZ	4:B:400:HOH:O	2.44	0.51
1:A:245:ASP:O	1:A:248:ARG:HD3	2.10	0.50
1:B:234:ILE:HD13	1:B:259:VAL:HG22	1.92	0.50
1:B:58:LEU:HD12	1:B:61:PHE:CZ	2.47	0.49
1:B:158:LYS:HD2	1:B:158:LYS:N	2.28	0.48
1:B:206:ARG:NH1	4:B:347:HOH:O	2.44	0.48
1:B:225:VAL:HA	1:B:229:GLU:HB2	1.95	0.48
1:B:45:ILE:HD12	1:B:71:SER:HB3	1.95	0.48
1:A:3:ILE:CD1	1:A:26:LEU:HB2	2.44	0.48
1:B:275:HIS:ND1	1:B:275:HIS:C	2.66	0.48
1:A:87:ILE:HD11	1:A:123:LEU:CD1	2.43	0.48
1:B:182:ALA:CB	1:B:234:ILE:HD11	2.40	0.48
1:A:44:GLY:HA2	1:B:105:SER:CB	2.44	0.48
1:B:121:PRO:CA	1:B:161:MSE:HE1	2.45	0.47
1:A:44:GLY:HA3	1:B:105:SER:HB2	1.97	0.46
1:B:200:VAL:CG1	1:B:204:GLY:HA2	2.45	0.46
1:A:256:ASN:ND2	4:A:459:HOH:O	2.46	0.46
1:B:3:ILE:CD1	1:B:26:LEU:HB2	2.45	0.46
1:B:121:PRO:CA	1:B:161:MSE:CE	2.94	0.45
1:A:274:GLU:C	1:A:276:HIS:N	2.69	0.45
1:A:44:GLY:HA2	1:B:105:SER:HB3	1.98	0.45
1:A:273:LEU:C	1:A:275:HIS:H	2.19	0.45
1:A:9:ASP:O	1:A:37:PRO:HG3	2.17	0.45
1:A:84:LYS:HA	4:A:538:HOH:O	2.18	0.44
1:A:41:THR:O	1:A:42:GLY:O	2.36	0.44
1:B:242:ASN:HB3	1:B:244:VAL:HG22	2.00	0.43
1:B:121:PRO:CB	1:B:161:MSE:CE	2.93	0.43
1:A:38:LYS:HA	1:A:41:THR:OG1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:CD1	1:B:259:VAL:HG22	2.47	0.43
1:B:187:ALA:HA	1:B:222:ASP:CG	2.39	0.43
1:B:244:VAL:HG23	1:B:245:ASP:H	1.82	0.43
1:A:45:ILE:CG2	1:A:47:LEU:HG	2.49	0.42
1:B:178:ARG:HG2	1:B:270:ALA:CB	2.48	0.42
1:A:34:PRO:HD2	4:A:456:HOH:O	2.18	0.42
1:B:269:LEU:O	1:B:273:LEU:HD23	2.19	0.42
1:B:38:LYS:O	1:B:41:THR:O	2.36	0.42
1:A:49:LYS:HB2	1:A:50:PRO:HD2	2.01	0.42
1:B:275:HIS:O	1:B:278:HIS:HB2	2.18	0.42
1:A:57:ASP:OD2	1:A:62:ARG:NH1	2.53	0.42
1:A:248:ARG:NH2	1:B:248:ARG:NH1	2.67	0.42
1:A:211:TYR:CD2	1:B:45:ILE:HG23	2.54	0.42
1:B:53:MSE:HE2	1:B:76:LEU:HD22	2.02	0.41
1:B:161:MSE:HG2	1:B:165:VAL:O	2.21	0.41
1:B:163:GLN:NE2	1:B:249:GLU:O	2.54	0.41
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.88	0.41
1:B:276:HIS:C	1:B:278:HIS:N	2.71	0.41
1:B:239:LEU:HA	1:B:239:LEU:HD23	1.74	0.41
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.96	0.41
1:A:168:ILE:HD13	1:A:258:MSE:SE	2.71	0.41
1:B:133:ASN:HD22	1:B:133:ASN:HA	1.73	0.40
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.95	0.40
1:B:120:ILE:HA	1:B:121:PRO:HD3	1.97	0.40
1:B:70:PRO:HD2	4:B:378:HOH:O	2.20	0.40
1:A:92:ILE:HG23	1:A:92:ILE:HD12	1.88	0.40
1:A:274:GLU:O	1:A:276:HIS:N	2.54	0.40
1:A:79:PHE:CD1	1:B:196:VAL:HB	2.57	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	274/280 (98%)	257 (94%)	13 (5%)	4 (2%)	13 5
1	B	276/280 (99%)	267 (97%)	7 (2%)	2 (1%)	26 19
All	All	550/560 (98%)	524 (95%)	20 (4%)	6 (1%)	17 9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ILE
1	B	92	ILE
1	A	42	GLY
1	B	59	CYS
1	A	40	ALA
1	A	275	HIS

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	225/223 (101%)	210 (93%)	15 (7%)	20 14
1	B	227/223 (102%)	218 (96%)	9 (4%)	38 33
All	All	452/446 (101%)	428 (95%)	24 (5%)	28 22

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	38	LYS
1	A	43	LEU
1	A	51	LEU
1	A	52	ARG
1	A	61	PHE
1	A	83	ARG
1	A	94	LEU
1	A	105	SER
1	A	134	GLU

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Mol	Chain	Res	Type
1	A	174	ARG
1	A	217	PRO
1	A	238	THR
1	A	248	ARG
1	A	273	LEU
1	B	2	LYS
1	B	41	THR
1	B	43	LEU
1	B	57	ASP
1	B	163	GLN
1	B	206	ARG
1	B	241	LEU
1	B	252	MSE
1	B	275	HIS

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

Mol	Chain	Res	Type
1	A	48	HIS
1	A	163	GLN
1	A	256	ASN
1	A	276	HIS
1	B	12	HIS
1	B	133	ASN
1	B	137	ASN
1	B	159	ASN
1	B	256	ASN

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 (i)

9 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	A	301	-	5,5,5	4.74	5 (100%)	5,5,5	5.68	3 (60%)
2	GOL	A	302	-	5,5,5	4.90	5 (100%)	5,5,5	5.57	3 (60%)
2	GOL	A	303	-	5,5,5	4.69	5 (100%)	5,5,5	5.72	3 (60%)
2	GOL	A	304	-	5,5,5	4.73	5 (100%)	5,5,5	5.63	3 (60%)
2	GOL	A	305	-	5,5,5	4.93	5 (100%)	5,5,5	5.63	3 (60%)
2	GOL	A	306	-	5,5,5	4.87	5 (100%)	5,5,5	5.75	3 (60%)
2	GOL	A	307	-	5,5,5	4.82	5 (100%)	5,5,5	5.70	3 (60%)
3	ACY	A	401	-	1,3,3	2.85	1 (100%)	0,3,3	0.00	-
3	ACY	A	402	-	1,3,3	1.97	0	0,3,3	0.00	-

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	301	-	-	0/4/4/4	0/0/0/0
2	GOL	A	302	-	-	0/4/4/4	0/0/0/0
2	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	GOL	A	304	-	-	0/4/4/4	0/0/0/0
2	GOL	A	305	-	-	0/4/4/4	0/0/0/0
2	GOL	A	306	-	-	0/4/4/4	0/0/0/0
2	GOL	A	307	-	-	0/4/4/4	0/0/0/0
3	ACY	A	401	-	-	0/0/0/0	0/0/0/0
3	ACY	A	402	-	-	0/0/0/0	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	GOL	C3-C2	-8.46	1.20	1.52
2	A	305	GOL	C3-C2	-8.30	1.20	1.52
2	A	307	GOL	C3-C2	-8.22	1.20	1.52
2	A	306	GOL	C3-C2	-8.18	1.21	1.52
2	A	304	GOL	C3-C2	-7.99	1.21	1.52
2	A	301	GOL	C3-C2	-7.97	1.21	1.52
2	A	303	GOL	C3-C2	-7.95	1.22	1.52
2	A	305	GOL	O2-C2	-3.57	1.32	1.43
2	A	301	GOL	C1-C2	-3.30	1.39	1.52
2	A	307	GOL	C1-C2	-3.23	1.40	1.52
2	A	306	GOL	C1-C2	-3.17	1.40	1.52
2	A	303	GOL	C1-C2	-3.10	1.40	1.52
2	A	302	GOL	C1-C2	-3.07	1.40	1.52
2	A	306	GOL	O2-C2	-3.03	1.34	1.43
2	A	305	GOL	C1-C2	-2.97	1.41	1.52
2	A	302	GOL	O2-C2	-2.89	1.34	1.43
2	A	304	GOL	C1-C2	-2.77	1.41	1.52
2	A	303	GOL	O2-C2	-2.69	1.35	1.43
2	A	304	GOL	O2-C2	-2.59	1.35	1.43
2	A	301	GOL	O2-C2	-2.59	1.35	1.43
2	A	307	GOL	O2-C2	-2.55	1.35	1.43
3	A	401	ACY	CH3-C	2.85	1.52	1.48
2	A	305	GOL	O3-C3	3.03	1.55	1.42
2	A	302	GOL	O3-C3	3.23	1.56	1.42
2	A	303	GOL	O3-C3	3.33	1.56	1.42
2	A	306	GOL	O3-C3	3.35	1.56	1.42
2	A	307	GOL	O3-C3	3.37	1.56	1.42
2	A	304	GOL	O3-C3	3.40	1.57	1.42
2	A	301	GOL	O3-C3	3.44	1.57	1.42
2	A	303	GOL	O1-C1	4.36	1.61	1.42
2	A	301	GOL	O1-C1	4.38	1.61	1.42
2	A	307	GOL	O1-C1	4.49	1.61	1.42
2	A	302	GOL	O1-C1	4.51	1.61	1.42
2	A	306	GOL	O1-C1	4.58	1.62	1.42
2	A	305	GOL	O1-C1	4.66	1.62	1.42
2	A	304	GOL	O1-C1	4.68	1.62	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	GOL	O1-C1-C2	3.16	125.48	110.18
2	A	306	GOL	O1-C1-C2	3.16	125.52	110.18
2	A	307	GOL	O1-C1-C2	3.22	125.82	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	GOL	O1-C1-C2	3.23	125.83	110.18
2	A	304	GOL	O1-C1-C2	3.31	126.24	110.18
2	A	305	GOL	O1-C1-C2	3.35	126.44	110.18
2	A	303	GOL	O1-C1-C2	3.39	126.64	110.18
2	A	305	GOL	O2-C2-C3	6.34	137.71	108.65
2	A	302	GOL	O2-C2-C3	6.35	137.79	108.65
2	A	304	GOL	O2-C2-C3	6.37	137.84	108.65
2	A	306	GOL	O2-C2-C3	6.51	138.50	108.65
2	A	303	GOL	O2-C2-C3	6.54	138.64	108.65
2	A	301	GOL	O2-C2-C3	6.55	138.69	108.65
2	A	307	GOL	O2-C2-C3	6.58	138.83	108.65
2	A	302	GOL	O3-C3-C2	10.18	159.54	110.18
2	A	304	GOL	O3-C3-C2	10.31	160.19	110.18
2	A	305	GOL	O3-C3-C2	10.33	160.28	110.18
2	A	307	GOL	O3-C3-C2	10.36	160.42	110.18
2	A	301	GOL	O3-C3-C2	10.37	160.49	110.18
2	A	303	GOL	O3-C3-C2	10.42	160.74	110.18
2	A	306	GOL	O3-C3-C2	10.58	161.48	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	270/280 (96%)	-0.22	11 (4%)	41	42	19, 30, 61, 93	0
1	B	272/280 (97%)	-0.13	14 (5%)	32	33	20, 33, 65, 106	0
All	All	542/560 (96%)	-0.18	25 (4%)	36	38	19, 31, 62, 106	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	HIS	6.8
1	B	275	HIS	6.5
1	B	246	ALA	5.7
1	B	277	HIS	5.3
1	B	247	HIS	4.8
1	B	278	HIS	4.4
1	A	59	CYS	4.1
1	B	59	CYS	4.0
1	A	276	HIS	3.9
1	B	43	LEU	3.1
1	A	247	HIS	3.1
1	A	274	GLU	2.9
1	A	60	GLY	2.9
1	A	43	LEU	2.9
1	A	137	ASN	2.8
1	B	60	GLY	2.7
1	A	42	GLY	2.6
1	A	275	HIS	2.6
1	A	246	ALA	2.4
1	B	44	GLY	2.3
1	B	40	ALA	2.3
1	B	137	ASN	2.3
1	B	273	LEU	2.2
1	B	274	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	44	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 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
2	GOL	A	306	6/6	0.61	0.36	9.84	89,90,91,92	0
2	GOL	A	305	6/6	0.71	0.25	9.13	65,69,70,72	0
2	GOL	A	304	6/6	0.78	0.20	4.57	71,71,72,72	0
2	GOL	A	301	6/6	0.54	0.25	3.28	92,93,94,95	0
2	GOL	A	302	6/6	0.84	0.16	2.40	65,66,67,68	0
2	GOL	A	307	6/6	0.93	0.27	2.22	54,56,57,59	0
3	ACY	A	401	4/4	0.77	0.24	0.96	50,51,52,53	0
3	ACY	A	402	4/4	0.83	0.15	0.65	66,67,67,67	0
2	GOL	A	303	6/6	0.66	0.27	-	63,68,68,69	0

6.5 Other polymers (i)

There are no such residues in this entry.