



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:52 AM GMT

PDB ID : 2V43  
Title : CRYSTAL STRUCTURE OF RSEB: A SENSOR FOR PERIPLASMIC STRESS RESPONSE IN E. COLI  
Authors : Wollmann, P.; Zeth, K.  
Deposited on : 2007-06-27  
Resolution : 2.37 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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

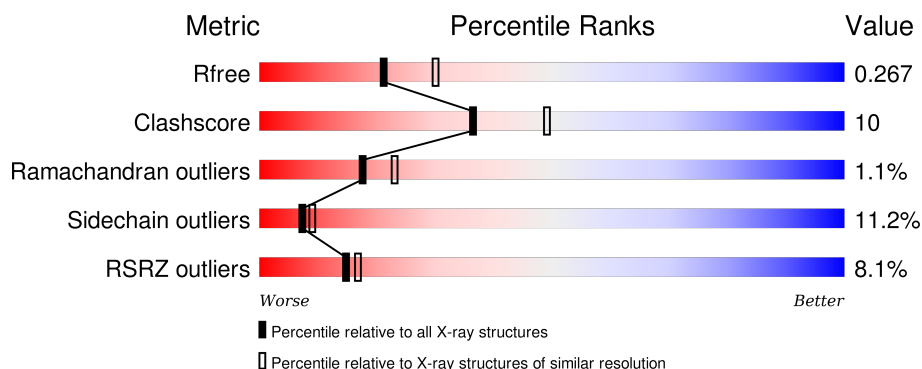
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	303	<div> <div>7%</div> <div>63% 19% •• 14%</div> </div>
1	B	303	<div> <div>3%</div> <div>67% 19% 5% 9%</div> </div>
1	C	303	<div> <div>12%</div> <div>67% 19% •• 9%</div> </div>

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	CYS	A	1315	-	-	X	X
2	CYS	A	1316	-	-	-	X
2	CYS	B	1317	-	-	-	X
2	CYS	B	1318	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6687 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.

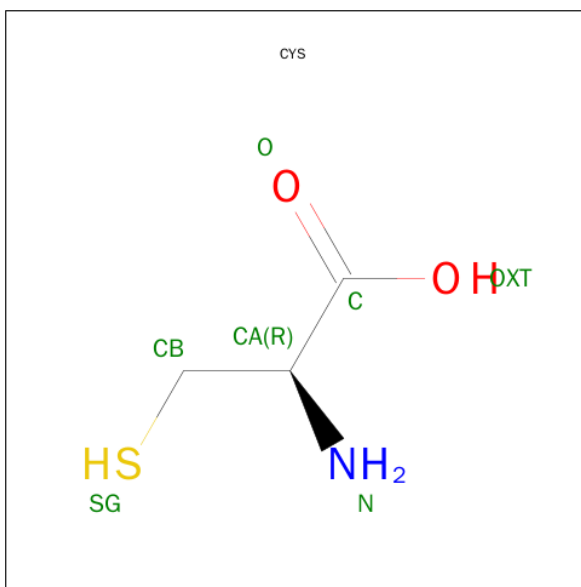
- Molecule 1 is a protein called SIGMA-E FACTOR REGULATORY PROTEIN RSEB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2077	1307	365	398	7			
1	B	276	Total	C	N	O	S	0	0	0
			2201	1382	391	420	8			
1	C	276	Total	C	N	O	S	0	1	0
			2187	1374	391	413	9			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	EXPRESSION TAG	UNP P0AFX9
A	319	HIS	-	EXPRESSION TAG	UNP P0AFX9
A	320	HIS	-	EXPRESSION TAG	UNP P0AFX9
A	321	HIS	-	EXPRESSION TAG	UNP P0AFX9
A	322	HIS	-	EXPRESSION TAG	UNP P0AFX9
A	323	HIS	-	EXPRESSION TAG	UNP P0AFX9
A	324	HIS	-	EXPRESSION TAG	UNP P0AFX9
B	22	MET	-	EXPRESSION TAG	UNP P0AFX9
B	319	HIS	-	EXPRESSION TAG	UNP P0AFX9
B	320	HIS	-	EXPRESSION TAG	UNP P0AFX9
B	321	HIS	-	EXPRESSION TAG	UNP P0AFX9
B	322	HIS	-	EXPRESSION TAG	UNP P0AFX9
B	323	HIS	-	EXPRESSION TAG	UNP P0AFX9
B	324	HIS	-	EXPRESSION TAG	UNP P0AFX9
C	22	MET	-	EXPRESSION TAG	UNP P0AFX9
C	319	HIS	-	EXPRESSION TAG	UNP P0AFX9
C	320	HIS	-	EXPRESSION TAG	UNP P0AFX9
C	321	HIS	-	EXPRESSION TAG	UNP P0AFX9
C	322	HIS	-	EXPRESSION TAG	UNP P0AFX9
C	323	HIS	-	EXPRESSION TAG	UNP P0AFX9
C	324	HIS	-	EXPRESSION TAG	UNP P0AFX9

- Molecule 2 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

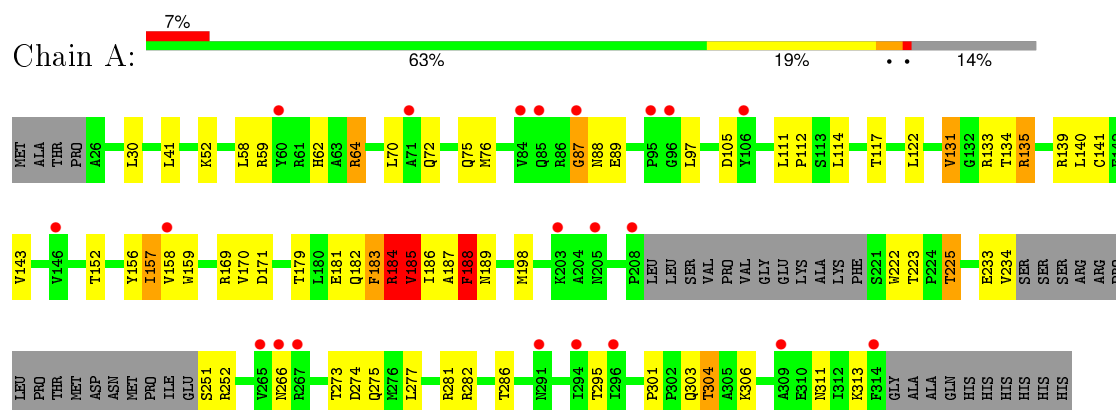
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	76	Total	O	0	0
			76	76		
3	C	37	Total	O	0	0
			37	37		

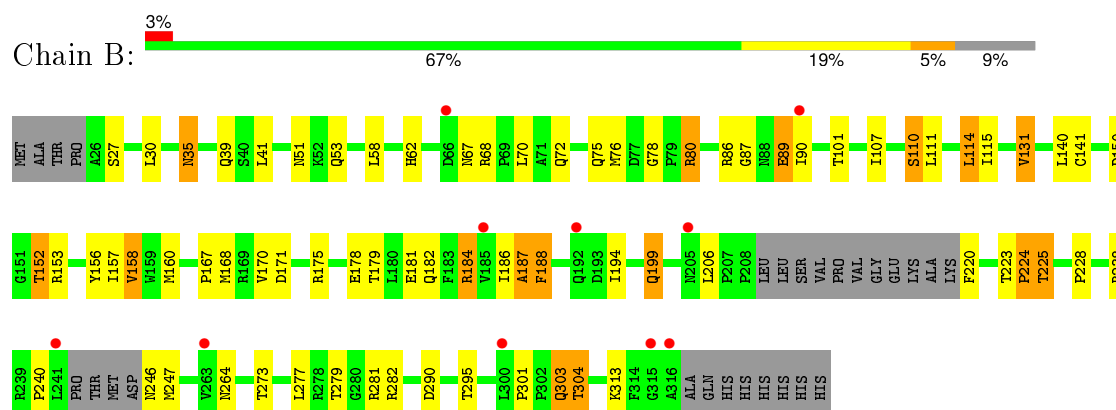
### 3 Residue-property plots [i](#)

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.

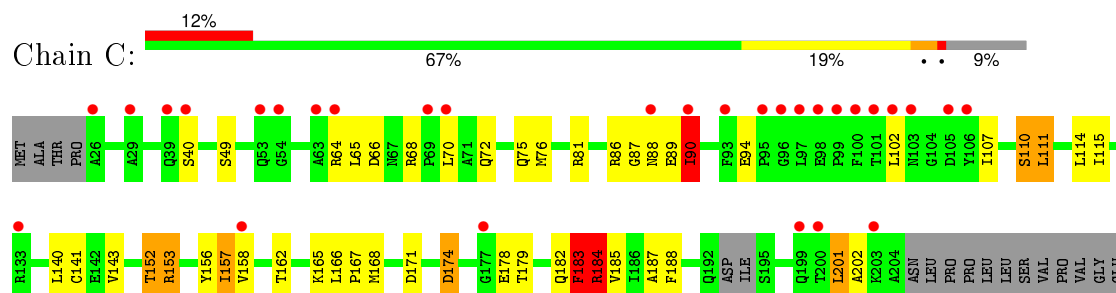
#### • Molecule 1: SIGMA-E FACTOR REGULATORY PROTEIN RSEB

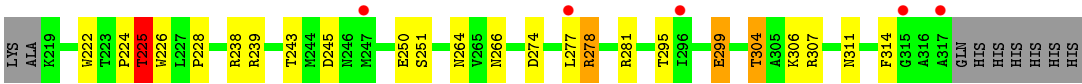


#### • Molecule 1: SIGMA-E FACTOR REGULATORY PROTEIN RSEB



#### • Molecule 1: SIGMA-E FACTOR REGULATORY PROTEIN RSEB





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.60Å 200.70Å 109.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.37 19.84 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.37) 98.5 (19.84-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.228 , 0.278 0.220 , 0.267	Depositor DCC
$R_{free}$ test set	2205 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43629 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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	0.56	1/2116 (0.0%)	0.85	10/2870 (0.3%)
1	B	0.56	1/2243 (0.0%)	0.86	10/3040 (0.3%)
1	C	0.46	0/2228	0.74	6/3018 (0.2%)
All	All	0.53	2/6587 (0.0%)	0.82	26/8928 (0.3%)

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	7
1	B	0	7
1	C	0	6
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	ASN	CG-ND2	6.67	1.49	1.32
1	A	313	LYS	C-N	5.54	1.46	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	THR	N-CA-C	-8.16	88.96	111.00
1	B	224	PRO	N-CA-C	8.15	133.29	112.10
1	A	185	VAL	N-CA-C	7.95	132.46	111.00
1	B	90	ILE	N-CA-C	7.57	131.43	111.00
1	A	184	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	C	76	MET	N-CA-C	-7.12	91.76	111.00
1	B	225	THR	N-CA-C	-7.03	92.02	111.00
1	B	225	THR	N-CA-CB	6.26	122.19	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	LEU	CA-CB-CG	6.16	129.47	115.30
1	C	157	ILE	N-CA-C	6.11	127.49	111.00
1	B	76	MET	N-CA-C	-5.91	95.04	111.00
1	B	188	PHE	N-CA-CB	5.90	121.21	110.60
1	A	184	ARG	N-CA-C	-5.85	95.20	111.00
1	A	76	MET	N-CA-C	-5.83	95.26	111.00
1	A	157	ILE	N-CA-C	5.69	126.36	111.00
1	C	184	ARG	N-CA-CB	5.68	120.82	110.60
1	B	187	ALA	N-CA-CB	-5.65	102.19	110.10
1	C	90	ILE	N-CA-C	-5.57	95.95	111.00
1	A	186	ILE	N-CA-C	-5.56	95.99	111.00
1	A	87	GLY	N-CA-C	-5.38	99.65	113.10
1	C	114	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	184	ARG	N-CA-CB	5.32	120.17	110.60
1	A	184	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	184	ARG	N-CA-CB	-5.12	101.38	110.60
1	B	157	ILE	N-CA-C	5.10	124.78	111.00
1	A	188	PHE	N-CA-CB	5.10	119.78	110.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	TYR	Peptide
1	A	183	PHE	Peptide
1	A	184	ARG	Peptide
1	A	185	VAL	Peptide
1	A	187	ALA	Peptide
1	A	75	GLN	Peptide
1	A	87	GLY	Peptide
1	B	156	TYR	Peptide
1	B	186	ILE	Peptide
1	B	187	ALA	Peptide
1	B	223	THR	Peptide
1	B	224	PRO	Peptide
1	B	75	GLN	Peptide
1	B	89	GLU	Peptide
1	C	156	TYR	Peptide
1	C	183	PHE	Peptide
1	C	187	ALA	Peptide
1	C	224	PRO	Peptide
1	C	75	GLN	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	C	89	GLU	Peptide

## 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	2077	0	2049	45	0
1	B	2201	0	2179	38	0
1	C	2187	0	2159	43	0
2	A	14	0	8	6	0
2	B	14	0	8	3	0
3	A	81	0	0	1	0
3	B	76	0	0	1	0
3	C	37	0	0	3	0
All	All	6687	0	6403	123	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 10.

All (123) 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:C:225:THR:HB	1:C:311:ASN:O	1.54	1.06
1:C:152:THR:HG21	1:C:228:PRO:HB3	1.40	1.00
1:A:183:PHE:HB2	2:A:1315:CYS:HB2	1.41	0.99
1:B:301:PRO:HB3	2:B:1317:CYS:HB3	1.47	0.96
1:C:182:GLN:NE2	1:C:184:ARG:HD3	1.81	0.95
1:C:152:THR:CG2	1:C:153:ARG:HD2	1.98	0.94
1:B:152:THR:HG22	1:B:153:ARG:HD2	1.50	0.93
1:A:183:PHE:CB	2:A:1315:CYS:HB2	2.00	0.91
1:A:182:GLN:HE22	1:A:184:ARG:HH11	1.18	0.90
1:A:64:ARG:HG2	1:A:64:ARG:HH11	1.34	0.90
1:A:182:GLN:NE2	1:A:184:ARG:HD3	1.89	0.87
1:B:182:GLN:HE22	1:B:184:ARG:HH11	1.20	0.86
1:A:152:THR:O	1:A:304:THR:HG21	1.79	0.83
1:B:152:THR:O	1:B:304:THR:HG21	1.78	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASP:OD1	1:C:182:GLN:HG3	1.81	0.81
1:B:152:THR:HG21	1:B:228:PRO:HB3	1.63	0.80
1:B:107:ILE:O	1:B:110:SER:HB2	1.81	0.79
1:C:182:GLN:HE22	1:C:184:ARG:HD3	1.46	0.78
1:A:112:PRO:HG3	2:A:1315:CYS:HB3	1.67	0.77
1:C:152:THR:HG23	1:C:153:ARG:HD2	1.68	0.76
1:A:225:THR:HB	1:A:311:ASN:O	1.85	0.76
1:C:152:THR:O	1:C:304:THR:HG21	1.86	0.75
1:A:59:ARG:HH21	1:A:72:GLN:HE22	1.34	0.74
1:A:64:ARG:HG2	1:A:64:ARG:NH1	1.97	0.74
1:B:295:THR:HG22	3:B:2072:HOH:O	1.88	0.74
1:A:182:GLN:HE21	1:A:184:ARG:HD3	1.51	0.73
1:C:152:THR:HG22	1:C:153:ARG:HD2	1.73	0.69
1:A:234:VAL:HG13	1:C:66:ASP:HB3	1.74	0.69
1:C:115:ILE:HG12	1:C:167:PRO:HG3	1.75	0.69
1:B:35:ASN:C	1:B:35:ASN:HD22	1.96	0.69
1:B:27:SER:H	2:B:1318:CYS:HB2	1.57	0.68
1:B:181:GLU:OE1	1:B:281:ARG:NH2	2.25	0.67
1:B:182:GLN:NE2	1:B:184:ARG:HD3	2.10	0.67
1:C:143:VAL:HG12	1:C:157:ILE:HD11	1.76	0.65
1:B:150:ASP:OD1	1:B:152:THR:HB	1.97	0.65
1:A:41:LEU:O	1:A:62:HIS:HD2	1.81	0.64
1:C:281:ARG:HG2	1:C:299:GLU:HG3	1.80	0.64
1:A:182:GLN:HE22	1:A:184:ARG:NH1	1.94	0.63
1:C:182:GLN:HE22	1:C:184:ARG:HH11	1.46	0.63
1:C:110:SER:OG	1:C:111:LEU:N	2.32	0.63
1:C:70:LEU:HD21	1:C:202:ALA:HB2	1.80	0.62
1:A:143:VAL:CG1	1:A:157:ILE:HD11	2.29	0.62
1:C:81:ARG:HB3	1:C:81:ARG:HH11	1.65	0.61
1:A:275:GLN:HG2	1:A:286:THR:HB	1.80	0.61
1:B:182:GLN:HE21	1:B:184:ARG:HD3	1.65	0.61
1:B:264:ASN:HB2	1:B:295:THR:HG23	1.83	0.60
1:C:40:SER:HA	1:C:64:ARG:HD2	1.84	0.60
1:C:143:VAL:CG1	1:C:157:ILE:HD11	2.32	0.59
1:B:41:LEU:O	1:B:62:HIS:HD2	1.86	0.58
1:A:273:THR:O	1:A:286:THR:HG22	2.02	0.58
1:A:198:MET:CE	3:A:2021:HOH:O	2.53	0.57
1:C:281:ARG:HG2	1:C:299:GLU:CG	2.35	0.56
1:A:135:ARG:HG3	1:B:78:GLY:O	2.06	0.56
1:B:35:ASN:C	1:B:35:ASN:ND2	2.59	0.56
1:A:233:GLU:OE2	1:A:252:ARG:HG2	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:THR:HG22	1:C:153:ARG:CD	2.36	0.55
1:C:251:SER:OG	1:C:264:ASN:ND2	2.36	0.55
1:B:152:THR:HG22	1:B:153:ARG:CD	2.30	0.55
1:C:182:GLN:HE21	1:C:184:ARG:HD3	1.68	0.54
1:B:194:ILE:HG12	1:B:199:GLN:HG2	1.88	0.54
1:B:301:PRO:CB	2:B:1317:CYS:HB3	2.30	0.54
1:A:133:ARG:CB	1:A:141:CYS:O	2.54	0.54
1:C:162:THR:O	1:C:165:LYS:HE3	2.07	0.54
1:A:181:GLU:OE2	1:A:281:ARG:HG3	2.07	0.54
1:A:59:ARG:HH21	1:A:72:GLN:NE2	2.05	0.54
1:C:182:GLN:HE21	1:C:184:ARG:HB2	1.73	0.54
1:C:183:PHE:C	1:C:183:PHE:CD2	2.81	0.53
1:B:152:THR:CG2	1:B:153:ARG:HD2	2.33	0.53
1:C:107:ILE:O	1:C:110:SER:HB3	2.09	0.52
1:B:89:GLU:HB3	1:B:101:THR:CG2	2.40	0.52
1:C:81:ARG:HG2	1:C:94:GLU:HG3	1.92	0.51
1:A:183:PHE:HB3	2:A:1315:CYS:HB2	1.86	0.51
1:A:301:PRO:HB2	1:A:304:THR:HG23	1.93	0.50
1:B:115:ILE:HG12	1:B:167:PRO:HG3	1.94	0.49
1:A:143:VAL:HG12	1:A:157:ILE:HD11	1.94	0.48
1:A:139:ARG:CZ	1:A:188:PHE:HE1	2.25	0.48
1:A:222:TRP:CH2	1:A:252:ARG:HD3	2.49	0.48
1:A:133:ARG:HA	1:A:143:VAL:HG23	1.96	0.47
1:C:174:ASP:HB2	1:C:178:GLU:O	2.14	0.47
1:A:112:PRO:CG	2:A:1315:CYS:HB3	2.41	0.47
1:A:64:ARG:HH11	1:A:64:ARG:CG	2.14	0.47
1:C:295:THR:HG22	3:C:2027:HOH:O	2.15	0.47
1:A:158:VAL:HG13	1:A:170:VAL:HG22	1.96	0.46
1:C:174:ASP:OD2	1:C:278:ARG:NH2	2.48	0.46
1:A:112:PRO:HG3	2:A:1315:CYS:CB	2.41	0.46
1:C:86:ARG:HD3	1:C:202:ALA:HA	1.97	0.46
1:B:89:GLU:HB3	1:B:101:THR:HG21	1.96	0.46
1:A:133:ARG:HB3	1:A:141:CYS:O	2.15	0.46
1:B:175:ARG:HH12	1:B:303:GLN:NE2	2.14	0.45
1:B:152:THR:HG21	1:B:228:PRO:CB	2.41	0.45
1:C:86:ARG:HG3	1:C:201:LEU:HD22	1.98	0.45
1:C:250:GLU:O	1:C:264:ASN:HA	2.17	0.45
1:A:171:ASP:OD1	1:A:182:GLN:HG3	2.16	0.45
1:A:303:GLN:HA	1:A:306:LYS:HE2	1.99	0.45
1:B:225:THR:HG21	1:B:313:LYS:CG	2.47	0.44
1:B:141:CYS:SG	1:B:168:MET:HG3	2.58	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:HG2	3:C:2025:HOH:O	2.18	0.44
1:C:266:ASN:ND2	3:C:2027:HOH:O	2.50	0.44
1:C:238:ARG:HD3	1:C:250:GLU:HG2	2.00	0.44
1:A:117:THR:HG21	1:A:122:LEU:HD22	1.98	0.44
1:B:158:VAL:HG13	1:B:170:VAL:HG22	2.00	0.43
1:B:131:VAL:HG22	1:B:131:VAL:O	2.18	0.43
1:A:182:GLN:HE21	1:A:184:ARG:HB2	1.83	0.43
1:C:226:TRP:CE3	1:C:307:ARG:HG2	2.54	0.43
1:B:51:ASN:OD1	1:B:53:GLN:HB2	2.19	0.42
1:C:65:LEU:O	1:C:68:ARG:HB3	2.19	0.42
1:A:135:ARG:CZ	1:B:80:ARG:HG3	2.49	0.42
1:C:141:CYS:SG	1:C:168:MET:HG3	2.60	0.42
1:C:90:ILE:HD13	1:C:90:ILE:HA	1.95	0.42
1:C:166:LEU:HD12	1:C:188:PHE:HE2	1.85	0.42
1:B:279:THR:OG1	1:B:282:ARG:HB3	2.20	0.41
1:A:59:ARG:NH2	1:A:72:GLN:HE22	2.10	0.41
1:A:169:ARG:HA	1:A:183:PHE:O	2.21	0.41
1:B:131:VAL:O	1:B:131:VAL:CG2	2.69	0.41
1:C:222:TRP:HB3	1:C:314:PHE:CD2	2.56	0.41
1:B:264:ASN:HB2	1:B:295:THR:CG2	2.48	0.41
1:B:175:ARG:HD3	1:B:301:PRO:CG	2.51	0.40
1:A:182:GLN:HE22	1:A:184:ARG:HD3	1.79	0.40
1:B:171:ASP:OD1	1:B:182:GLN:HG3	2.21	0.40
1:A:157:ILE:HG12	1:A:159:TRP:CZ3	2.56	0.40
1:A:131:VAL:HG12	1:A:143:VAL:HB	2.04	0.40
1:A:117:THR:HG21	1:A:122:LEU:CD2	2.51	0.40
1:B:68:ARG:NH1	1:B:86:ARG:HG2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	255/303 (84%)	244 (96%)	9 (4%)	2 (1%)	24	33
1	B	270/303 (89%)	258 (96%)	9 (3%)	3 (1%)	17	23
1	C	271/303 (89%)	258 (95%)	9 (3%)	4 (2%)	13	15
All	All	796/909 (88%)	760 (96%)	27 (3%)	9 (1%)	17	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	PRO
1	C	90	ILE
1	A	188	PHE
1	B	188	PHE
1	A	88	ASN
1	C	174	ASP
1	C	184	ARG
1	B	87	GLY
1	C	87	GLY

### 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	231/270 (86%)	204 (88%)	27 (12%)	7	8
1	B	246/270 (91%)	218 (89%)	28 (11%)	7	9
1	C	240/270 (89%)	216 (90%)	24 (10%)	9	12
All	All	717/810 (88%)	638 (89%)	79 (11%)	7	10

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	52	LYS
1	A	58	LEU
1	A	64	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	70	LEU
1	A	89	GLU
1	A	97	LEU
1	A	105	ASP
1	A	111	LEU
1	A	114	LEU
1	A	131	VAL
1	A	134	THR
1	A	135	ARG
1	A	140	LEU
1	A	179	THR
1	A	184	ARG
1	A	185	VAL
1	A	189	ASN
1	A	223	THR
1	A	225	THR
1	A	251	SER
1	A	266	ASN
1	A	274	ASP
1	A	277	LEU
1	A	282	ARG
1	A	295	THR
1	A	304	THR
1	B	30	LEU
1	B	35	ASN
1	B	39	GLN
1	B	58	LEU
1	B	67	ASN
1	B	70	LEU
1	B	72	GLN
1	B	80	ARG
1	B	110	SER
1	B	111	LEU
1	B	114	LEU
1	B	131	VAL
1	B	140	LEU
1	B	152	THR
1	B	158	VAL
1	B	160	MET
1	B	178	GLU
1	B	179	THR
1	B	199	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	206	LEU
1	B	220	PHE
1	B	238	ARG
1	B	247	MET
1	B	273	THR
1	B	277	LEU
1	B	290	ASP
1	B	303	GLN
1	B	304	THR
1	C	49	SER
1	C	72	GLN
1	C	88	ASN
1	C	102	LEU
1	C	110	SER
1	C	111	LEU
1	C	140	LEU
1	C	152	THR
1	C	153	ARG
1	C	158	VAL
1	C	179	THR
1	C	183	PHE
1	C	184	ARG
1	C	185	VAL
1	C	201	LEU
1	C	225	THR
1	C	243	THR
1	C	245	ASP
1	C	274	ASP
1	C	277	LEU
1	C	278	ARG
1	C	299	GLU
1	C	304	THR
1	C	306	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	62	HIS
1	A	72	GLN
1	A	182	GLN
1	A	189	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	264	ASN
1	B	35	ASN
1	B	39	GLN
1	B	62	HIS
1	B	182	GLN
1	B	189	ASN
1	B	191	ASN
1	B	264	ASN
1	B	266	ASN
1	B	303	GLN
1	C	33	GLN
1	C	62	HIS
1	C	182	GLN
1	C	189	ASN
1	C	264	ASN
1	C	266	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 carbohydrates 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	CYS	A	1315	-	3,6,6	1.02	0	1,7,7	2.94	1 (100%)
2	CYS	A	1316	-	3,6,6	0.31	0	1,7,7	0.23	0
2	CYS	B	1317	-	3,6,6	0.59	0	1,7,7	0.13	0
2	CYS	B	1318	-	3,6,6	1.17	0	1,7,7	1.02	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	CYS	A	1315	-	-	0/2/6/6	0/0/0/0
2	CYS	A	1316	-	-	0/2/6/6	0/0/0/0
2	CYS	B	1317	-	-	0/2/6/6	0/0/0/0
2	CYS	B	1318	-	-	0/2/6/6	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1315	CYS	CA-CB-SG	2.94	121.22	114.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1315	CYS	6	0
2	B	1317	CYS	2	0
2	B	1318	CYS	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	261/303 (86%)	0.55	21 (8%) 15 17	36, 48, 63, 72	0
1	B	276/303 (91%)	0.43	10 (3%) 46 51	35, 49, 67, 75	0
1	C	276/303 (91%)	0.80	35 (12%) 5 6	36, 49, 68, 71	0
All	All	813/909 (89%)	0.59	66 (8%) 15 17	35, 49, 67, 75	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	GLY	6.1
1	B	316	ALA	5.3
1	C	99	PRO	5.2
1	A	71	ALA	4.7
1	A	266	ASN	4.4
1	C	100	PHE	4.3
1	C	29	ALA	4.3
1	C	203	LYS	4.2
1	B	192	GLN	4.2
1	C	317	ALA	4.1
1	A	291	ASN	4.0
1	B	315	GLY	3.9
1	A	84	VAL	3.8
1	C	106	TYR	3.7
1	C	64	ARG	3.7
1	C	93	PHE	3.7
1	C	26	ALA	3.7
1	C	200	THR	3.6
1	C	277	LEU	3.1
1	C	199	GLN	3.0
1	A	314	PHE	3.0
1	B	241	LEU	2.9
1	B	263	VAL	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	106	TYR	2.8
1	C	98	GLU	2.8
1	C	177	GLY	2.8
1	C	158	VAL	2.7
1	C	90	ILE	2.7
1	C	315	GLY	2.7
1	B	185	VAL	2.7
1	C	97	LEU	2.7
1	A	208	PRO	2.7
1	B	66	ASP	2.7
1	A	146	VAL	2.7
1	C	103	ASN	2.7
1	C	296	ILE	2.6
1	A	158	VAL	2.6
1	B	205	ASN	2.6
1	C	88	ASN	2.6
1	C	95	PRO	2.6
1	C	39	GLN	2.6
1	C	40	SER	2.5
1	A	296	ILE	2.5
1	A	95	PRO	2.5
1	C	102	LEU	2.4
1	C	247	MET	2.4
1	A	309	ALA	2.4
1	A	294	ILE	2.4
1	C	133	ARG	2.4
1	A	267	ARG	2.4
1	A	60	TYR	2.4
1	A	265	VAL	2.3
1	A	203	LYS	2.3
1	A	96	GLY	2.3
1	C	101	THR	2.3
1	A	85	GLN	2.3
1	C	54	GLY	2.2
1	B	300	LEU	2.2
1	C	70	LEU	2.2
1	B	90	ILE	2.2
1	C	105	ASP	2.1
1	C	53	GLN	2.1
1	C	63	ALA	2.1
1	A	205	ASN	2.1
1	C	69	PRO	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	87	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CYS	A	1316	7/7	0.79	0.47	11.50	97,97,97,97	0
2	CYS	B	1318	7/7	0.54	0.43	10.42	90,90,90,90	0
2	CYS	A	1315	7/7	0.83	0.36	6.74	52,53,54,54	0
2	CYS	B	1317	7/7	0.81	0.35	4.40	63,64,64,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.