



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:40 PM GMT

PDB ID : 4TXO  
Title : Crystal structure of the mixed disulfide complex of thioredoxin-like Tl-pAs(C110S) and copper chaperone ScoIs(C74S)  
Authors : Scharer, M.A.; Abicht, H.K.; Glockshuber, R.; Hennecke, H.  
Deposited on : 2014-07-04  
Resolution : 2.20 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.

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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

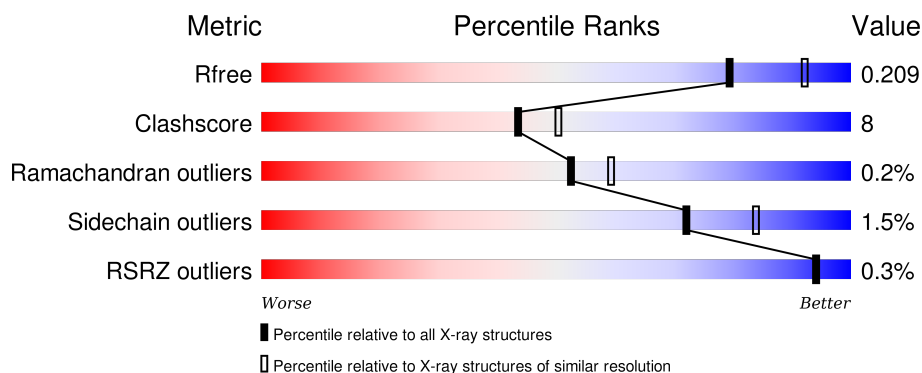
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	184	<div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	C	184	<div> <div>73%</div> <div>22%</div> <div>..</div> </div>
1	E	184	<div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	G	184	<div> <div>2%</div> <div>77%</div> <div>18%</div> <div>.</div> </div>
2	B	175	<div> <div>76%</div> <div>13%</div> <div>.</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	175	
2	F	175	
2	H	175	

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	SCN	C	301	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10798 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 Thiol:disulfide interchange protein TlpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	177	Total	C	N	O	S	0	0	0
			1330	846	229	249	6			
1	A	177	Total	C	N	O	S	0	0	0
			1328	845	228	249	6			
1	E	178	Total	C	N	O	S	0	0	0
			1337	851	230	250	6			
1	G	176	Total	C	N	O	S	0	0	0
			1321	840	227	248	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	110	SER	CYS	engineered mutation	UNP P43221
A	110	SER	CYS	engineered mutation	UNP P43221
E	110	SER	CYS	engineered mutation	UNP P43221
G	110	SER	CYS	engineered mutation	UNP P43221

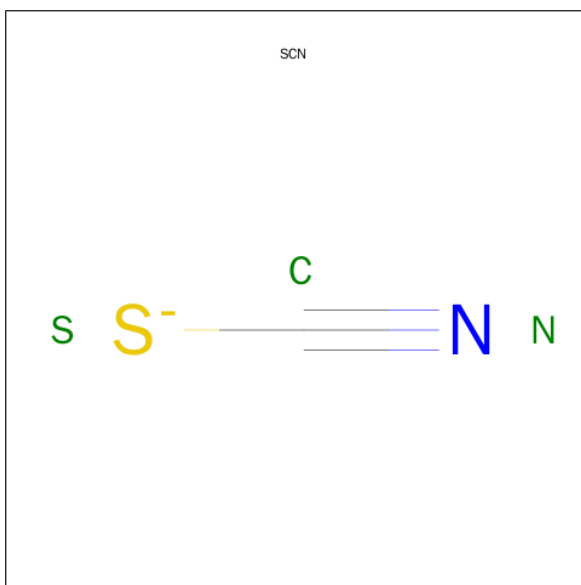
- Molecule 2 is a protein called Blr1131 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	159	Total	C	N	O	S	0	0	0
			1233	785	204	239	5			
2	B	158	Total	C	N	O	S	0	0	0
			1227	782	204	236	5			
2	F	158	Total	C	N	O	S	0	0	0
			1230	783	204	238	5			
2	H	152	Total	C	N	O	S	0	0	0
			1187	757	196	229	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	22	TRP	-	expression tag	UNP Q89VB6
D	23	SER	-	expression tag	UNP Q89VB6
D	24	HIS	-	expression tag	UNP Q89VB6
D	25	PRO	-	expression tag	UNP Q89VB6
D	26	GLN	-	expression tag	UNP Q89VB6
D	27	PHE	-	expression tag	UNP Q89VB6
D	28	GLU	-	expression tag	UNP Q89VB6
D	29	LYS	-	expression tag	UNP Q89VB6
D	74	SER	CYS	engineered mutation	UNP Q89VB6
B	22	TRP	-	expression tag	UNP Q89VB6
B	23	SER	-	expression tag	UNP Q89VB6
B	24	HIS	-	expression tag	UNP Q89VB6
B	25	PRO	-	expression tag	UNP Q89VB6
B	26	GLN	-	expression tag	UNP Q89VB6
B	27	PHE	-	expression tag	UNP Q89VB6
B	28	GLU	-	expression tag	UNP Q89VB6
B	29	LYS	-	expression tag	UNP Q89VB6
B	74	SER	CYS	engineered mutation	UNP Q89VB6
F	22	TRP	-	expression tag	UNP Q89VB6
F	23	SER	-	expression tag	UNP Q89VB6
F	24	HIS	-	expression tag	UNP Q89VB6
F	25	PRO	-	expression tag	UNP Q89VB6
F	26	GLN	-	expression tag	UNP Q89VB6
F	27	PHE	-	expression tag	UNP Q89VB6
F	28	GLU	-	expression tag	UNP Q89VB6
F	29	LYS	-	expression tag	UNP Q89VB6
F	74	SER	CYS	engineered mutation	UNP Q89VB6
H	22	TRP	-	expression tag	UNP Q89VB6
H	23	SER	-	expression tag	UNP Q89VB6
H	24	HIS	-	expression tag	UNP Q89VB6
H	25	PRO	-	expression tag	UNP Q89VB6
H	26	GLN	-	expression tag	UNP Q89VB6
H	27	PHE	-	expression tag	UNP Q89VB6
H	28	GLU	-	expression tag	UNP Q89VB6
H	29	LYS	-	expression tag	UNP Q89VB6
H	74	SER	CYS	engineered mutation	UNP Q89VB6

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		

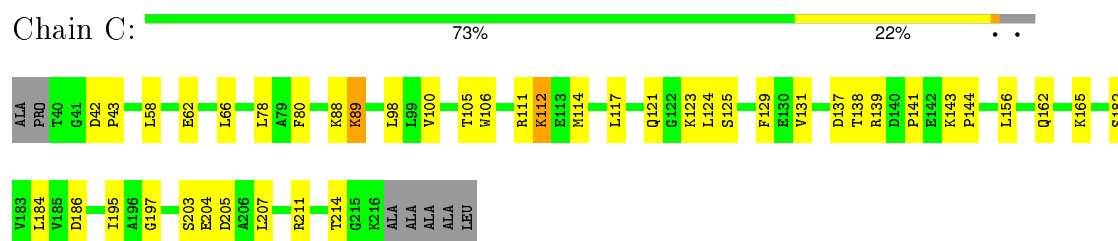
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	91	Total	O	0	0
			91	91		
6	D	116	Total	O	0	0
			116	116		
6	A	101	Total	O	0	0
			101	101		
6	B	125	Total	O	0	0
			125	125		
6	E	47	Total	O	0	0
			47	47		
6	F	44	Total	O	0	0
			44	44		
6	G	34	Total	O	0	0
			34	34		
6	H	32	Total	O	0	0
			32	32		

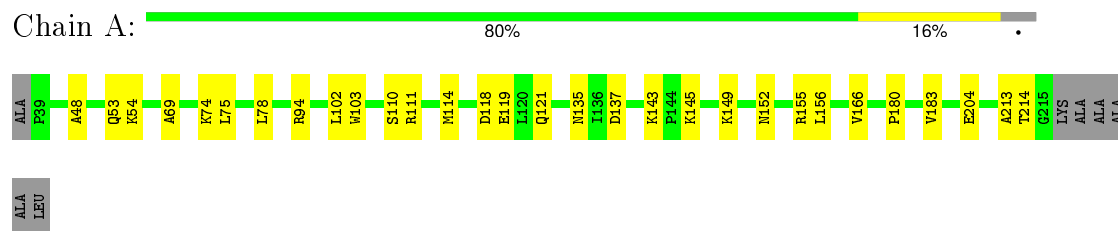
### 3 Residue-property plots [i](#)

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.

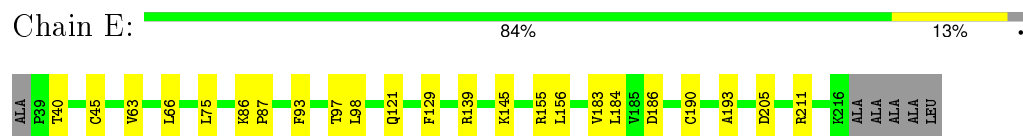
- Molecule 1: Thiol:disulfide interchange protein TlpA



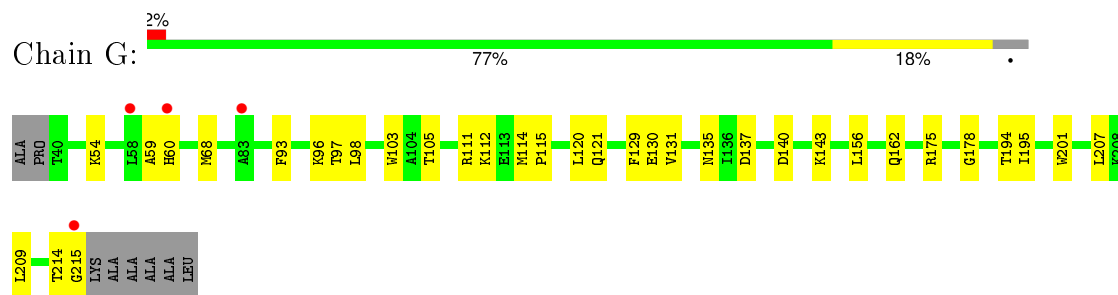
- Molecule 1: Thiol:disulfide interchange protein TlpA



- Molecule 1: Thiol:disulfide interchange protein TlpA

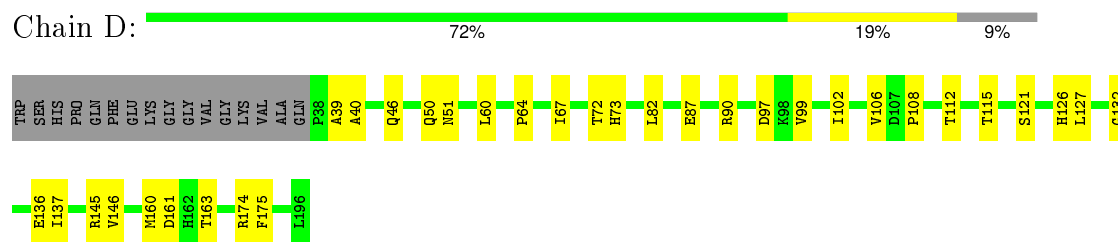


- Molecule 1: Thiol:disulfide interchange protein TlpA

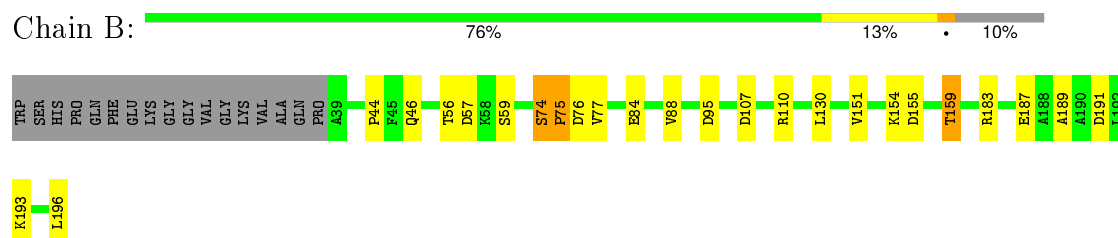


- Molecule 2: Blr1131 protein

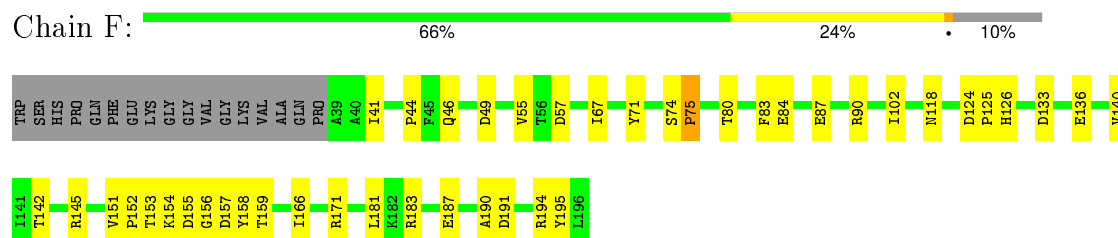




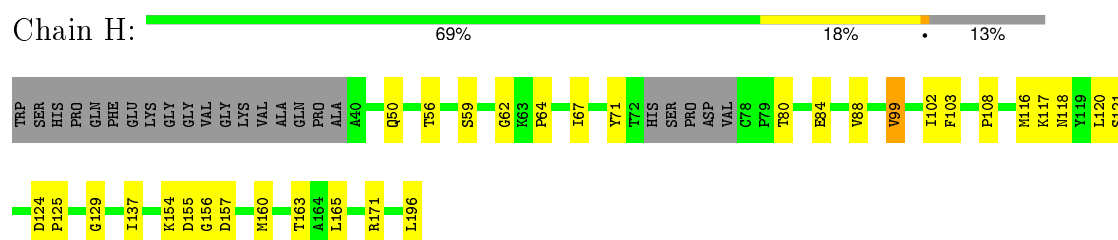
• Molecule 2: Blr1131 protein



• Molecule 2: Blr1131 protein



• Molecule 2: Blr1131 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.03Å 173.22Å 66.69Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	49.34 – 2.20 49.34 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.34-2.20) 98.7 (49.34-2.20)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.174 , 0.207 0.174 , 0.209	Depositor DCC
$R_{free}$ test set	1363 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 25.5	EDS
Estimated twinning fraction	0.500 for h,-k,-l 0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 68109 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PEG, SCN

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	0.32	0/1355	0.54	0/1840
1	C	0.34	0/1356	0.58	0/1840
1	E	0.28	0/1364	0.51	0/1851
1	G	0.28	0/1347	0.49	0/1829
2	B	0.34	0/1255	0.56	0/1699
2	D	0.35	0/1262	0.55	0/1710
2	F	0.28	0/1258	0.53	0/1703
2	H	0.28	0/1212	0.50	0/1637
All	All	0.31	0/10409	0.53	0/14109

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1328	0	1357	25	0
1	C	1330	0	1362	27	1
1	E	1337	0	1370	16	0
1	G	1321	0	1349	18	1
2	B	1227	0	1218	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1233	0	1217	21	0
2	F	1230	0	1220	28	0
2	H	1187	0	1182	19	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
4	C	7	0	10	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	101	0	0	11	1
6	B	125	0	0	3	0
6	C	91	0	0	5	0
6	D	116	0	0	4	0
6	E	47	0	0	4	1
6	F	44	0	0	3	0
6	G	34	0	0	0	0
6	H	32	0	0	1	0
All	All	10798	0	10285	165	2

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 8.

All (165) 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)
2:D:50:GLN:O	6:D:268:HOH:O	2.03	0.77
1:C:204:GLU:OE1	1:C:211:ARG:NH2	2.18	0.75
2:B:46:GLN:NE2	6:B:301:HOH:O	2.24	0.70
1:G:121:GLN:HG2	1:G:131:VAL:HB	1.73	0.70
1:G:111:ARG:HA	1:G:114:MET:HG2	1.73	0.70
1:C:143:LYS:NZ	6:C:441:HOH:O	2.24	0.68
2:D:60:LEU:O	6:D:228:HOH:O	2.12	0.68
2:H:80:THR:OG1	6:H:221:HOH:O	2.13	0.67
2:D:174:ARG:NH1	2:D:175:PHE:H	1.93	0.66
2:B:56:THR:HG23	2:B:59:SER:H	1.61	0.66
2:F:191:ASP:OD1	2:F:194:ARG:NH2	2.29	0.66
1:G:68:MET:HE1	1:G:209:LEU:HD11	1.78	0.65
2:B:110:ARG:NH1	6:B:398:HOH:O	2.31	0.64
1:A:121:GLN:HG3	1:A:156:LEU:HD23	1.77	0.64
1:C:58:LEU:O	6:C:473:HOH:O	2.15	0.64
2:D:108:PRO:HB3	2:D:137:ILE:HG13	1.80	0.64
1:C:112:LYS:HA	4:C:302:PEG:H22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:GLN:HG3	1:E:156:LEU:HD23	1.79	0.63
1:A:75:LEU:HD21	1:A:183:VAL:HG11	1.80	0.62
1:C:121:GLN:HG3	1:C:156:LEU:HD23	1.81	0.62
2:H:67:ILE:HD13	2:H:102:ILE:HB	1.81	0.62
1:G:120:LEU:HD22	1:G:201:TRP:HB3	1.82	0.61
2:F:41:ILE:HD11	2:F:145:ARG:HD2	1.82	0.61
1:E:93:PHE:HB3	1:E:98:LEU:HD21	1.83	0.61
1:G:96:LYS:NZ	1:G:130:GLU:OE2	2.26	0.60
1:A:53:GLN:NE2	1:A:69:ALA:O	2.34	0.59
2:D:39:ALA:HA	2:D:145:ARG:HH22	1.69	0.58
2:H:62:GLY:O	2:H:171:ARG:NH1	2.36	0.58
1:E:186:ASP:OD2	6:E:332:HOH:O	2.18	0.58
1:C:139:ARG:NH1	2:D:121:SER:O	2.37	0.57
1:A:48:ALA:N	6:A:416:HOH:O	2.27	0.57
2:F:152:PRO:HB2	2:F:154:LYS:HG3	1.87	0.57
2:F:153:THR:N	2:F:157:ASP:O	2.36	0.57
1:A:121:GLN:NE2	1:A:155:ARG:O	2.37	0.56
1:G:93:PHE:HB3	1:G:98:LEU:HD21	1.87	0.55
1:E:75:LEU:HD11	1:E:183:VAL:HG11	1.88	0.55
1:A:152:ASN:O	6:A:428:HOH:O	2.18	0.55
2:F:142:THR:O	6:F:201:HOH:O	2.18	0.54
6:A:474:HOH:O	2:B:74:SER:HB3	2.07	0.54
1:A:213:ALA:O	6:A:465:HOH:O	2.19	0.54
2:D:132:GLY:O	6:D:278:HOH:O	2.18	0.54
2:H:56:THR:HG23	2:H:59:SER:H	1.73	0.54
2:B:151:VAL:HB	2:B:159:THR:HG23	1.89	0.54
2:D:64:PRO:HG2	2:D:99:VAL:HG12	1.89	0.54
1:A:75:LEU:O	6:A:495:HOH:O	2.19	0.53
1:C:121:GLN:HG2	1:C:131:VAL:HB	1.90	0.52
1:E:155:ARG:NH1	6:E:301:HOH:O	2.35	0.52
2:H:118:ASN:O	2:H:121:SER:OG	2.21	0.52
1:A:135:ASN:ND2	1:A:137:ASP:OD1	2.30	0.52
1:A:74:LYS:NZ	6:A:426:HOH:O	2.44	0.52
1:A:143:LYS:NZ	6:A:444:HOH:O	2.42	0.52
1:E:97:THR:O	1:E:129:PHE:HA	2.10	0.51
1:C:78:LEU:O	1:C:89:LYS:HA	2.11	0.51
2:F:87:GLU:OE1	2:F:90:ARG:NH1	2.43	0.51
1:E:145:LYS:NZ	6:E:303:HOH:O	2.44	0.50
2:B:193:LYS:HA	2:B:196:LEU:HG	1.93	0.50
1:C:197:GLY:O	6:C:438:HOH:O	2.19	0.50
1:C:137:ASP:OD2	1:C:144:PRO:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:152:PRO:HA	2:F:158:TYR:HA	1.93	0.50
2:H:99:VAL:HG23	2:H:196:LEU:HD21	1.94	0.49
2:D:112:THR:H	2:D:115:THR:HG1	1.55	0.49
2:F:67:ILE:HD13	2:F:102:ILE:HB	1.95	0.49
1:A:111:ARG:HA	1:A:114:MET:HE2	1.95	0.49
2:D:97:ASP:OD1	2:D:126:HIS:NE2	2.46	0.49
1:A:111:ARG:HA	1:A:114:MET:CE	2.43	0.48
1:C:138:THR:HA	1:C:162:GLN:HG2	1.96	0.48
1:G:59:ALA:HB2	1:G:68:MET:CE	2.44	0.48
2:F:124:ASP:OD1	2:F:126:HIS:ND1	2.29	0.48
2:F:151:VAL:O	2:F:159:THR:HG22	2.13	0.48
2:D:72:THR:OG1	2:D:73:HIS:N	2.46	0.48
1:E:139:ARG:CZ	2:F:125:PRO:HD3	2.43	0.48
2:D:87:GLU:OE1	6:D:242:HOH:O	2.20	0.48
1:E:211:ARG:NH2	6:E:304:HOH:O	2.46	0.48
1:G:121:GLN:HG3	1:G:156:LEU:HD23	1.96	0.47
2:F:46:GLN:O	2:F:136:GLU:HG2	2.14	0.47
2:H:50:GLN:HB2	2:H:117:LYS:HA	1.95	0.47
2:F:155:ASP:HA	2:F:156:GLY:HA2	1.58	0.47
1:C:106:TRP:O	6:C:447:HOH:O	2.19	0.47
1:A:78:LEU:HD22	1:A:166:VAL:HG13	1.97	0.47
2:B:189:ALA:O	2:B:193:LYS:HG3	2.16	0.46
2:B:154:LYS:HA	2:B:155:ASP:HA	1.49	0.46
1:C:62:GLU:HB2	1:C:205:ASP:HB2	1.97	0.46
1:A:94:ARG:NH1	6:A:473:HOH:O	2.33	0.46
1:A:118:ASP:O	1:A:121:GLN:HB2	2.16	0.46
1:C:165:LYS:HE3	6:C:413:HOH:O	2.16	0.46
2:F:83:PHE:O	2:F:87:GLU:HG2	2.16	0.46
2:D:39:ALA:HA	2:D:145:ARG:NH2	2.31	0.46
2:H:155:ASP:HA	2:H:156:GLY:HA2	1.67	0.46
2:F:118:ASN:HB2	6:F:218:HOH:O	2.15	0.45
2:B:183:ARG:NH2	2:B:191:ASP:OD2	2.43	0.45
1:A:121:GLN:NE2	6:A:490:HOH:O	2.50	0.45
2:B:44:PRO:HA	2:B:57:ASP:CG	2.37	0.45
2:F:44:PRO:HA	2:F:57:ASP:CG	2.37	0.45
1:C:111:ARG:HG3	4:C:302:PEG:H11	1.99	0.45
2:D:106:VAL:HG23	2:D:160:MET:HG2	1.98	0.45
1:A:54:LYS:HB2	1:A:54:LYS:HE3	1.72	0.45
1:C:203:SER:O	1:C:207:LEU:HG	2.17	0.45
1:G:175:ARG:HD2	1:G:194:THR:HG21	1.98	0.45
1:A:110:SER:HB2	1:A:180:PRO:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ASP:OD1	6:B:339:HOH:O	2.21	0.45
1:G:195:ILE:HG21	1:G:201:TRP:HZ2	1.81	0.44
1:A:119:GLU:OE2	1:A:155:ARG:NH2	2.50	0.44
2:B:183:ARG:HB2	2:B:187:GLU:OE1	2.16	0.44
1:E:98:LEU:O	1:E:184:LEU:HD12	2.16	0.44
2:H:116:MET:HB3	2:H:116:MET:HE2	1.72	0.44
1:G:137:ASP:O	1:G:162:GLN:HA	2.17	0.44
2:F:136:GLU:O	2:F:140:VAL:HG23	2.17	0.44
2:B:84:GLU:O	2:B:88:VAL:HG23	2.18	0.44
2:H:103:PHE:O	2:H:129:GLY:HA2	2.18	0.44
2:H:64:PRO:HG2	2:H:99:VAL:HG23	1.99	0.44
2:F:183:ARG:NH2	2:F:191:ASP:OD2	2.45	0.43
1:E:93:PHE:HB2	1:E:98:LEU:HD11	2.00	0.43
2:F:80:THR:O	2:F:84:GLU:HG3	2.17	0.43
1:C:100:VAL:O	1:C:182:SER:HA	2.18	0.43
2:D:51:ASN:ND2	1:E:40:THR:OG1	2.51	0.43
2:F:166:ILE:HG13	2:F:181:LEU:HD11	1.99	0.43
2:F:171:ARG:NH2	2:F:195:TYR:O	2.47	0.43
2:F:190:ALA:O	2:F:194:ARG:HG3	2.18	0.43
2:H:71:TYR:CE1	2:H:160:MET:HB3	2.54	0.43
2:H:163:THR:HG22	2:H:165:LEU:H	1.84	0.43
2:D:82:LEU:HD11	2:D:127:LEU:HD13	2.00	0.43
1:C:112:LYS:HE3	4:C:302:PEG:H32	2.01	0.43
1:A:204:GLU:OE1	6:A:401:HOH:O	2.21	0.42
2:B:95:ASP:OD2	2:B:193:LYS:NZ	2.26	0.42
2:D:46:GLN:O	2:D:136:GLU:HG2	2.19	0.42
1:C:80:PHE:O	1:C:88:LYS:N	2.38	0.42
1:C:125:SER:HA	1:C:129:PHE:O	2.19	0.42
1:C:114:MET:HE1	1:C:117:LEU:HD12	2.02	0.42
1:G:214:THR:HA	1:G:215:GLY:HA3	1.57	0.42
2:F:154:LYS:HA	2:F:155:ASP:HA	1.71	0.42
2:H:84:GLU:O	2:H:88:VAL:HG23	2.18	0.42
1:E:66:LEU:HG	1:E:193:ALA:HB1	2.02	0.42
2:H:108:PRO:HG3	2:H:137:ILE:HG13	2.02	0.42
2:H:124:ASP:HA	2:H:125:PRO:HD3	1.80	0.42
2:B:75:PRO:HB2	2:B:76:ASP:H	1.72	0.42
1:A:145:LYS:O	1:A:149:LYS:HG3	2.20	0.42
1:C:98:LEU:O	1:C:184:LEU:HD12	2.20	0.42
1:C:121:GLN:CG	1:C:131:VAL:HB	2.50	0.42
1:A:102:LEU:HD11	1:A:166:VAL:HG12	2.00	0.42
1:G:97:THR:O	1:G:129:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:ASP:OD2	1:G:143:LYS:HB2	2.20	0.42
1:G:114:MET:N	1:G:115:PRO:HD2	2.35	0.41
1:A:103:TRP:CB	1:A:114:MET:HE1	2.50	0.41
2:H:154:LYS:HA	2:H:155:ASP:HA	1.81	0.41
1:C:66:LEU:HD23	1:C:195:ILE:HB	2.02	0.41
2:D:146:VAL:HG13	2:D:163:THR:HB	2.02	0.41
2:D:87:GLU:OE2	2:D:90:ARG:NH1	2.53	0.41
2:F:71:TYR:HB2	6:F:213:HOH:O	2.19	0.41
1:G:178:GLY:HA2	2:H:80:THR:HG23	2.02	0.41
2:F:49:ASP:HB3	2:F:55:VAL:HG21	2.02	0.41
2:H:120:LEU:HD11	2:H:129:GLY:N	2.35	0.41
2:F:166:ILE:HG13	2:F:181:LEU:CD1	2.51	0.41
1:A:214:THR:O	6:A:402:HOH:O	2.22	0.41
1:E:63:VAL:HG22	1:E:205:ASP:HB3	2.03	0.41
1:G:103:TRP:CE2	1:G:135:ASN:HB2	2.56	0.41
1:G:111:ARG:HA	1:G:114:MET:CG	2.47	0.41
2:D:40:ALA:HB1	2:D:174:ARG:NH2	2.36	0.41
1:C:141:PRO:HG3	1:C:162:GLN:NE2	2.35	0.41
1:E:45:CYS:HB3	1:E:190:CYS:HB3	1.95	0.41
2:D:67:ILE:HD13	2:D:102:ILE:HB	2.02	0.41
1:C:123:LYS:O	1:C:124:LEU:HD23	2.22	0.40
1:E:86:LYS:HA	1:E:87:PRO:HD3	1.91	0.40
2:F:74:SER:HA	2:F:75:PRO:HD3	1.89	0.40
1:C:42:ASP:HA	1:C:43:PRO:HD3	1.94	0.40
2:F:183:ARG:HB2	2:F:187:GLU:OE2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:413:HOH:O	6:E:310:HOH:O[1_655]	2.07	0.13
1:C:214:THR:O	1:G:54:LYS:NZ[1_456]	2.14	0.06

## 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	175/184 (95%)	169 (97%)	6 (3%)	0	100	100
1	C	175/184 (95%)	168 (96%)	7 (4%)	0	100	100
1	E	176/184 (96%)	167 (95%)	9 (5%)	0	100	100
1	G	174/184 (95%)	166 (95%)	8 (5%)	0	100	100
2	B	156/175 (89%)	153 (98%)	2 (1%)	1 (1%)	30	29
2	D	157/175 (90%)	149 (95%)	8 (5%)	0	100	100
2	F	156/175 (89%)	150 (96%)	5 (3%)	1 (1%)	30	29
2	H	148/175 (85%)	143 (97%)	5 (3%)	0	100	100
All	All	1317/1436 (92%)	1265 (96%)	50 (4%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	75	PRO
2	F	75	PRO

### 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	138/140 (99%)	138 (100%)	0	100	100
1	C	138/140 (99%)	134 (97%)	4 (3%)	50	62
1	E	139/140 (99%)	139 (100%)	0	100	100
1	G	137/140 (98%)	133 (97%)	4 (3%)	50	62
2	B	133/147 (90%)	129 (97%)	4 (3%)	48	60
2	D	134/147 (91%)	133 (99%)	1 (1%)	88	94
2	F	134/147 (91%)	133 (99%)	1 (1%)	88	94
2	H	129/147 (88%)	127 (98%)	2 (2%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1082/1148 (94%)	1066 (98%)	16 (2%)	72 84

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

Mol	Chain	Res	Type
1	C	89	LYS
1	C	105	THR
1	C	112	LYS
1	C	186	ASP
2	D	161	ASP
2	B	74	SER
2	B	77	VAL
2	B	130	LEU
2	B	159	THR
2	F	133	ASP
1	G	60	HIS
1	G	105	THR
1	G	112	LYS
1	G	207	LEU
2	H	99	VAL
2	H	157	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	GLN
1	C	101	ASN
1	C	160	ASN
2	D	51	ASN
2	D	100	ASN
1	A	101	ASN
2	B	46	GLN
2	B	126	HIS
1	E	101	ASN
1	E	160	ASN

### 5.3.3 RNA ⓘ

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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	SCN	A	301	-	2,2,2	1.90	1 (50%)	1,1,1	0.15	0
3	SCN	C	301	-	2,2,2	1.75	1 (50%)	1,1,1	0.43	0
4	PEG	C	302	-	6,6,6	0.60	0	5,5,5	0.67	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	SCN	A	301	-	-	0/0/0/0	0/0/0/0
3	SCN	C	301	-	-	0/0/0/0	0/0/0/0
4	PEG	C	302	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	SCN	C-S	2.43	1.79	1.63
3	A	301	SCN	C-S	2.63	1.80	1.63

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	PEG	3	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, 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(Å²)	Q<0.9	
1	A	177/184 (96%)	-0.87	0	100	100	25, 35, 50, 71	0
1	C	177/184 (96%)	-0.87	0	100	100	19, 34, 54, 95	0
1	E	178/184 (96%)	-0.55	0	100	100	37, 53, 77, 102	0
1	G	176/184 (95%)	-0.47	4 (2%)	64	63	33, 55, 90, 120	0
2	B	158/175 (90%)	-0.85	0	100	100	22, 29, 56, 84	0
2	D	159/175 (90%)	-0.90	0	100	100	19, 28, 49, 94	0
2	F	158/175 (90%)	-0.62	0	100	100	27, 50, 82, 111	0
2	H	152/175 (86%)	-0.66	0	100	100	31, 50, 74, 95	0
All	All	1335/1436 (92%)	-0.72	4 (0%)	94	94	19, 43, 73, 120	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	83	ALA	4.4
1	G	58	LEU	3.9
1	G	215	GLY	2.1
1	G	60	HIS	2.1

### 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
3	SCN	C	301	3/3	0.98	0.14	3.54	11,11,12,58	0
4	PEG	C	302	7/7	0.96	0.12	1.12	26,32,42,46	0
3	SCN	A	301	3/3	0.96	0.10	0.78	37,37,37,37	0
5	NA	A	302	1/1	0.99	0.09	-0.87	30,30,30,30	0
5	NA	B	201	1/1	0.99	0.06	-1.70	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.