Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:10 AM GMT

PDB ID	:	2ZU0
Title	:	Crystal structure of SufC-SufD complex involved in the iron-sulfur cluster biosynthesis
Authors	:	Wada, K.
Deposited on	:	2008-10-11
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
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:

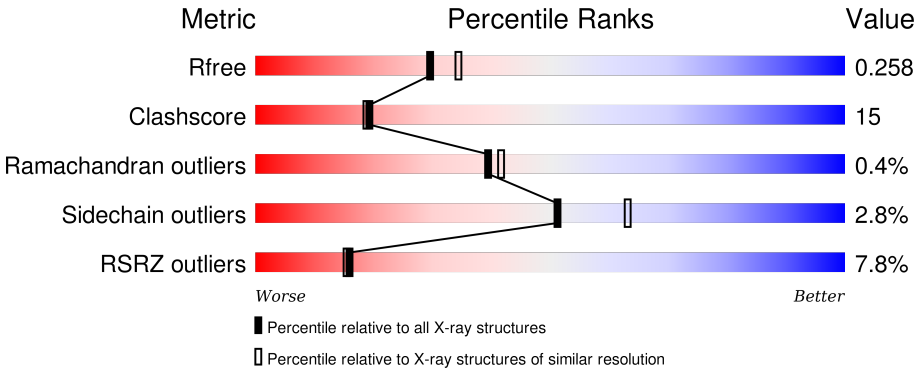
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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 >=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	423	4% 75% 22%
1	B	423	3% 77% 19%
2	C	267	10% 64% 24% 7%
2	D	267	12% 10% 6% 84%

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	MES	C	2000	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9043 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 Protein sufD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3255	2028	604	615	8			
1	B	414	Total	C	N	O	S	0	0	0
			3237	2019	599	611	8			

- Molecule 2 is a protein called Probable ATP-dependent transporter sufC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	247	Total	C	N	O	S	0	0	0
			1931	1223	325	376	7			
2	D	42	Total	C	N	O	S	0	0	0
			319	205	51	62	1			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	EXPRESSION TAG	UNP P77499
C	-17	GLY	-	EXPRESSION TAG	UNP P77499
C	-16	SER	-	EXPRESSION TAG	UNP P77499
C	-15	SER	-	EXPRESSION TAG	UNP P77499
C	-14	HIS	-	EXPRESSION TAG	UNP P77499
C	-13	HIS	-	EXPRESSION TAG	UNP P77499
C	-12	HIS	-	EXPRESSION TAG	UNP P77499
C	-11	HIS	-	EXPRESSION TAG	UNP P77499
C	-10	HIS	-	EXPRESSION TAG	UNP P77499
C	-9	SER	-	EXPRESSION TAG	UNP P77499
C	-8	SER	-	EXPRESSION TAG	UNP P77499
C	-7	GLY	-	EXPRESSION TAG	UNP P77499
C	-6	LEU	-	EXPRESSION TAG	UNP P77499
C	-5	VAL	-	EXPRESSION TAG	UNP P77499
C	-4	PRO	-	EXPRESSION TAG	UNP P77499
C	-3	ARG	-	EXPRESSION TAG	UNP P77499

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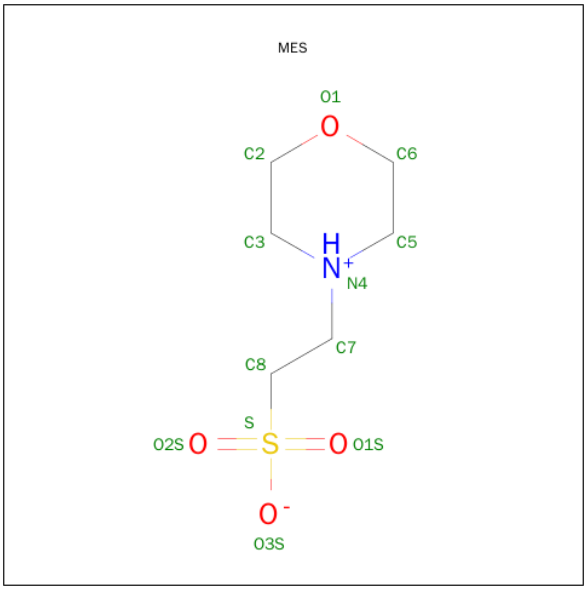
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P77499
C	-1	SER	-	EXPRESSION TAG	UNP P77499
C	0	HIS	-	EXPRESSION TAG	UNP P77499
D	-18	MET	-	EXPRESSION TAG	UNP P77499
D	-17	GLY	-	EXPRESSION TAG	UNP P77499
D	-16	SER	-	EXPRESSION TAG	UNP P77499
D	-15	SER	-	EXPRESSION TAG	UNP P77499
D	-14	HIS	-	EXPRESSION TAG	UNP P77499
D	-13	HIS	-	EXPRESSION TAG	UNP P77499
D	-12	HIS	-	EXPRESSION TAG	UNP P77499
D	-11	HIS	-	EXPRESSION TAG	UNP P77499
D	-10	HIS	-	EXPRESSION TAG	UNP P77499
D	-9	SER	-	EXPRESSION TAG	UNP P77499
D	-8	SER	-	EXPRESSION TAG	UNP P77499
D	-7	GLY	-	EXPRESSION TAG	UNP P77499
D	-6	LEU	-	EXPRESSION TAG	UNP P77499
D	-5	VAL	-	EXPRESSION TAG	UNP P77499
D	-4	PRO	-	EXPRESSION TAG	UNP P77499
D	-3	ARG	-	EXPRESSION TAG	UNP P77499
D	-2	GLY	-	EXPRESSION TAG	UNP P77499
D	-1	SER	-	EXPRESSION TAG	UNP P77499
D	0	HIS	-	EXPRESSION TAG	UNP P77499

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

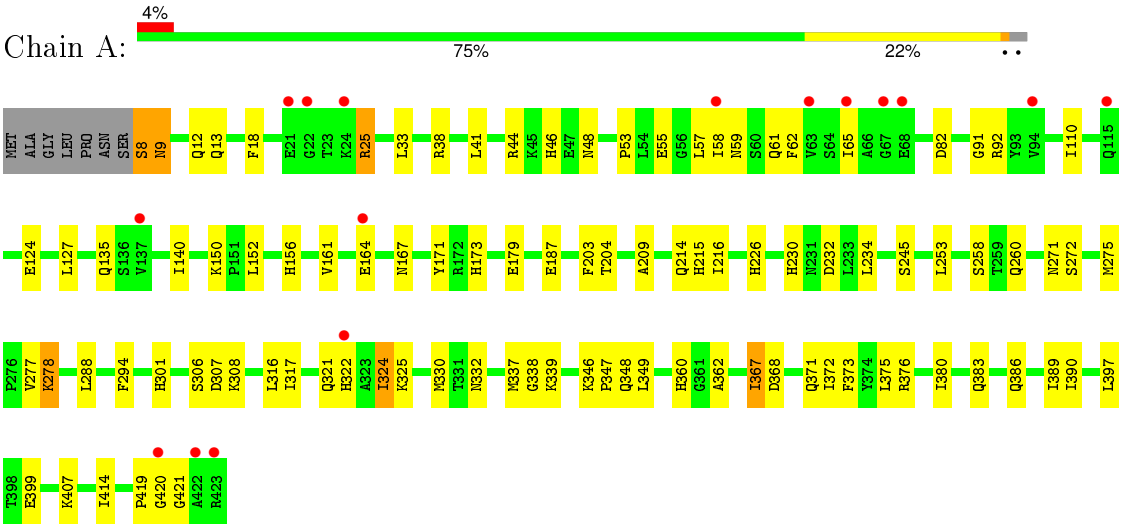
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	126	Total	O	0	0
			126	126		
4	C	47	Total	O	0	0
			47	47		

3 Residue-property plots

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.

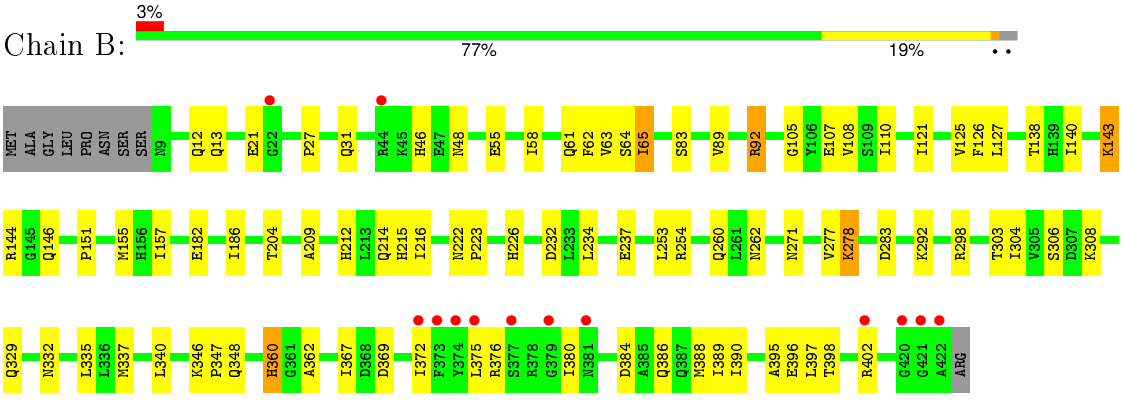
- Molecule 1: Protein sufD

Chain A:



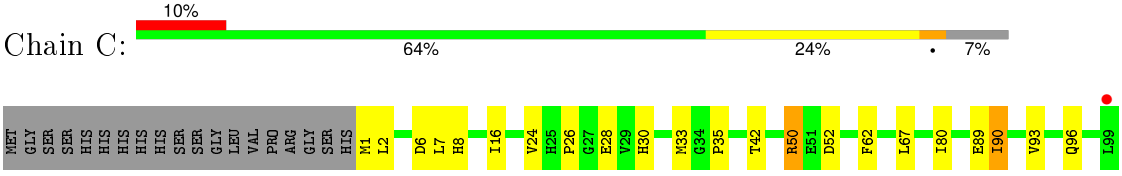
- Molecule 1: Protein sufD

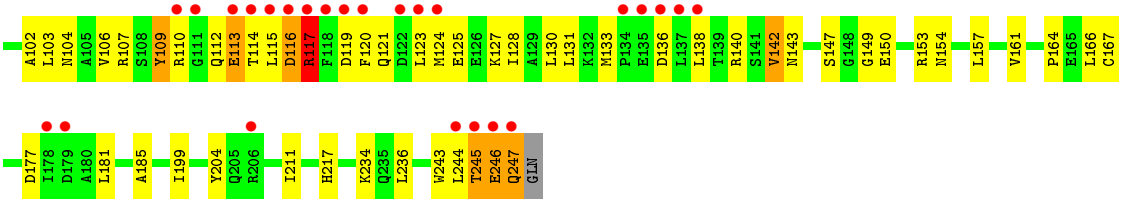
Chain B:



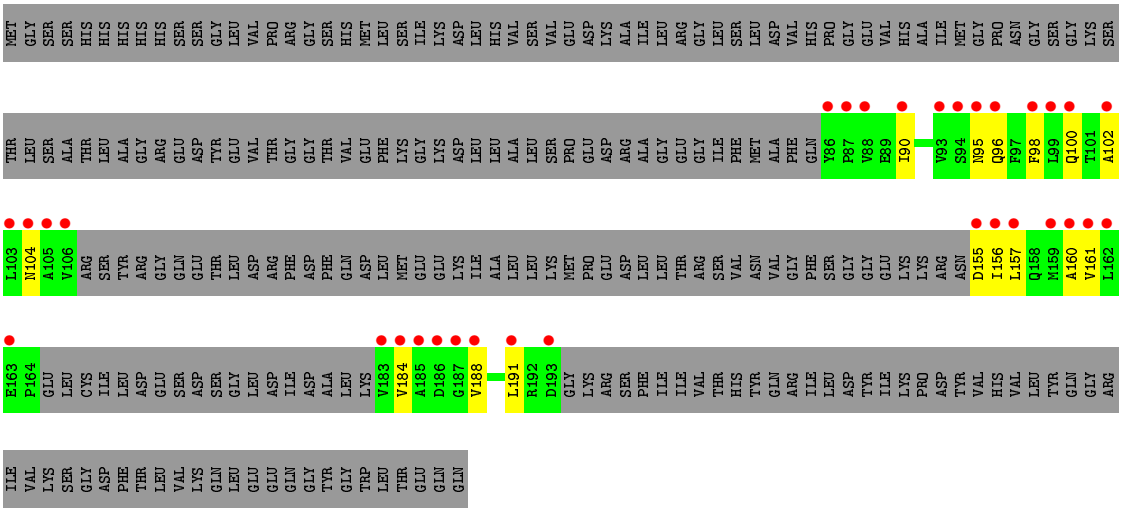
- Molecule 2: Probable ATP-dependent transporter sufC

Chain C:





- Molecule 2: Probable ATP-dependent transporter sufC



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.11Å 106.15Å 171.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.14 – 2.20 45.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (45.14-2.20) 97.2 (45.14-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.48 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.259 0.234 , 0.258	Depositor DCC
R_{free} test set	8712 reflections (9.99%)	DCC
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 89820 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9043	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: MES

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	0.33	0/3317	0.62	0/4494
1	B	0.34	0/3299	0.63	0/4472
2	C	0.37	0/1963	0.66	2/2649 (0.1%)
2	D	0.35	0/322	0.49	0/438
All	All	0.34	0/8901	0.63	2/12053 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	109	TYR	N-CA-C	-5.57	95.97	111.00
2	C	246	GLU	N-CA-C	5.43	125.66	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3255	0	3202	97	0
1	B	3237	0	3184	84	0
2	C	1931	0	1928	80	0
2	D	319	0	316	12	0
3	C	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	116	0	0	1	0
4	B	126	0	0	3	0
4	C	47	0	0	0	0
All	All	9043	0	8643	263	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (263) 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:B:121:ILE:HD11	1:B:234:LEU:HD21	1.36	1.07
1:B:143:LYS:H	1:B:143:LYS:HD2	1.20	1.05
1:A:65:ILE:HD12	1:A:161:VAL:HG11	1.49	0.95
1:A:367:ILE:HD13	1:A:368:ASP:N	1.84	0.93
2:C:124:MET:HG2	2:C:138:LEU:HD11	1.51	0.90
1:A:46:HIS:HD2	1:A:48:ASN:H	1.23	0.84
2:C:185:ALA:HA	2:C:211:ILE:HD11	1.59	0.83
1:B:46:HIS:HD2	1:B:48:ASN:H	1.22	0.83
1:B:13:GLN:HE22	1:B:62:PHE:H	1.27	0.82
2:C:90:ILE:N	2:C:90:ILE:HD12	1.95	0.81
2:C:90:ILE:HD13	2:C:142:VAL:CG1	2.11	0.81
1:B:13:GLN:NE2	1:B:62:PHE:H	1.77	0.81
2:C:24:VAL:HG21	2:C:199:ILE:HD11	1.64	0.78
1:B:143:LYS:N	1:B:143:LYS:HD2	1.98	0.76
1:A:367:ILE:HD11	1:A:389:ILE:HG21	1.67	0.75
1:A:367:ILE:HD13	1:A:368:ASP:H	1.55	0.72
1:A:38:ARG:HB3	1:A:38:ARG:HH21	1.54	0.71
1:B:107:GLU:HG2	1:B:143:LYS:HE2	1.73	0.71
2:C:114:THR:HG22	2:C:115:LEU:N	2.06	0.71
1:A:46:HIS:CD2	1:A:48:ASN:H	2.08	0.70
1:A:383:GLN:HG2	1:A:420:GLY:O	1.91	0.70
2:C:124:MET:HG3	2:C:128:ILE:HD11	1.74	0.69
2:C:90:ILE:HD13	2:C:142:VAL:HB	1.74	0.69
1:A:41:LEU:HD13	1:A:58:ILE:HG22	1.75	0.69
1:A:386:GLN:HE22	1:A:420:GLY:H	1.43	0.67
2:C:143:ASN:ND2	2:C:154:ASN:HD22	1.93	0.67
1:A:18:PHE:O	1:A:25:ARG:HD2	1.94	0.67
2:C:204:TYR:CE2	2:C:247:GLN:HA	2.31	0.66
1:B:262:ASN:C	1:B:292:LYS:HG3	2.15	0.66
2:C:114:THR:HG22	2:C:115:LEU:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HD12	1:A:59:ASN:N	2.11	0.66
1:A:8:SER:HB3	1:A:61:GLN:NE2	2.10	0.66
2:D:160:ALA:HA	2:D:191:LEU:HD21	1.78	0.65
1:B:380:ILE:HD12	1:B:380:ILE:H	1.61	0.65
1:B:105:GLY:O	1:B:143:LYS:HE3	1.97	0.65
2:C:116:ASP:O	2:C:119:ASP:N	2.30	0.64
1:A:38:ARG:NH2	1:A:38:ARG:HB3	2.13	0.64
2:C:90:ILE:HD13	2:C:142:VAL:CB	2.27	0.64
1:B:143:LYS:H	1:B:143:LYS:CD	1.90	0.63
1:B:277:VAL:HG23	1:B:278:LYS:HG2	1.80	0.63
1:A:346:LYS:HG3	1:B:348:GLN:HG2	1.81	0.63
2:D:96:GLN:HG3	2:D:100:GLN:NE2	2.14	0.63
1:B:55:GLU:H	1:B:55:GLU:CD	2.03	0.62
1:A:156:HIS:HE1	1:A:173:HIS:NE2	1.97	0.62
2:C:89:GLU:C	2:C:90:ILE:HD12	2.20	0.62
2:C:109:TYR:O	2:C:110:ARG:CB	2.47	0.61
1:A:13:GLN:HE21	1:A:62:PHE:H	1.46	0.61
2:C:96:GLN:HB2	2:C:138:LEU:HD12	1.82	0.61
1:B:13:GLN:HE22	1:B:62:PHE:N	1.98	0.61
1:A:324:ILE:H	1:A:324:ILE:HD13	1.65	0.61
1:A:13:GLN:HE21	1:A:61:GLN:HA	1.67	0.60
1:A:317:ILE:HD11	1:A:330:MET:HE3	1.83	0.60
2:C:185:ALA:CA	2:C:211:ILE:HD11	2.30	0.60
1:B:121:ILE:HD11	1:B:234:LEU:CD2	2.22	0.60
1:A:317:ILE:HB	1:A:349:LEU:HD23	1.83	0.60
2:C:90:ILE:CD1	2:C:90:ILE:N	2.65	0.60
1:B:138:THR:HG22	1:B:140:ILE:HD11	1.84	0.59
1:B:386:GLN:O	1:B:390:ILE:HG12	2.01	0.59
2:C:116:ASP:O	2:C:117:ARG:C	2.40	0.59
1:B:46:HIS:CD2	1:B:48:ASN:H	2.13	0.59
1:B:214:GLN:HG2	1:B:216:ILE:HD11	1.85	0.59
1:A:9:ASN:ND2	1:A:12:GLN:H	1.99	0.59
2:C:236:LEU:HB3	2:C:244:LEU:HD11	1.85	0.59
2:C:131:LEU:HD12	2:C:157:LEU:HB2	1.85	0.58
2:C:245:THR:HG22	2:C:246:GLU:H	1.68	0.58
1:B:63:VAL:HB	1:B:65:ILE:HD11	1.84	0.58
2:C:104:ASN:OD1	2:C:114:THR:HG21	2.03	0.58
1:B:335:LEU:HD21	1:B:367:ILE:CD1	2.33	0.58
2:C:131:LEU:HD13	2:C:153:ARG:O	2.04	0.58
2:D:96:GLN:HG3	2:D:100:GLN:HE21	1.69	0.58
2:C:130:LEU:HD23	2:C:130:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:ASN:HA	2:C:114:THR:HG1	1.69	0.57
2:C:109:TYR:O	2:C:110:ARG:HB3	2.05	0.57
1:A:278:LYS:HG3	1:A:308:LYS:HE2	1.85	0.57
2:D:157:LEU:O	2:D:161:VAL:HG23	2.04	0.57
1:B:372:ILE:CD1	1:B:389:ILE:HD12	2.35	0.57
1:A:65:ILE:H	1:A:167:ASN:ND2	2.02	0.57
1:B:335:LEU:HD21	1:B:367:ILE:HD11	1.87	0.57
2:C:104:ASN:HA	2:C:114:THR:OG1	2.04	0.56
1:B:380:ILE:HD11	2:D:102:ALA:HB2	1.87	0.56
2:C:110:ARG:HG2	2:C:112:GLN:HE21	1.70	0.56
1:A:347:PRO:HG3	1:A:360:HIS:CD2	2.40	0.56
2:C:124:MET:HG3	2:C:128:ILE:CD1	2.34	0.56
1:A:9:ASN:C	1:A:9:ASN:HD22	2.09	0.56
2:C:136:ASP:OD2	2:C:140:ARG:HD2	2.06	0.56
2:C:120:PHE:CE1	2:C:124:MET:HE3	2.41	0.56
1:A:65:ILE:H	1:A:167:ASN:HD21	1.54	0.56
1:A:339:LYS:NZ	1:A:339:LYS:HB2	2.21	0.55
1:B:367:ILE:HD11	1:B:390:ILE:HD13	1.88	0.55
2:C:136:ASP:O	2:C:140:ARG:HG3	2.06	0.55
1:B:372:ILE:O	1:B:376:ARG:HG3	2.07	0.55
1:A:324:ILE:HD13	1:A:324:ILE:N	2.21	0.55
1:B:64:SER:C	1:B:65:ILE:HD13	2.27	0.55
1:B:340:LEU:N	1:B:340:LEU:HD22	2.22	0.55
2:C:204:TYR:CZ	2:C:246:GLU:O	2.60	0.54
2:C:30:HIS:HD2	2:C:217:HIS:NE2	2.05	0.54
1:A:275:MET:SD	1:A:414:ILE:HD12	2.47	0.54
1:A:306:SER:HA	1:A:337:MET:HB2	1.90	0.54
2:C:133:MET:HE2	2:C:133:MET:HA	1.89	0.54
2:C:90:ILE:HD13	2:C:142:VAL:HG11	1.89	0.54
1:B:157:ILE:HD12	1:B:157:ILE:N	2.23	0.53
1:B:367:ILE:HD11	1:B:390:ILE:CD1	2.37	0.53
2:C:143:ASN:HD21	2:C:154:ASN:HD22	1.54	0.53
1:B:186:ILE:HD12	1:B:186:ILE:N	2.23	0.53
1:B:253:LEU:HD23	1:B:253:LEU:C	2.29	0.53
1:B:110:ILE:N	1:B:110:ILE:HD12	2.23	0.53
1:A:346:LYS:HE2	1:B:348:GLN:HE21	1.74	0.53
2:C:62:PHE:CD2	2:C:80:ILE:HD11	2.43	0.53
1:B:204:THR:HG22	1:B:232:ASP:HB2	1.91	0.53
2:C:114:THR:CG2	2:C:115:LEU:N	2.72	0.53
1:B:348:GLN:NE2	4:B:548:HOH:O	2.42	0.53
2:C:106:VAL:O	2:C:109:TYR:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ILE:N	1:B:380:ILE:HD12	2.24	0.52
1:A:216:ILE:N	1:A:216:ILE:HD12	2.25	0.52
1:A:399:GLU:OE1	1:A:407:LYS:HE2	2.10	0.52
1:A:321:GLN:O	1:A:322:HIS:HB2	2.08	0.52
2:C:52:ASP:N	2:C:52:ASP:OD2	2.34	0.52
1:A:127:LEU:C	1:A:127:LEU:HD23	2.30	0.52
2:C:107:ARG:HD2	2:C:112:GLN:HG3	1.91	0.52
1:B:121:ILE:HD12	1:B:260:GLN:CD	2.29	0.52
1:B:375:LEU:HD21	2:D:90:ILE:HD13	1.90	0.51
1:B:376:ARG:HA	1:B:380:ILE:O	2.10	0.51
1:A:164:GLU:OE2	1:A:164:GLU:N	2.43	0.51
2:C:123:LEU:HD12	2:C:127:LYS:HZ3	1.76	0.51
1:A:271:ASN:HB3	1:A:397:LEU:HD22	1.93	0.51
1:A:9:ASN:HD22	1:A:12:GLN:H	1.59	0.51
1:A:215:HIS:C	1:A:216:ILE:HD12	2.31	0.51
1:B:143:LYS:HD3	1:B:146:GLN:HG3	1.93	0.51
2:D:156:ILE:HD12	2:D:156:ILE:H	1.77	0.50
1:A:230:HIS:HE1	1:A:258:SER:OG	1.95	0.50
2:C:147:SER:OG	2:C:150:GLU:HG3	2.11	0.50
2:C:42:THR:N	3:C:2000:MES:O2S	2.41	0.50
1:B:254:ARG:HA	1:B:283:ASP:HB3	1.92	0.50
1:B:83:SER:HB2	1:B:151:PRO:O	2.11	0.50
1:B:308:LYS:NZ	1:B:308:LYS:HB3	2.26	0.50
1:A:368:ASP:CG	1:A:371:GLN:HG3	2.32	0.50
1:A:324:ILE:H	1:A:324:ILE:CD1	2.24	0.50
1:B:304:ILE:HD12	1:B:304:ILE:N	2.27	0.50
2:C:16:ILE:HG21	2:C:42:THR:OG1	2.11	0.50
1:A:380:ILE:HD11	2:C:102:ALA:HB2	1.94	0.49
2:C:128:ILE:HG23	2:C:133:MET:HB2	1.93	0.49
1:A:380:ILE:HD12	1:A:380:ILE:N	2.27	0.49
1:B:214:GLN:HG2	1:B:216:ILE:CD1	2.43	0.49
1:A:8:SER:HB3	1:A:61:GLN:HE21	1.77	0.49
2:C:33:MET:HE1	2:C:236:LEU:HD12	1.94	0.49
1:A:278:LYS:HE3	1:A:308:LYS:HE3	1.93	0.49
1:A:204:THR:HG22	1:A:232:ASP:HB2	1.93	0.49
1:A:348:GLN:HG3	1:B:346:LYS:HG2	1.94	0.49
1:B:216:ILE:HD12	1:B:216:ILE:N	2.27	0.48
1:A:317:ILE:HD12	1:A:349:LEU:HD21	1.94	0.48
2:C:164:PRO:HG2	2:C:167:CYS:SG	2.53	0.48
1:A:367:ILE:HD12	1:A:372:ILE:CD1	2.42	0.48
1:B:21:GLU:HA	1:B:21:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:VAL:O	2:D:188:VAL:HG23	2.12	0.48
1:A:13:GLN:NE2	1:A:62:PHE:H	2.12	0.48
1:B:372:ILE:HD13	1:B:389:ILE:HD12	1.95	0.48
2:C:1:MET:HE3	2:C:26:PRO:HG3	1.95	0.48
1:A:245:SER:O	1:A:272:SER:HA	2.14	0.48
2:C:103:LEU:HG	2:C:114:THR:HG23	1.96	0.48
2:C:114:THR:CG2	2:C:115:LEU:H	2.24	0.48
2:C:67:LEU:HD11	2:C:80:ILE:HD13	1.96	0.48
1:B:13:GLN:HE22	1:B:61:GLN:HA	1.78	0.48
1:B:271:ASN:HB3	1:B:397:LEU:HD22	1.96	0.47
1:B:27:PRO:O	1:B:31:GLN:HG3	2.14	0.47
1:B:303:THR:C	1:B:304:ILE:HD12	2.35	0.47
1:A:332:ASN:O	1:A:362:ALA:HA	2.14	0.47
1:A:386:GLN:HE22	1:A:420:GLY:N	2.11	0.47
1:B:138:THR:CG2	1:B:140:ILE:HD11	2.44	0.47
1:A:110:ILE:HD12	1:A:110:ILE:N	2.29	0.47
1:B:260:GLN:HE21	1:B:262:ASN:HD21	1.62	0.47
1:A:316:LEU:C	1:A:316:LEU:HD13	2.34	0.47
1:A:372:ILE:HG12	1:A:389:ILE:HD12	1.98	0.46
1:B:298:ARG:HD3	1:B:329:GLN:HB2	1.97	0.46
1:A:33:LEU:HD13	1:A:33:LEU:C	2.36	0.46
1:A:179:GLU:HG3	1:A:209:ALA:O	2.15	0.46
1:A:372:ILE:CG1	1:A:389:ILE:HD12	2.46	0.46
1:A:386:GLN:O	1:A:390:ILE:HD13	2.14	0.46
1:A:9:ASN:HB3	1:A:12:GLN:HB3	1.98	0.46
1:B:155:MET:HG2	1:B:157:ILE:HD11	1.98	0.46
1:A:271:ASN:HB3	1:A:397:LEU:CD2	2.46	0.46
2:C:2:LEU:HD22	2:C:166:LEU:HD21	1.97	0.46
1:A:18:PHE:CD1	1:A:25:ARG:HD3	2.52	0.45
1:B:396:GLU:HB2	4:B:543:HOH:O	2.15	0.45
2:C:113:GLU:CD	2:C:114:THR:H	2.19	0.45
1:A:275:MET:SD	1:A:414:ILE:HG23	2.57	0.45
1:B:306:SER:HA	1:B:337:MET:HB2	1.98	0.45
1:A:253:LEU:C	1:A:253:LEU:HD23	2.36	0.45
1:B:395:ALA:HA	1:B:398:THR:OG1	2.17	0.45
1:A:301:HIS:O	1:A:332:ASN:HA	2.15	0.45
1:A:82:ASP:OD2	1:A:150:LYS:HE2	2.17	0.45
1:A:18:PHE:CE1	1:A:25:ARG:HD3	2.52	0.45
1:A:234:LEU:HD23	1:A:260:GLN:HB2	1.99	0.45
1:B:127:LEU:HD23	1:B:127:LEU:C	2.36	0.45
1:A:44:ARG:HH21	1:A:53:PRO:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:HG2	1:B:212:HIS:HB2	1.98	0.45
1:B:125:VAL:HG13	1:B:126:PHE:CD1	2.51	0.44
1:B:384:ASP:O	1:B:388:MET:HG3	2.17	0.44
1:B:360:HIS:HD2	1:B:360:HIS:O	2.00	0.44
1:A:226:HIS:HE1	4:A:461:HOH:O	2.01	0.44
1:A:92:ARG:NE	1:A:135:GLN:OE1	2.49	0.44
2:C:30:HIS:HB2	2:C:199:ILE:HD13	1.99	0.44
1:A:92:ARG:HH11	1:A:92:ARG:HG3	1.81	0.44
2:C:120:PHE:CE1	2:C:124:MET:CE	3.01	0.44
1:A:321:GLN:O	1:A:322:HIS:CB	2.65	0.44
2:D:95:ASN:HA	2:D:98:PHE:HB3	1.99	0.44
1:B:332:ASN:O	1:B:362:ALA:HA	2.18	0.44
1:A:140:ILE:HD13	1:A:152:LEU:HD21	2.00	0.43
1:B:108:VAL:HG22	1:B:140:ILE:HD12	2.01	0.43
2:C:6:ASP:O	2:C:8:HIS:HD2	2.00	0.43
2:D:157:LEU:O	2:D:157:LEU:HD23	2.17	0.43
2:C:149:GLY:O	2:C:153:ARG:HG3	2.19	0.43
1:B:138:THR:HG22	1:B:140:ILE:CD1	2.47	0.43
2:C:138:LEU:HD22	2:C:138:LEU:H	1.84	0.43
2:C:28:GLU:OE1	2:C:30:HIS:HE1	2.01	0.43
2:C:113:GLU:OE1	2:C:114:THR:N	2.52	0.43
2:C:121:GLN:O	2:C:125:GLU:HG3	2.19	0.43
1:A:41:LEU:CD1	1:A:58:ILE:HG22	2.47	0.43
2:C:107:ARG:O	2:C:109:TYR:O	2.37	0.43
1:A:362:ALA:HB3	1:B:360:HIS:NE2	2.34	0.43
1:A:92:ARG:HE	1:A:135:GLN:CD	2.22	0.43
1:A:91:GLY:HA2	1:A:171:TYR:CE1	2.54	0.43
1:A:307:ASP:O	1:A:308:LYS:HB2	2.19	0.43
2:D:156:ILE:N	2:D:156:ILE:HD12	2.34	0.43
1:B:335:LEU:HD21	1:B:367:ILE:HD13	2.01	0.43
1:A:307:ASP:OD1	1:A:338:GLY:HA3	2.19	0.42
1:A:294:PHE:CE2	1:A:325:LYS:HG3	2.54	0.42
2:C:124:MET:C	2:C:128:ILE:HD13	2.40	0.42
2:C:204:TYR:CD2	2:C:247:GLN:HB3	2.55	0.42
2:C:33:MET:HE1	2:C:236:LEU:CD1	2.49	0.42
1:A:373:PHE:CZ	2:C:50:ARG:HD2	2.53	0.42
1:B:89:VAL:O	1:B:92:ARG:HD3	2.20	0.42
2:D:100:GLN:O	2:D:104:ASN:ND2	2.52	0.42
1:A:13:GLN:NE2	1:A:61:GLN:HA	2.31	0.42
1:B:215:HIS:C	1:B:216:ILE:HD12	2.40	0.42
1:B:209:ALA:HA	1:B:237:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:PRO:HB3	2:C:243:TRP:CD1	2.55	0.42
1:B:144:ARG:HH21	1:B:144:ARG:HG3	1.85	0.41
2:C:124:MET:O	2:C:128:ILE:HD13	2.20	0.41
1:A:347:PRO:HB3	1:A:360:HIS:CE1	2.54	0.41
1:B:402:ARG:HA	1:B:402:ARG:HD3	1.82	0.41
1:B:253:LEU:HD23	1:B:254:ARG:N	2.34	0.41
1:A:373:PHE:CE1	2:C:50:ARG:HD2	2.56	0.41
1:A:419:PRO:C	1:A:421:GLY:H	2.24	0.41
2:C:120:PHE:CZ	2:C:124:MET:HE1	2.55	0.41
1:A:380:ILE:HD12	1:A:380:ILE:H	1.84	0.41
2:C:116:ASP:OD2	2:C:116:ASP:N	2.53	0.41
1:A:277:VAL:O	1:A:278:LYS:C	2.59	0.41
1:B:58:ILE:C	1:B:58:ILE:HD12	2.41	0.41
2:C:128:ILE:HD12	2:C:157:LEU:HD11	2.01	0.41
1:A:347:PRO:HD2	1:B:347:PRO:O	2.20	0.41
1:A:92:ARG:HG3	1:A:92:ARG:NH1	2.36	0.41
2:C:93:VAL:O	2:C:142:VAL:HG23	2.20	0.41
1:B:226:HIS:HE1	4:B:449:HOH:O	2.02	0.41
1:A:55:GLU:C	1:A:57:LEU:H	2.24	0.40
2:C:177:ASP:O	2:C:181:LEU:HB2	2.22	0.40
1:B:143:LYS:HB2	1:B:146:GLN:HG2	2.02	0.40
2:C:130:LEU:C	2:C:130:LEU:HD23	2.41	0.40
1:B:222:ASN:HB2	1:B:223:PRO:CD	2.50	0.40
1:A:376:ARG:HA	1:A:380:ILE:O	2.22	0.40
1:A:372:ILE:O	1:A:376:ARG:HG3	2.21	0.40
1:B:367:ILE:HG21	1:B:372:ILE:HD11	2.02	0.40
2:C:157:LEU:O	2:C:161:VAL:HG23	2.21	0.40
1:A:124:GLU:OE2	1:A:230:HIS:HD2	2.04	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	414/423 (98%)	394 (95%)	19 (5%)	1 (0%)	52 59
1	B	412/423 (97%)	398 (97%)	13 (3%)	1 (0%)	52 59
2	C	245/267 (92%)	233 (95%)	10 (4%)	2 (1%)	24 22
2	D	36/267 (14%)	35 (97%)	1 (3%)	0	100 100
All	All	1107/1380 (80%)	1060 (96%)	43 (4%)	4 (0%)	39 42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	117	ARG
1	B	278	LYS
2	C	142	VAL
1	A	278	LYS

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	345/350 (99%)	335 (97%)	10 (3%)	50 62
1	B	343/350 (98%)	337 (98%)	6 (2%)	68 81
2	C	211/228 (92%)	202 (96%)	9 (4%)	35 43
2	D	36/228 (16%)	35 (97%)	1 (3%)	51 63
All	All	935/1156 (81%)	909 (97%)	26 (3%)	51 63

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	9	ASN
1	A	25	ARG
1	A	187	GLU
1	A	203	PHE
1	A	214	GLN
1	A	288	LEU

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Mol	Chain	Res	Type
1	A	324	ILE
1	A	367	ILE
1	A	375	LEU
1	B	12	GLN
1	B	65	ILE
1	B	92	ARG
1	B	143	LYS
1	B	360	HIS
1	B	369	ASP
2	C	7	LEU
2	C	50	ARG
2	C	90	ILE
2	C	113	GLU
2	C	116	ASP
2	C	117	ARG
2	C	234	LYS
2	C	245	THR
2	C	247	GLN
2	D	155	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	13	GLN
1	A	46	HIS
1	A	59	ASN
1	A	61	GLN
1	A	156	HIS
1	A	167	ASN
1	A	212	HIS
1	A	226	HIS
1	A	230	HIS
1	A	260	GLN
1	A	299	GLN
1	A	322	HIS
1	A	329	GLN
1	A	371	GLN
1	A	386	GLN
1	A	408	GLN
1	B	13	GLN
1	B	31	GLN

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Mol	Chain	Res	Type
1	B	46	HIS
1	B	115	GLN
1	B	122	GLN
1	B	226	HIS
1	B	260	GLN
1	B	291	ASN
1	B	329	GLN
1	B	333	ASN
1	B	348	GLN
1	B	371	GLN
1	B	386	GLN
1	B	387	GLN
1	B	416	GLN
2	C	8	HIS
2	C	30	HIS
2	C	36	ASN
2	C	95	ASN
2	C	112	GLN
2	C	121	GLN
2	C	143	ASN
2	C	189	ASN
2	C	203	HIS
2	D	100	GLN
2	D	104	ASN
2	D	189	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)

1 ligand is 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	$\#\|Z\| > 2$
3	MES	C	2000	-	11,12,12	0.37	0	14,16,16	1.28	2 (14%)

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	MES	C	2000	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2000	MES	O1S-S-C8	2.77	109.27	106.91
3	C	2000	MES	O2S-S-C8	2.85	109.33	106.91

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
3	C	2000	MES	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	416/423 (98%)	0.18	16 (3%) 44 43	19, 30, 50, 83	0
1	B	414/423 (97%)	0.10	13 (3%) 52 51	17, 28, 51, 72	0
2	C	247/267 (92%)	0.45	26 (10%) 8 7	21, 35, 67, 84	0
2	D	42/267 (15%)	4.33	32 (76%) 0 0	55, 72, 92, 95	0
All	All	1119/1380 (81%)	0.36	87 (7%) 16 15	17, 31, 64, 95	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	184	VAL	18.1
2	D	185	ALA	13.0
1	A	422	ALA	10.0
2	C	118	PHE	10.0
2	D	86	TYR	9.5
2	D	156	ILE	8.4
1	B	422	ALA	8.1
2	D	87	PRO	7.4
2	D	193	ASP	7.0
2	D	160	ALA	6.7
2	C	115	LEU	6.1
2	C	114	THR	6.0
2	C	116	ASP	5.9
2	D	106	VAL	5.7
2	D	103	LEU	5.7
2	D	157	LEU	5.5
1	B	22	GLY	5.3
2	D	188	VAL	5.3
2	C	246	GLU	5.2
1	A	423	ARG	5.1
2	C	111	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	C	119	ASP	4.7
2	D	105	ALA	4.6
2	D	99	LEU	4.5
2	D	186	ASP	4.4
2	C	120	PHE	4.3
1	A	22	GLY	4.1
1	A	21	GLU	4.1
2	D	98	PHE	4.1
2	D	187	GLY	3.9
2	D	96	GLN	3.8
2	D	102	ALA	3.7
2	D	95	ASN	3.7
1	A	164	GLU	3.7
1	B	421	GLY	3.7
2	D	88	VAL	3.7
2	C	117	ARG	3.6
2	D	155	ASP	3.5
2	D	161	VAL	3.5
2	D	162	LEU	3.5
1	A	94	VAL	3.4
2	D	90	ILE	3.4
2	C	137	LEU	3.4
1	A	67	GLY	3.4
2	D	93	VAL	3.3
2	C	124	MET	3.3
1	B	374	TYR	3.3
2	D	94	SER	3.3
1	A	63	VAL	3.2
2	D	159	MET	3.2
1	A	137	VAL	3.2
1	B	379	GLY	3.1
2	D	183	VAL	3.1
1	A	68	GLU	3.1
2	C	245	THR	3.0
1	B	44	ARG	3.0
2	D	191	LEU	3.0
1	A	58	ILE	3.0
2	D	104	ASN	2.9
2	D	100	GLN	2.8
2	C	178	ILE	2.8
1	A	24	LYS	2.7
1	B	373	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	115	GLN	2.7
2	C	247	GLN	2.6
2	C	135	GLU	2.5
2	C	206	ARG	2.5
1	B	381	ASN	2.5
1	B	420	GLY	2.4
2	D	163	GLU	2.4
1	B	402	ARG	2.4
2	C	122	ASP	2.4
2	C	136	ASP	2.4
1	A	322	HIS	2.3
1	A	65	ILE	2.3
2	C	123	LEU	2.3
2	C	99	LEU	2.3
2	C	134	PRO	2.3
2	C	244	LEU	2.3
2	C	113	GLU	2.3
2	C	179	ASP	2.2
1	B	377	SER	2.2
2	C	138	LEU	2.2
1	B	372	ILE	2.1
2	C	110	ARG	2.1
1	A	420	GLY	2.1
1	B	375	LEU	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
3	MES	C	2000	12/12	0.81	0.29	9.76	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.