Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:53 PM GMT

PDB ID	:	1R30
Title	:	The Crystal Structure of Biotin Synthase, an S-Adenosylmethionine-Dependent Radical Enzyme
Authors	:	Berkovitch, F.; Nicolet, Y.; Wan, J.T.; Jarrett, J.T.; Drennan, C.L.
Deposited on	:	2003-09-30
Resolution	:	3.40 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:

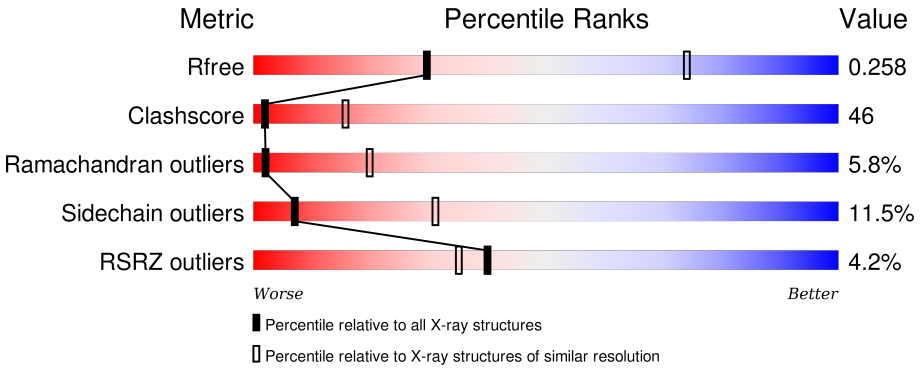
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	369	2% 32% 44% 8% 15%
1	B	369	5% 33% 42% 9% 15%

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	SAM	A	501	-	-	X	-
2	SAM	B	501	-	-	X	-
5	DTB	A	502	-	-	X	X
5	DTB	B	502	-	-	X	-
6	TRS	A	503	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4982 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 Biotin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2425	1517	422	466	20			
1	B	313	Total	C	N	O	S	0	0	0
			2441	1526	428	467	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	EXPRESSION TAG	UNP P12996
A	-21	SER	-	EXPRESSION TAG	UNP P12996
A	-20	SER	-	EXPRESSION TAG	UNP P12996
A	-19	HIS	-	EXPRESSION TAG	UNP P12996
A	-18	HIS	-	EXPRESSION TAG	UNP P12996
A	-17	HIS	-	EXPRESSION TAG	UNP P12996
A	-16	HIS	-	EXPRESSION TAG	UNP P12996
A	-15	HIS	-	EXPRESSION TAG	UNP P12996
A	-14	HIS	-	EXPRESSION TAG	UNP P12996
A	-13	ASP	-	LINKER	UNP P12996
A	-12	TYR	-	LINKER	UNP P12996
A	-11	ASP	-	LINKER	UNP P12996
A	-10	ILE	-	LINKER	UNP P12996
A	-9	PRO	-	LINKER	UNP P12996
A	-8	THR	-	LINKER	UNP P12996
A	-7	THR	-	LINKER	UNP P12996
A	-6	GLU	-	LINKER	UNP P12996
A	-5	ASN	-	LINKER	UNP P12996
A	-4	LEU	-	LINKER	UNP P12996
A	-3	TYR	-	LINKER	UNP P12996
A	-2	PHE	-	LINKER	UNP P12996
A	-1	GLN	-	LINKER	UNP P12996
A	0	GLY	-	LINKER	UNP P12996
A	1	SER	-	LINKER	UNP P12996
B	-22	GLY	-	EXPRESSION TAG	UNP P12996

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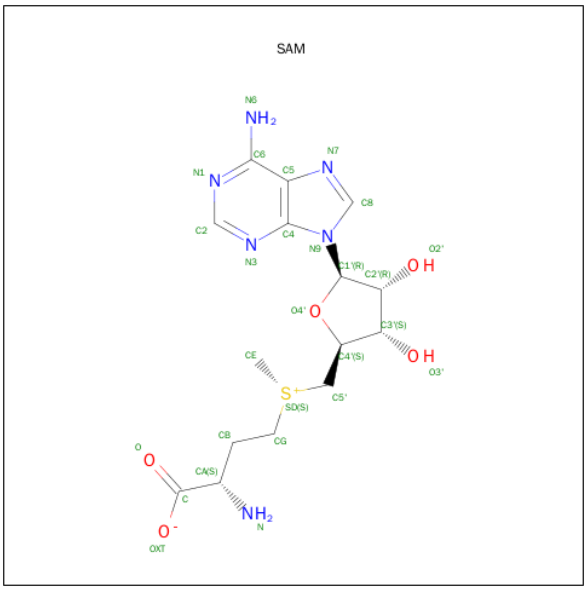
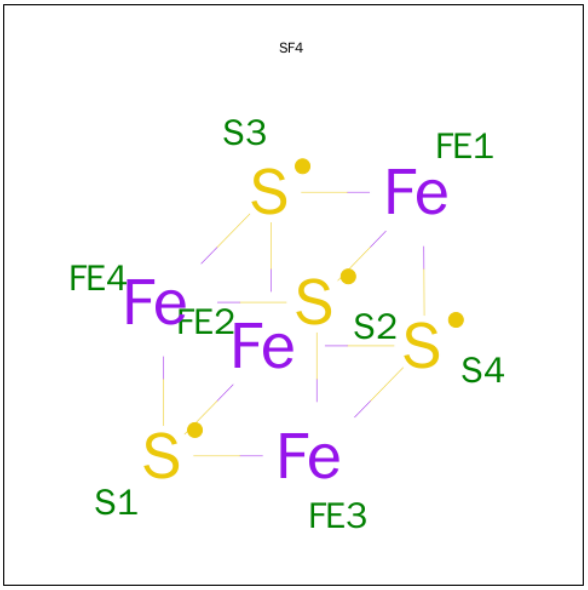
Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	SER	-	EXPRESSION TAG	UNP P12996
B	-20	SER	-	EXPRESSION TAG	UNP P12996
B	-19	HIS	-	EXPRESSION TAG	UNP P12996
B	-18	HIS	-	EXPRESSION TAG	UNP P12996
B	-17	HIS	-	EXPRESSION TAG	UNP P12996
B	-16	HIS	-	EXPRESSION TAG	UNP P12996
B	-15	HIS	-	EXPRESSION TAG	UNP P12996
B	-14	HIS	-	EXPRESSION TAG	UNP P12996
B	-13	ASP	-	LINKER	UNP P12996
B	-12	TYR	-	LINKER	UNP P12996
B	-11	ASP	-	LINKER	UNP P12996
B	-10	ILE	-	LINKER	UNP P12996
B	-9	PRO	-	LINKER	UNP P12996
B	-8	THR	-	LINKER	UNP P12996
B	-7	THR	-	LINKER	UNP P12996
B	-6	GLU	-	LINKER	UNP P12996
B	-5	ASN	-	LINKER	UNP P12996
B	-4	LEU	-	LINKER	UNP P12996
B	-3	TYR	-	LINKER	UNP P12996
B	-2	PHE	-	LINKER	UNP P12996
B	-1	GLN	-	LINKER	UNP P12996
B	0	GLY	-	LINKER	UNP P12996
B	1	SER	-	LINKER	UNP P12996

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



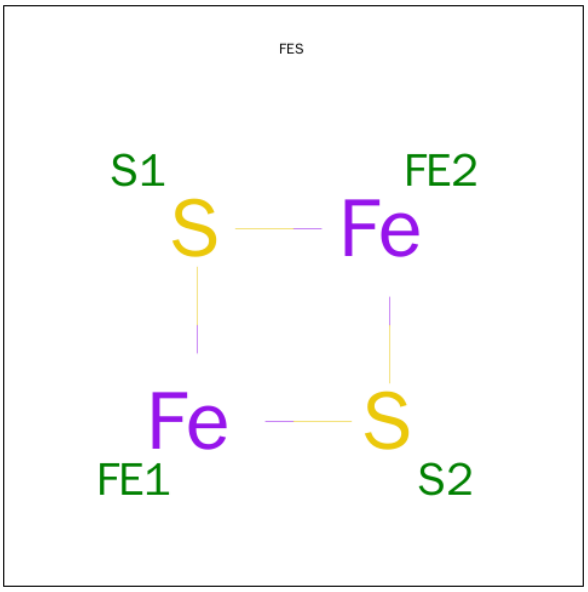
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



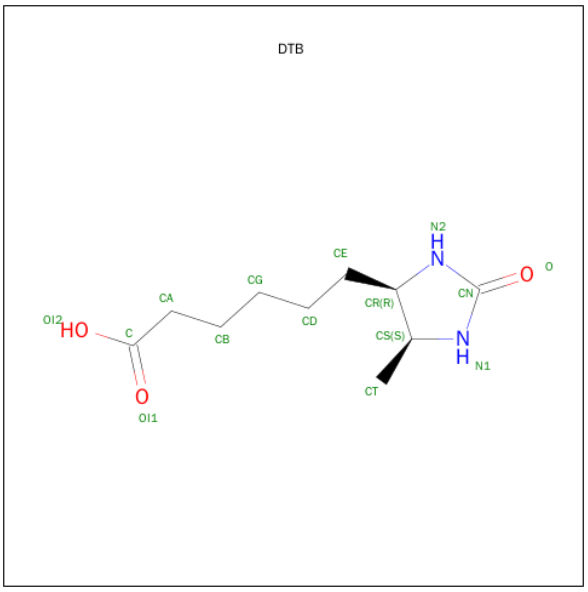
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Fe	S		0	0
			8	4	4			
3	B	1	Total	Fe	S		0	0
			8	4	4			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	B	1	Total Fe S 4 2 2	0	0

- Molecule 5 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (three-letter code: DTB) (formula: $C_{10}H_{18}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 15 10 2 3	0	0

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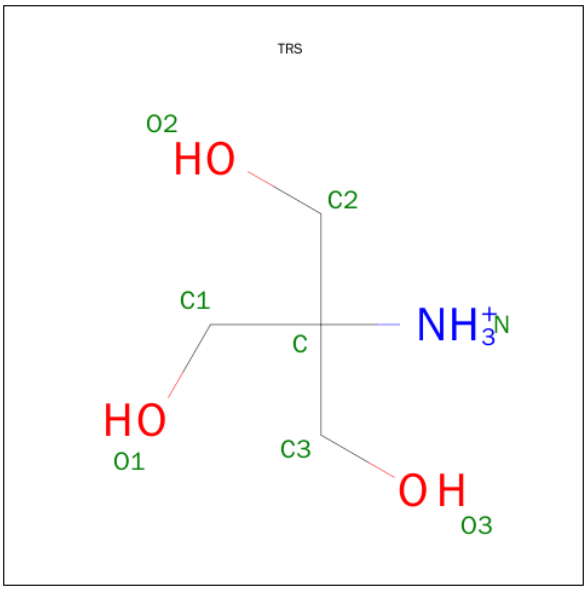
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			15	10	2	3		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

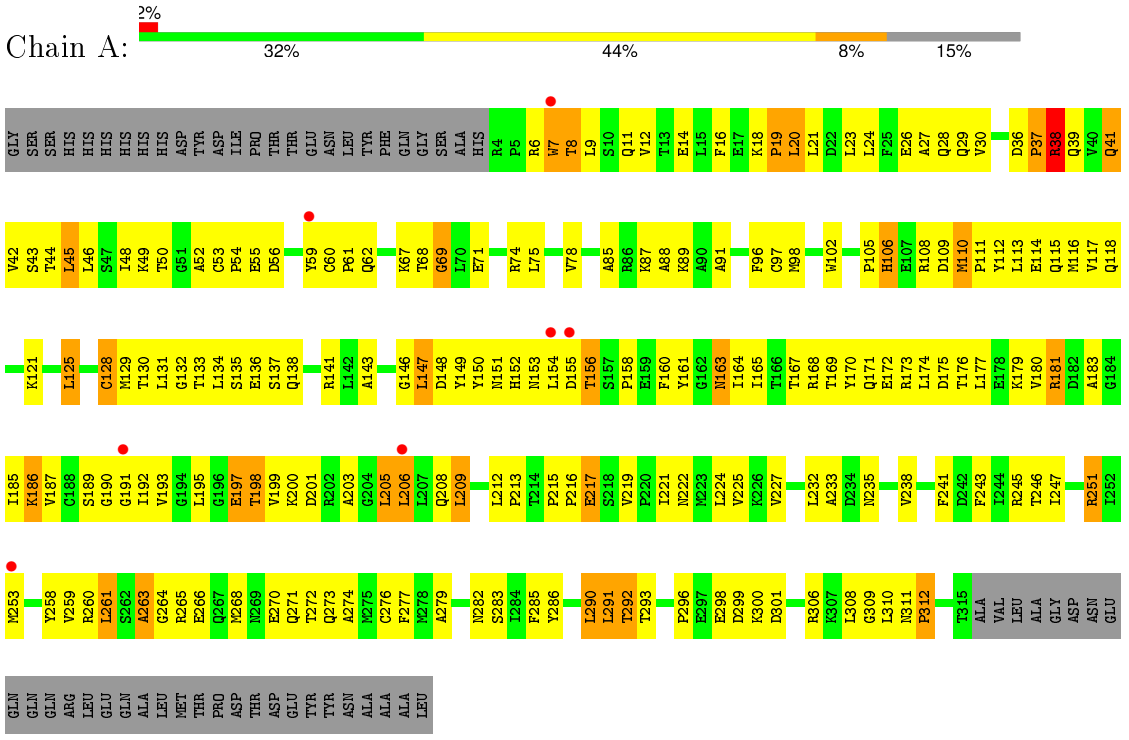


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		

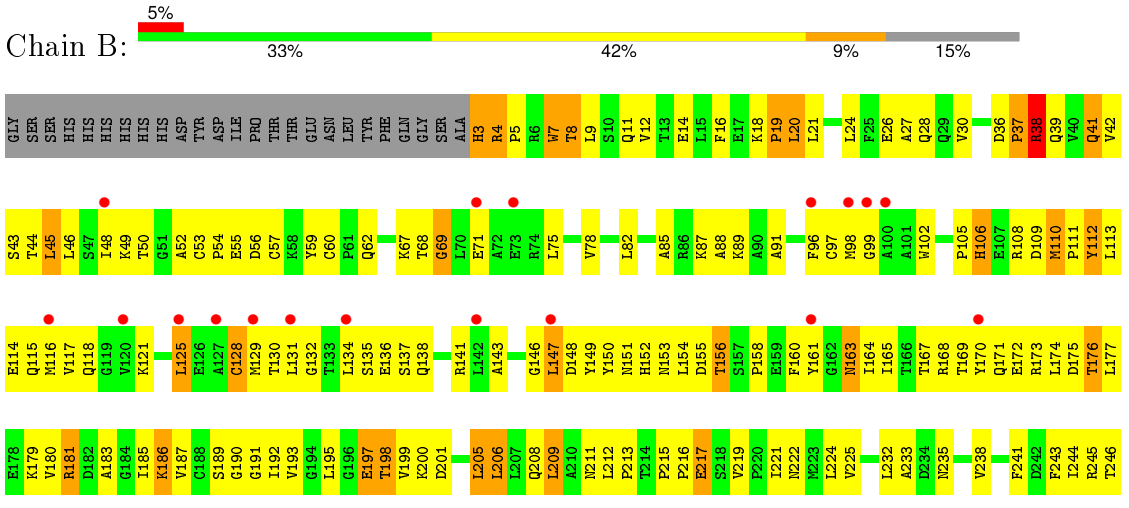
3 Residue-property plots (i)

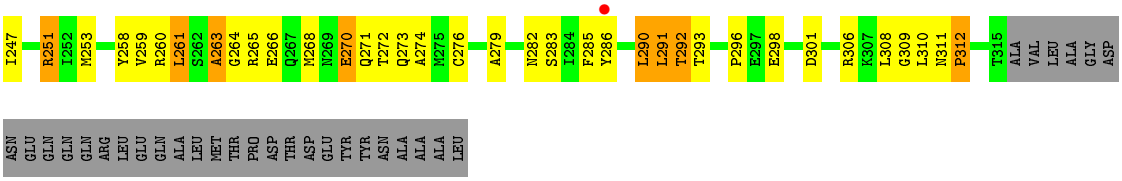
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Biotin synthase



- Molecule 1: Biotin synthase




I247 R251 I252 M253 Y258 V259 R260 L261 S262 A263 G264 R265 E266 Q267 M268 N269 E270 Q271 T272 Q273 A274 N275 C276 A279 N282 S283 I284 F285 Y286 L290 L291 T292 T293 P296 E297 E298 D301 R306 K307 L308 G309 L310 N311 P312 T315 ALA VAL LEU ALA GLY ASP
ASN GLU GLN GLN GLN ARG LEU GLU GLN ALA LEU MET THR PRO ASP THR ASP GLU TYR TYR ASN ALA ALA ALA LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.69Å 155.69Å 90.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.45 – 3.40 44.45 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.45-3.40) 98.2 (44.45-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 3.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.256 , 0.300 0.224 , 0.258	Depositor DCC
R_{free} test set	1242 reflections (7.66%)	DCC
Wilson B-factor (Å^2)	113.1	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 108.8	EDS
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 17464 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4982	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: DTB, TRS, SF4, SAM, FES

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	0.39	0/2468	0.67	0/3342
1	B	0.40	0/2485	0.67	0/3364
All	All	0.40	0/4953	0.67	0/6706

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

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	2425	0	2400	228	0
1	B	2441	0	2418	233	0
2	A	27	0	22	11	0
2	B	27	0	22	13	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	15	0	17	9	0
5	B	15	0	17	11	0
6	A	8	0	12	1	0
All	All	4982	0	4908	459	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 46.

All (459) 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:128:CYS:HB2	1:A:149:TYR:HB2	1.43	1.00
1:A:165:ILE:HD13	1:A:168:ARG:HH22	1.29	0.98
1:B:128:CYS:HB2	1:B:149:TYR:HB2	1.43	0.98
1:B:165:ILE:HD13	1:B:168:ARG:HH22	1.29	0.97
5:A:502:DTB:OI1	5:A:502:DTB:HCD1	1.65	0.97
1:A:310:LEU:HD21	1:B:21:LEU:HD12	1.47	0.94
1:A:291:LEU:HD22	2:A:501:SAM:HE1	1.50	0.94
1:A:293:THR:HG23	5:A:502:DTB:OI2	1.67	0.94
1:A:28:GLN:HE22	1:B:28:GLN:HE22	0.96	0.91
5:B:502:DTB:HCD1	5:B:502:DTB:OI1	1.69	0.91
1:A:44:THR:HG21	1:A:88:ALA:HB1	1.52	0.91
1:B:44:THR:HG21	1:B:88:ALA:HB1	1.51	0.90
1:A:21:LEU:HD12	1:B:310:LEU:HD21	1.53	0.90
1:B:130:THR:HB	1:B:151:ASN:HB3	1.56	0.87
1:A:117:VAL:HG11	1:A:147:LEU:H	1.38	0.87
1:B:117:VAL:HG11	1:B:147:LEU:H	1.39	0.87
1:A:28:GLN:NE2	1:B:28:GLN:HE22	1.73	0.86
1:B:165:ILE:HD13	1:B:168:ARG:NH2	1.92	0.85
1:A:130:THR:HB	1:A:151:ASN:HB3	1.57	0.84
1:A:165:ILE:HD13	1:A:168:ARG:NH2	1.91	0.83
1:B:125:LEU:H	1:B:125:LEU:HD12	1.42	0.83
1:A:163:ASN:HD22	1:A:163:ASN:N	1.76	0.83
1:B:163:ASN:HD22	1:B:163:ASN:N	1.75	0.82
1:A:28:GLN:HE22	1:B:28:GLN:NE2	1.76	0.82
1:A:125:LEU:H	1:A:125:LEU:HD12	1.42	0.82
1:A:132:GLY:HA2	2:A:501:SAM:OXT	1.79	0.81
1:B:198:THR:HG23	1:B:201:ASP:OD2	1.81	0.80
1:B:192:ILE:HB	1:B:195:LEU:HD11	1.63	0.80
1:A:192:ILE:HB	1:A:195:LEU:HD11	1.62	0.80
1:A:198:THR:HG23	1:A:201:ASP:OD2	1.82	0.79
2:B:501:SAM:C5	5:B:502:DTB:HCA2	2.11	0.79
2:A:501:SAM:C5	5:A:502:DTB:HCA2	2.14	0.78
1:A:222:ASN:HB3	1:A:263:ALA:HB3	1.66	0.76
1:B:291:LEU:HD22	2:B:501:SAM:HE1	1.68	0.76
1:B:38:ARG:HA	1:B:310:LEU:HD22	1.67	0.76
1:B:222:ASN:HB3	1:B:263:ALA:HB3	1.66	0.75
1:A:38:ARG:HA	1:A:310:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD13	1:A:131:LEU:HD13	1.69	0.75
1:B:105:PRO:HG3	1:B:131:LEU:HB3	1.70	0.73
1:A:105:PRO:HG3	1:A:131:LEU:HB3	1.70	0.73
1:A:45:LEU:HD13	1:A:285:PHE:CE2	2.24	0.73
1:B:221:ILE:HD12	1:B:247:ILE:HD13	1.70	0.73
1:A:38:ARG:HA	1:A:310:LEU:CD2	2.19	0.72
1:B:113:LEU:HD13	1:B:131:LEU:HD13	1.70	0.72
1:B:38:ARG:HA	1:B:310:LEU:CD2	2.19	0.72
1:A:113:LEU:HD23	1:A:116:MET:HE1	1.71	0.72
1:B:45:LEU:HD13	1:B:285:PHE:CE2	2.24	0.72
1:A:8:THR:HG23	1:A:11:GLN:OE1	1.89	0.71
1:A:310:LEU:HD21	1:B:21:LEU:CD1	2.20	0.71
1:A:45:LEU:HB2	1:A:97:CYS:O	1.91	0.71
1:A:221:ILE:HD12	1:A:247:ILE:HD13	1.72	0.70
1:B:8:THR:HG23	1:B:11:GLN:OE1	1.91	0.70
1:B:170:TYR:OH	1:B:208:GLN:HG2	1.92	0.69
1:A:291:LEU:HD13	5:A:502:DTB:HCE2	1.73	0.69
1:A:170:TYR:OH	1:A:208:GLN:HG2	1.93	0.69
1:A:224:LEU:HD12	1:A:225:VAL:N	2.08	0.68
1:B:26:GLU:O	1:B:30:VAL:HG23	1.93	0.68
1:B:45:LEU:HB2	1:B:97:CYS:O	1.93	0.68
1:A:62:GLN:HE22	1:A:291:LEU:HD23	1.58	0.68
1:A:26:GLU:O	1:A:30:VAL:HG23	1.93	0.68
1:A:97:CYS:HA	1:A:128:CYS:O	1.94	0.68
1:B:97:CYS:HA	1:B:128:CYS:O	1.94	0.68
1:B:62:GLN:HE22	1:B:291:LEU:HD23	1.57	0.67
1:A:308:LEU:HD23	1:B:20:LEU:HD23	1.75	0.67
1:A:8:THR:OG1	1:A:11:GLN:HB2	1.94	0.67
1:A:271:GLN:HG2	1:B:272:THR:OG1	1.94	0.67
1:B:8:THR:OG1	1:B:11:GLN:HB2	1.95	0.67
1:B:224:LEU:HD12	1:B:225:VAL:N	2.08	0.67
1:A:169:THR:HB	1:A:172:GLU:HB2	1.77	0.66
1:B:169:THR:HB	1:B:172:GLU:HB2	1.77	0.66
1:A:266:GLU:OE1	6:A:503:TRS:H12	1.95	0.66
1:B:153:ASN:HB3	1:B:190:GLY:O	1.96	0.66
1:A:21:LEU:CD1	1:B:310:LEU:HD21	2.24	0.66
1:A:290:LEU:H	1:A:290:LEU:HD12	1.60	0.66
1:B:163:ASN:HD22	1:B:163:ASN:H	1.43	0.65
1:B:290:LEU:H	1:B:290:LEU:HD12	1.61	0.65
1:A:291:LEU:HD22	2:A:501:SAM:CE	2.23	0.65
1:A:258:TYR:HD1	1:A:282:ASN:HD21	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:SAM:N7	5:A:502:DTB:HCA2	2.12	0.65
1:B:56:ASP:OD2	1:B:167:THR:HG23	1.97	0.65
1:B:45:LEU:CB	1:B:97:CYS:HB2	2.27	0.64
1:B:113:LEU:HD23	1:B:116:MET:HE1	1.80	0.64
1:A:56:ASP:OD2	1:A:167:THR:HG23	1.98	0.64
1:A:176:THR:O	1:A:180:VAL:HG23	1.98	0.64
1:A:45:LEU:CB	1:A:97:CYS:HB2	2.27	0.64
1:B:258:TYR:HD1	1:B:282:ASN:HD21	1.46	0.63
1:A:163:ASN:HD22	1:A:163:ASN:H	1.44	0.63
1:B:176:THR:O	1:B:180:VAL:HG23	1.98	0.63
2:B:501:SAM:N7	5:B:502:DTB:HCA2	2.13	0.63
1:B:117:VAL:CG1	1:B:147:LEU:H	2.12	0.62
1:B:78:VAL:HG11	1:B:115:GLN:HG2	1.80	0.62
1:A:78:VAL:HG11	1:A:115:GLN:HG2	1.81	0.62
1:A:158:PRO:HG3	1:A:170:TYR:CZ	2.35	0.62
1:A:113:LEU:HD13	1:A:131:LEU:CD1	2.29	0.62
1:B:113:LEU:HD13	1:B:131:LEU:CD1	2.29	0.62
1:B:134:LEU:HD13	1:B:150:TYR:CE1	2.35	0.62
1:A:221:ILE:HD13	1:A:246:THR:HG22	1.82	0.62
1:A:134:LEU:HD13	1:A:150:TYR:CE1	2.35	0.61
1:A:45:LEU:HB3	1:A:97:CYS:HB2	1.81	0.61
1:A:117:VAL:CG1	1:A:147:LEU:H	2.12	0.61
1:B:163:ASN:ND2	1:B:163:ASN:N	2.48	0.61
1:B:263:ALA:HB2	5:B:502:DTB:HCG1	1.81	0.61
1:B:4:ARG:HB2	1:B:5:PRO:CD	2.31	0.61
1:B:3:HIS:N	1:B:3:HIS:HD1	1.99	0.61
1:B:221:ILE:HD13	1:B:246:THR:HG22	1.82	0.61
1:B:41:GLN:HE21	1:B:41:GLN:HA	1.66	0.60
1:A:271:GLN:O	1:A:274:ALA:HB3	2.02	0.60
1:B:216:PRO:HG2	1:B:219:VAL:HG22	1.83	0.60
1:B:291:LEU:HD22	2:B:501:SAM:CE	2.31	0.60
1:A:308:LEU:HD21	1:B:241:PHE:CE1	2.37	0.60
1:B:291:LEU:CD2	2:B:501:SAM:HE1	2.31	0.60
1:A:191:GLY:HA3	1:A:205:LEU:HD11	1.84	0.60
1:B:45:LEU:HB3	1:B:97:CYS:HB2	1.83	0.60
1:A:41:GLN:HA	1:A:41:GLN:HE21	1.65	0.59
1:B:271:GLN:O	1:B:274:ALA:HB3	2.02	0.59
1:A:181:ARG:HG3	1:A:181:ARG:NH1	2.16	0.59
1:B:181:ARG:NH1	1:B:181:ARG:HG3	2.16	0.59
1:A:181:ARG:HH11	1:A:181:ARG:HG3	1.67	0.59
1:A:153:ASN:HB3	1:A:190:GLY:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD23	1:B:308:LEU:HD23	1.84	0.59
1:A:152:HIS:CE1	1:A:173:ARG:HH21	2.21	0.59
1:B:152:HIS:CE1	1:B:173:ARG:HH21	2.21	0.59
1:B:181:ARG:HH11	1:B:181:ARG:HG3	1.67	0.59
1:A:216:PRO:HG2	1:A:219:VAL:HG22	1.83	0.59
1:B:158:PRO:HG3	1:B:170:TYR:CZ	2.36	0.58
1:A:59:TYR:HB3	1:A:232:LEU:HD12	1.84	0.58
1:B:191:GLY:HA3	1:B:205:LEU:HD11	1.85	0.58
1:A:18:LYS:HG3	1:A:19:PRO:HD2	1.85	0.58
1:A:186:LYS:CG	1:A:217:GLU:HG3	2.34	0.58
1:B:42:VAL:O	1:B:42:VAL:HG13	2.02	0.58
1:B:293:THR:HG23	5:B:502:DTB:OI2	2.03	0.58
1:A:222:ASN:CB	1:A:263:ALA:HB3	2.34	0.58
1:B:59:TYR:HB3	1:B:232:LEU:HD12	1.86	0.58
1:B:24:LEU:O	1:B:28:GLN:HG3	2.04	0.57
1:B:263:ALA:HB1	5:B:502:DTB:HCB2	1.85	0.57
5:B:502:DTB:HCD1	5:B:502:DTB:C	2.35	0.57
1:B:113:LEU:HD22	1:B:129:MET:CE	2.34	0.57
1:B:37:PRO:O	1:B:39:GLN:N	2.38	0.57
1:A:113:LEU:HD22	1:A:129:MET:CE	2.35	0.57
1:A:42:VAL:O	1:A:42:VAL:HG13	2.03	0.57
1:B:113:LEU:HD23	1:B:116:MET:CE	2.34	0.57
1:A:186:LYS:HG2	1:A:217:GLU:HG3	1.87	0.57
1:A:224:LEU:HD12	1:A:225:VAL:H	1.69	0.57
1:A:135:SER:O	1:A:137:SER:N	2.38	0.57
1:A:37:PRO:O	1:A:39:GLN:N	2.38	0.57
2:B:501:SAM:H5'1	5:B:502:DTB:HCT3	1.85	0.57
1:B:87:LYS:O	1:B:91:ALA:HB2	2.05	0.56
1:B:18:LYS:HG3	1:B:19:PRO:HD2	1.85	0.56
1:B:224:LEU:HD12	1:B:225:VAL:H	1.69	0.56
1:B:37:PRO:C	1:B:39:GLN:H	2.09	0.56
1:B:130:THR:O	1:B:130:THR:HG23	2.06	0.56
1:A:113:LEU:HD23	1:A:116:MET:CE	2.35	0.56
1:A:272:THR:OG1	1:B:271:GLN:HG2	2.04	0.56
1:A:24:LEU:O	1:A:28:GLN:HG3	2.05	0.56
1:A:112:TYR:HD1	1:A:112:TYR:N	2.04	0.56
1:B:141:ARG:HH11	1:B:141:ARG:HG2	1.70	0.56
1:B:129:MET:H	1:B:147:LEU:HD11	1.69	0.56
1:B:186:LYS:CG	1:B:217:GLU:HG3	2.35	0.56
1:A:9:LEU:C	1:A:9:LEU:HD23	2.26	0.56
1:B:135:SER:O	1:B:137:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LYS:HG2	1:B:217:GLU:HG3	1.88	0.56
1:A:75:LEU:HD23	1:A:75:LEU:C	2.27	0.56
1:B:112:TYR:CD1	1:B:112:TYR:N	2.74	0.56
1:B:112:TYR:HD1	1:B:112:TYR:N	2.03	0.56
1:B:75:LEU:HD23	1:B:75:LEU:C	2.26	0.56
1:B:45:LEU:HD21	1:B:290:LEU:HA	1.88	0.56
1:B:174:LEU:H	1:B:174:LEU:HD22	1.71	0.56
1:B:171:GLN:HA	1:B:174:LEU:HD23	1.88	0.56
1:B:222:ASN:CB	1:B:263:ALA:HB3	2.33	0.56
1:A:129:MET:H	1:A:147:LEU:HD11	1.70	0.56
1:A:37:PRO:C	1:A:39:GLN:H	2.09	0.55
1:A:141:ARG:HG2	1:A:141:ARG:HH11	1.71	0.55
1:A:125:LEU:HD12	1:A:125:LEU:N	2.19	0.55
1:B:264:GLY:O	1:B:268:MET:HE2	2.06	0.55
1:B:113:LEU:HA	1:B:116:MET:HE3	1.89	0.55
1:B:9:LEU:HD23	1:B:9:LEU:C	2.27	0.55
1:A:45:LEU:HD21	1:A:290:LEU:HA	1.88	0.55
1:A:171:GLN:HA	1:A:174:LEU:HD23	1.89	0.55
1:A:87:LYS:O	1:A:91:ALA:HB2	2.07	0.55
1:A:161:TYR:OH	1:A:168:ARG:NH2	2.40	0.55
1:A:12:VAL:CG2	1:A:253:MET:SD	2.95	0.55
1:A:169:THR:HB	1:A:172:GLU:H	1.72	0.54
1:B:149:TYR:CD1	1:B:186:LYS:HB3	2.42	0.54
1:A:130:THR:O	1:A:130:THR:HG23	2.07	0.54
1:A:112:TYR:N	1:A:112:TYR:CD1	2.74	0.54
1:A:271:GLN:CD	1:A:271:GLN:H	2.11	0.54
1:A:41:GLN:CA	1:A:41:GLN:HE21	2.19	0.54
1:B:161:TYR:OH	1:B:168:ARG:NH2	2.41	0.54
1:A:161:TYR:OH	1:A:173:ARG:HD2	2.07	0.54
1:B:161:TYR:OH	1:B:173:ARG:HD2	2.08	0.54
1:A:45:LEU:HD21	1:A:290:LEU:CA	2.38	0.54
1:B:169:THR:HB	1:B:172:GLU:H	1.72	0.54
1:B:146:GLY:O	1:B:147:LEU:C	2.47	0.54
1:A:163:ASN:ND2	1:A:163:ASN:N	2.49	0.54
1:B:271:GLN:CD	1:B:271:GLN:H	2.12	0.54
1:B:125:LEU:N	1:B:125:LEU:HD12	2.19	0.53
1:B:132:GLY:HA2	2:B:501:SAM:OXT	2.08	0.53
1:B:192:ILE:HD11	2:B:501:SAM:H2'	1.91	0.53
1:A:225:VAL:HG11	1:A:293:THR:HG21	1.90	0.53
1:B:45:LEU:HD21	1:B:290:LEU:CA	2.39	0.53
1:A:174:LEU:H	1:A:174:LEU:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLY:O	1:A:268:MET:HE2	2.08	0.53
1:A:68:THR:O	1:A:69:GLY:C	2.47	0.53
1:A:149:TYR:CD1	1:A:186:LYS:HB3	2.43	0.53
1:A:41:GLN:HG3	1:A:283:SER:OG	2.09	0.53
1:A:146:GLY:O	1:A:147:LEU:C	2.47	0.52
1:A:7:TRP:CH2	1:A:253:MET:HA	2.44	0.52
1:A:121:LYS:HE3	1:A:148:ASP:OD2	2.08	0.52
1:B:129:MET:N	1:B:147:LEU:HD11	2.24	0.52
1:B:134:LEU:HD22	1:B:150:TYR:CZ	2.44	0.52
1:B:174:LEU:CD2	1:B:174:LEU:H	2.22	0.52
1:B:7:TRP:CH2	1:B:253:MET:HA	2.44	0.52
1:B:68:THR:O	1:B:69:GLY:C	2.48	0.52
1:A:24:LEU:O	1:A:27:ALA:HB3	2.09	0.52
1:B:225:VAL:HG11	1:B:293:THR:HG21	1.91	0.52
1:A:261:LEU:HD13	1:A:265:ARG:HD2	1.91	0.52
1:B:265:ARG:NH2	1:B:301:ASP:OD2	2.42	0.52
1:B:46:LEU:HD21	1:B:98:MET:HG3	1.91	0.52
1:A:46:LEU:HD21	1:A:98:MET:HG3	1.92	0.52
1:B:121:LYS:HE3	1:B:148:ASP:OD2	2.09	0.52
1:B:114:GLU:O	1:B:118:GLN:HG2	2.09	0.52
1:A:62:GLN:HE22	1:A:291:LEU:CD2	2.23	0.52
1:B:41:GLN:HE21	1:B:41:GLN:CA	2.20	0.51
1:A:174:LEU:CD2	1:A:174:LEU:H	2.23	0.51
1:A:143:ALA:HB2	1:A:185:ILE:HD11	1.92	0.51
1:B:12:VAL:CG2	1:B:253:MET:SD	2.98	0.51
1:B:143:ALA:HB2	1:B:185:ILE:HD11	1.91	0.51
1:B:9:LEU:C	1:B:11:GLN:H	2.13	0.51
1:B:3:HIS:ND1	1:B:3:HIS:N	2.58	0.51
1:A:129:MET:N	1:A:147:LEU:HD11	2.26	0.51
1:B:41:GLN:HG3	1:B:283:SER:OG	2.10	0.51
1:B:153:ASN:ND2	2:B:501:SAM:H4'	2.25	0.51
1:A:59:TYR:CD2	1:A:60:CYS:N	2.79	0.51
1:A:114:GLU:O	1:A:118:GLN:HG2	2.10	0.50
1:A:9:LEU:C	1:A:11:GLN:H	2.14	0.50
1:B:260:ARG:HB2	1:B:283:SER:HB3	1.94	0.50
1:A:134:LEU:HD22	1:A:150:TYR:CZ	2.46	0.50
1:A:192:ILE:HD11	2:A:501:SAM:H2'	1.93	0.50
1:A:170:TYR:CD2	1:A:174:LEU:HD21	2.47	0.50
1:B:62:GLN:HE22	1:B:291:LEU:CD2	2.23	0.50
1:B:261:LEU:HD13	1:B:265:ARG:HD2	1.94	0.50
1:B:4:ARG:CB	1:B:5:PRO:CD	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HD22	1:B:129:MET:HE2	1.93	0.50
1:B:24:LEU:O	1:B:27:ALA:HB3	2.12	0.49
1:A:49:LYS:HD3	1:A:49:LYS:C	2.33	0.49
1:A:41:GLN:OE1	1:A:43:SER:OG	2.30	0.49
1:A:158:PRO:HG3	1:A:170:TYR:CE2	2.48	0.49
1:B:212:LEU:HB3	1:B:213:PRO:HD2	1.95	0.49
1:B:59:TYR:CD2	1:B:60:CYS:N	2.80	0.49
1:B:149:TYR:CE1	1:B:186:LYS:HB3	2.48	0.49
1:B:41:GLN:OE1	1:B:43:SER:OG	2.31	0.49
1:A:113:LEU:HD22	1:A:129:MET:HE2	1.94	0.49
1:B:4:ARG:HB2	1:B:5:PRO:HD2	1.95	0.49
1:B:205:LEU:O	1:B:208:GLN:HB3	2.13	0.49
1:A:265:ARG:HA	1:A:268:MET:HE3	1.94	0.49
1:A:260:ARG:HB2	1:A:283:SER:HB3	1.95	0.48
1:A:149:TYR:CE1	1:A:186:LYS:HB3	2.48	0.48
1:A:134:LEU:H	1:A:134:LEU:HD23	1.77	0.48
1:B:158:PRO:HG3	1:B:170:TYR:CE2	2.49	0.48
1:A:181:ARG:HA	1:A:181:ARG:HH11	1.78	0.48
1:A:158:PRO:HA	1:A:170:TYR:CD1	2.48	0.48
1:B:170:TYR:CD2	1:B:174:LEU:HD21	2.48	0.48
1:A:45:LEU:HD23	1:A:45:LEU:O	2.14	0.48
1:A:43:SER:O	1:A:285:PHE:HA	2.13	0.48
1:B:154:LEU:O	1:B:156:THR:N	2.42	0.48
1:B:291:LEU:HD13	5:B:502:DTB:HCE2	1.94	0.48
1:B:216:PRO:HG2	1:B:219:VAL:CG2	2.43	0.48
1:B:175:ASP:O	1:B:179:LYS:HG3	2.13	0.48
1:B:49:LYS:C	1:B:49:LYS:HD3	2.33	0.48
1:B:37:PRO:C	1:B:39:GLN:N	2.67	0.48
1:A:217:GLU:H	1:A:217:GLU:CD	2.17	0.48
1:A:180:VAL:O	1:A:183:ALA:HB3	2.14	0.48
1:B:158:PRO:HA	1:B:170:TYR:CD1	2.49	0.48
1:B:181:ARG:HH11	1:B:181:ARG:HA	1.79	0.48
1:A:181:ARG:HH11	1:A:181:ARG:CG	2.27	0.48
1:A:205:LEU:O	1:A:208:GLN:HB3	2.14	0.47
1:B:106:HIS:O	1:B:109:ASP:HB2	2.15	0.47
1:B:134:LEU:H	1:B:134:LEU:HD23	1.78	0.47
1:B:36:ASP:OD2	1:B:39:GLN:HB2	2.14	0.47
1:A:265:ARG:NH2	1:A:301:ASP:OD2	2.43	0.47
1:B:206:LEU:HA	1:B:209:LEU:HD21	1.97	0.47
1:A:160:PHE:HE2	1:A:164:ILE:HD11	1.79	0.47
1:A:175:ASP:O	1:A:179:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:HIS:O	1:A:109:ASP:HB2	2.14	0.47
1:B:199:VAL:HG23	1:B:200:LYS:N	2.29	0.47
1:B:42:VAL:HG23	1:B:286:TYR:HB2	1.97	0.47
1:B:27:ALA:HB1	1:B:279:ALA:O	2.15	0.47
1:B:192:ILE:HG22	1:B:193:VAL:N	2.30	0.47
1:B:181:ARG:HH11	1:B:181:ARG:CG	2.28	0.47
1:A:216:PRO:HG2	1:A:219:VAL:CG2	2.43	0.47
1:B:160:PHE:HE2	1:B:164:ILE:HD11	1.79	0.47
1:B:7:TRP:H	1:B:211:ASN:HD21	1.62	0.47
1:A:45:LEU:HD13	1:A:285:PHE:HE2	1.79	0.47
1:A:37:PRO:C	1:A:39:GLN:N	2.67	0.47
1:B:38:ARG:NH1	1:B:309:GLY:O	2.48	0.47
1:A:232:LEU:O	1:A:233:ALA:C	2.53	0.47
1:A:53:CYS:HA	1:A:54:PRO:HD3	1.79	0.47
1:A:199:VAL:HG23	1:A:200:LYS:N	2.30	0.47
1:A:42:VAL:HG23	1:A:286:TYR:HB2	1.97	0.47
1:B:276:CYS:O	1:B:279:ALA:HB3	2.15	0.47
1:B:192:ILE:HD11	2:B:501:SAM:C2'	2.45	0.47
1:A:212:LEU:HB3	1:A:213:PRO:HD2	1.96	0.47
1:B:43:SER:O	1:B:285:PHE:HA	2.14	0.46
1:A:36:ASP:OD2	1:A:39:GLN:HB2	2.15	0.46
1:A:310:LEU:O	1:A:311:ASN:HB2	2.15	0.46
1:B:105:PRO:HG3	1:B:131:LEU:CB	2.42	0.46
1:B:232:LEU:O	1:B:233:ALA:C	2.54	0.46
1:A:276:CYS:O	1:A:279:ALA:HB3	2.15	0.46
1:A:265:ARG:HE	1:A:273:GLN:NE2	2.14	0.46
2:A:501:SAM:O4'	5:A:502:DTB:HCE1	2.15	0.46
1:A:45:LEU:HB2	1:A:97:CYS:HB2	1.98	0.46
1:B:217:GLU:CD	1:B:217:GLU:H	2.17	0.46
1:B:180:VAL:O	1:B:183:ALA:HB3	2.16	0.46
1:B:306:ARG:O	1:B:309:GLY:N	2.48	0.46
1:A:241:PHE:CE2	1:B:270:GLU:HB3	2.51	0.46
1:A:27:ALA:HB1	1:A:279:ALA:O	2.15	0.46
1:A:206:LEU:HA	1:A:209:LEU:HD21	1.97	0.46
1:A:286:TYR:CE1	1:A:298:GLU:HA	2.51	0.46
1:A:192:ILE:HD11	2:A:501:SAM:C2'	2.46	0.46
1:A:308:LEU:HD21	1:B:241:PHE:CZ	2.51	0.46
1:B:247:ILE:HG23	1:B:259:VAL:HG11	1.98	0.46
1:B:206:LEU:HA	1:B:209:LEU:CD2	2.46	0.46
1:B:110:MET:HB2	1:B:111:PRO:HD3	1.98	0.46
1:B:85:ALA:HB2	1:B:96:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TYR:CE1	1:B:298:GLU:HA	2.51	0.45
1:B:53:CYS:HA	1:B:54:PRO:HD3	1.79	0.45
1:A:41:GLN:CA	1:A:41:GLN:NE2	2.79	0.45
1:A:169:THR:O	1:A:170:TYR:C	2.55	0.45
1:B:310:LEU:O	1:B:311:ASN:HB2	2.16	0.45
1:A:12:VAL:HG21	1:A:253:MET:SD	2.57	0.45
1:A:206:LEU:HA	1:A:209:LEU:CD2	2.46	0.45
1:A:110:MET:HB2	1:A:111:PRO:HD3	1.97	0.45
1:A:154:LEU:O	1:A:156:THR:N	2.41	0.45
1:B:45:LEU:O	1:B:45:LEU:HD23	2.17	0.45
1:B:45:LEU:HB2	1:B:97:CYS:HB2	1.96	0.45
1:A:105:PRO:HG3	1:A:131:LEU:CB	2.42	0.45
1:B:198:THR:N	1:B:201:ASP:OD2	2.48	0.45
1:B:221:ILE:HG22	1:B:243:PHE:CE1	2.51	0.45
1:B:148:ASP:O	1:B:186:LYS:HB2	2.17	0.45
1:A:192:ILE:HG22	1:A:193:VAL:N	2.31	0.45
1:B:129:MET:HG2	1:B:147:LEU:CD1	2.47	0.45
1:A:135:SER:O	1:A:138:GLN:N	2.50	0.45
1:A:12:VAL:HG22	1:A:253:MET:SD	2.56	0.45
1:A:290:LEU:H	1:A:290:LEU:CD1	2.24	0.44
1:A:113:LEU:HA	1:A:116:MET:HE3	1.98	0.44
1:B:141:ARG:NH1	1:B:141:ARG:HG2	2.32	0.44
1:B:212:LEU:HB3	1:B:213:PRO:CD	2.47	0.44
1:A:173:ARG:O	1:A:176:THR:N	2.50	0.44
1:A:273:GLN:O	1:A:277:PHE:CD2	2.70	0.44
1:B:169:THR:O	1:B:170:TYR:C	2.55	0.44
1:A:113:LEU:CD1	1:A:131:LEU:HD13	2.45	0.44
1:A:212:LEU:HB3	1:A:213:PRO:CD	2.48	0.44
1:B:173:ARG:O	1:B:176:THR:N	2.50	0.44
1:B:173:ARG:O	1:B:174:LEU:C	2.56	0.44
1:A:221:ILE:HG22	1:A:243:PHE:CE1	2.51	0.44
1:A:198:THR:N	1:A:201:ASP:OD2	2.47	0.44
1:B:251:ARG:NH2	1:B:259:VAL:HG23	2.33	0.44
1:B:12:VAL:HG21	1:B:253:MET:SD	2.57	0.44
1:A:306:ARG:O	1:A:309:GLY:N	2.50	0.44
1:B:263:ALA:CB	5:B:502:DTB:HCB2	2.48	0.43
1:B:102:TRP:CZ3	1:B:131:LEU:HD22	2.52	0.43
1:B:221:ILE:CD1	1:B:246:THR:HG22	2.48	0.43
1:A:251:ARG:NH2	1:A:259:VAL:HG23	2.33	0.43
1:B:169:THR:CB	1:B:172:GLU:HB2	2.46	0.43
1:A:291:LEU:O	1:A:292:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLN:NE2	1:B:41:GLN:CA	2.80	0.43
1:A:225:VAL:O	1:A:227:VAL:HG23	2.19	0.43
1:B:265:ARG:HA	1:B:268:MET:HE3	2.01	0.43
1:B:265:ARG:HE	1:B:273:GLN:NE2	2.16	0.43
1:B:135:SER:O	1:B:138:GLN:N	2.52	0.43
1:A:200:LYS:O	1:A:203:ALA:HB3	2.19	0.43
1:A:85:ALA:HB2	1:A:96:PHE:CE2	2.53	0.43
1:A:173:ARG:O	1:A:174:LEU:C	2.56	0.43
1:A:38:ARG:NH1	1:A:309:GLY:O	2.51	0.43
1:A:37:PRO:O	1:A:38:ARG:HG2	2.18	0.43
1:A:169:THR:CB	1:A:172:GLU:HB2	2.46	0.43
1:B:20:LEU:O	1:B:24:LEU:HD23	2.19	0.43
1:A:129:MET:HG2	1:A:147:LEU:CD1	2.49	0.43
1:A:41:GLN:NE2	1:A:42:VAL:N	2.67	0.43
1:B:41:GLN:NE2	1:B:42:VAL:N	2.67	0.43
1:B:59:TYR:CE2	2:B:501:SAM:H2'	2.53	0.43
1:B:102:TRP:HZ3	1:B:113:LEU:HD11	1.84	0.43
1:A:141:ARG:HG2	1:A:141:ARG:NH1	2.33	0.43
1:B:48:ILE:HD13	1:B:116:MET:SD	2.59	0.43
1:B:150:TYR:HB3	1:B:180:VAL:HG11	2.01	0.43
1:A:102:TRP:CZ3	1:A:131:LEU:HD22	2.54	0.43
1:A:89:LYS:HB2	1:A:125:LEU:HD21	2.01	0.43
1:B:291:LEU:O	1:B:292:THR:HG23	2.19	0.42
1:B:225:VAL:HB	2:B:501:SAM:HN62	1.84	0.42
1:A:102:TRP:HZ3	1:A:113:LEU:HD11	1.84	0.42
1:B:9:LEU:C	1:B:11:GLN:N	2.72	0.42
1:A:154:LEU:HD12	1:A:170:TYR:CZ	2.54	0.42
1:A:271:GLN:OE1	1:A:271:GLN:N	2.52	0.42
1:B:219:VAL:O	1:B:219:VAL:HG12	2.19	0.42
1:A:219:VAL:O	1:A:219:VAL:HG12	2.20	0.42
1:B:57:CYS:SG	1:B:165:ILE:HG12	2.59	0.42
1:A:48:ILE:HD13	1:A:116:MET:SD	2.60	0.42
1:A:148:ASP:O	1:A:186:LYS:HB2	2.18	0.42
1:A:170:TYR:CE2	1:A:174:LEU:HD21	2.54	0.42
1:A:263:ALA:HB2	5:A:502:DTB:HCG1	2.01	0.42
1:A:247:ILE:HG23	1:A:259:VAL:HG11	2.01	0.42
1:B:154:LEU:HD23	1:B:189:SER:OG	2.20	0.42
1:A:195:LEU:HA	1:A:224:LEU:HD22	2.02	0.42
1:B:221:ILE:O	1:B:221:ILE:HG22	2.20	0.42
1:A:26:GLU:O	1:A:29:GLN:HB2	2.20	0.42
1:A:108:ARG:O	1:A:111:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ILE:HD13	1:B:244:ILE:HA	1.93	0.42
1:B:134:LEU:HD23	1:B:176:THR:CG2	2.50	0.42
1:B:261:LEU:C	1:B:261:LEU:CD2	2.88	0.42
1:A:187:VAL:HG12	1:A:216:PRO:HB3	2.02	0.42
1:B:206:LEU:O	1:B:209:LEU:HD23	2.20	0.42
1:A:130:THR:CB	1:A:151:ASN:HB3	2.40	0.42
1:A:221:ILE:O	1:A:221:ILE:HG22	2.19	0.42
1:A:23:LEU:HD23	1:A:245:ARG:HG3	2.02	0.42
1:B:170:TYR:CE2	1:B:174:LEU:HD21	2.56	0.41
1:B:152:HIS:HB3	1:B:177:LEU:HD11	2.01	0.41
2:A:501:SAM:HE3	5:A:502:DTB:CE	2.50	0.41
1:A:9:LEU:C	1:A:11:GLN:N	2.73	0.41
1:B:266:GLU:HB2	1:B:296:PRO:HD3	2.02	0.41
1:A:154:LEU:HD23	1:A:189:SER:OG	2.19	0.41
1:B:195:LEU:HA	1:B:224:LEU:HD22	2.01	0.41
1:B:108:ARG:O	1:B:111:PRO:HD2	2.21	0.41
2:A:501:SAM:HE3	5:A:502:DTB:HCE1	2.01	0.41
1:B:37:PRO:O	1:B:38:ARG:HG2	2.21	0.41
1:B:271:GLN:OE1	1:B:271:GLN:N	2.54	0.41
1:B:266:GLU:HA	1:B:296:PRO:HG3	2.02	0.41
1:A:299:ASP:O	1:A:300:LYS:C	2.58	0.41
1:A:266:GLU:HB2	1:A:296:PRO:HD3	2.02	0.41
1:A:128:CYS:HB2	1:A:149:TYR:CB	2.31	0.41
1:A:61:PRO:HD3	2:A:501:SAM:HN61	1.85	0.41
1:A:206:LEU:O	1:A:209:LEU:HD23	2.21	0.41
1:B:154:LEU:HD12	1:B:170:TYR:CZ	2.56	0.41
1:B:113:LEU:CD1	1:B:131:LEU:HD13	2.45	0.41
1:A:16:PHE:HA	1:A:245:ARG:HD3	2.02	0.41
1:A:152:HIS:HB3	1:A:177:LEU:HD11	2.03	0.41
1:A:174:LEU:N	1:A:174:LEU:HD22	2.36	0.41
1:A:134:LEU:HD23	1:A:176:THR:CG2	2.50	0.41
1:A:265:ARG:HA	1:A:268:MET:CE	2.50	0.41
1:B:174:LEU:N	1:B:174:LEU:HD22	2.34	0.41
1:A:18:LYS:HA	1:A:19:PRO:HD3	1.95	0.41
1:B:89:LYS:HB2	1:B:125:LEU:HD21	2.03	0.41
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.91	0.41
1:A:19:PRO:O	1:A:20:LEU:C	2.60	0.41
1:B:16:PHE:HA	1:B:245:ARG:HD3	2.02	0.41
1:B:217:GLU:N	1:B:217:GLU:CD	2.74	0.40
1:A:20:LEU:O	1:A:24:LEU:HD23	2.21	0.40
1:A:221:ILE:CD1	1:A:246:THR:HG22	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:O	1:A:75:LEU:C	2.59	0.40
1:A:217:GLU:N	1:A:217:GLU:CD	2.74	0.40
1:B:48:ILE:HG22	1:B:99:GLY:C	2.42	0.40
1:B:187:VAL:HG12	1:B:216:PRO:HB3	2.04	0.40
1:A:272:THR:O	1:A:273:GLN:C	2.60	0.40
1:B:21:LEU:O	1:B:24:LEU:HB2	2.21	0.40
2:B:501:SAM:HE2	5:B:502:DTB:HCT3	2.03	0.40
1:B:265:ARG:HA	1:B:268:MET:CE	2.51	0.40
1:A:133:THR:HA	1:A:176:THR:HG21	2.04	0.40
1:B:38:ARG:HA	1:B:310:LEU:HD23	2.01	0.40
1:B:272:THR:O	1:B:273:GLN:C	2.59	0.40
1:B:12:VAL:HG22	1:B:253:MET:SD	2.61	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	310/369 (84%)	243 (78%)	49 (16%)	18 (6%)	2 20
1	B	311/369 (84%)	244 (78%)	49 (16%)	18 (6%)	2 20
All	All	621/738 (84%)	487 (78%)	98 (16%)	36 (6%)	2 20

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	67	LYS
1	A	136	GLU
1	A	263	ALA
1	B	38	ARG
1	B	67	LYS

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Mol	Chain	Res	Type
1	B	136	GLU
1	B	263	ALA
1	A	20	LEU
1	A	52	ALA
1	A	69	GLY
1	A	147	LEU
1	A	197	GLU
1	A	312	PRO
1	B	20	LEU
1	B	52	ALA
1	B	69	GLY
1	B	147	LEU
1	B	197	GLU
1	B	312	PRO
1	A	71	GLU
1	B	71	GLU
1	A	55	GLU
1	A	155	ASP
1	B	155	ASP
1	A	37	PRO
1	A	110	MET
1	B	37	PRO
1	B	55	GLU
1	A	19	PRO
1	A	270	GLU
1	B	19	PRO
1	B	110	MET
1	B	270	GLU
1	A	215	PRO
1	B	215	PRO

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	264/314 (84%)	235 (89%)	29 (11%)	8 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	266/314 (85%)	234 (88%)	32 (12%)	6 29
All	All	530/628 (84%)	469 (88%)	61 (12%)	7 31

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	TRP
1	A	8	THR
1	A	14	GLU
1	A	38	ARG
1	A	41	GLN
1	A	45	LEU
1	A	50	THR
1	A	106	HIS
1	A	125	LEU
1	A	128	CYS
1	A	156	THR
1	A	163	ASN
1	A	181	ARG
1	A	186	LYS
1	A	197	GLU
1	A	198	THR
1	A	205	LEU
1	A	206	LEU
1	A	209	LEU
1	A	217	GLU
1	A	235	ASN
1	A	238	VAL
1	A	251	ARG
1	A	261	LEU
1	A	290	LEU
1	A	291	LEU
1	A	292	THR
1	A	312	PRO
1	B	3	HIS
1	B	4	ARG
1	B	7	TRP
1	B	8	THR
1	B	14	GLU
1	B	38	ARG
1	B	41	GLN

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	50	THR
1	B	106	HIS
1	B	112	TYR
1	B	125	LEU
1	B	128	CYS
1	B	156	THR
1	B	163	ASN
1	B	176	THR
1	B	181	ARG
1	B	186	LYS
1	B	197	GLU
1	B	198	THR
1	B	205	LEU
1	B	206	LEU
1	B	209	LEU
1	B	217	GLU
1	B	235	ASN
1	B	238	VAL
1	B	251	ARG
1	B	261	LEU
1	B	290	LEU
1	B	291	LEU
1	B	292	THR
1	B	312	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	62	GLN
1	A	80	GLN
1	A	115	GLN
1	A	140	GLN
1	A	144	ASN
1	A	151	ASN
1	A	152	HIS
1	A	163	ASN
1	A	211	ASN
1	A	235	ASN
1	A	273	GLN
1	B	28	GLN

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Mol	Chain	Res	Type
1	B	41	GLN
1	B	62	GLN
1	B	80	GLN
1	B	115	GLN
1	B	140	GLN
1	B	144	ASN
1	B	152	HIS
1	B	163	ASN
1	B	211	ASN
1	B	235	ASN
1	B	273	GLN

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

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	$\#\|Z\| > 2$
3	SF4	A	401	1,2	0,12,12	0.00	-	0,24,24	0.00	-
4	FES	A	402	1	0,4,4	0.00	-	0,4,4	0.00	-
2	SAM	A	501	3	21,29,29	1.19	2 (9%)	17,42,42	3.12	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DTB	A	502	-	12,15,15	1.45	2 (16%)	14,19,19	1.95	2 (14%)
6	TRS	A	503	-	7,7,7	0.92	1 (14%)	9,9,9	0.61	0
3	SF4	B	401	1,2	0,12,12	0.00	-	0,24,24	0.00	-
4	FES	B	402	1	0,4,4	0.00	-	0,4,4	0.00	-
2	SAM	B	501	3	21,29,29	1.42	2 (9%)	17,42,42	3.02	2 (11%)
5	DTB	B	502	-	12,15,15	1.42	1 (8%)	14,19,19	1.77	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	SF4	A	401	1,2	-	0/0/48/48	0/6/5/5
4	FES	A	402	1	-	0/0/4/4	0/1/1/1
2	SAM	A	501	3	-	0/8/33/33	0/3/3/3
5	DTB	A	502	-	-	0/6/20/20	0/1/1/1
6	TRS	A	503	-	-	0/9/9/9	0/0/0/0
3	SF4	B	401	1,2	-	0/0/48/48	0/6/5/5
4	FES	B	402	1	-	0/0/4/4	0/1/1/1
2	SAM	B	501	3	-	0/8/33/33	0/3/3/3
5	DTB	B	502	-	-	0/6/20/20	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	DTB	CN-N1	-3.47	1.30	1.35
5	B	502	DTB	CN-N1	-2.87	1.31	1.35
5	A	502	DTB	CN-N2	-2.29	1.32	1.35
2	A	501	SAM	C5-N7	-2.08	1.32	1.39
6	A	503	TRS	C-N	-2.04	1.47	1.50
2	B	501	SAM	C5-N7	-2.00	1.32	1.39
2	A	501	SAM	O4'-C1'	4.20	1.46	1.41
2	B	501	SAM	O4'-C1'	5.68	1.48	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	SAM	N3-C2-N1	-11.13	120.37	128.89
2	B	501	SAM	N3-C2-N1	-10.88	120.57	128.89
2	A	501	SAM	C4'-O4'-C1'	-4.88	104.36	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	SAM	C4'-O4'-C1'	-4.49	104.78	109.72
5	B	502	DTB	O-CN-N1	-2.44	123.08	125.90
5	A	502	DTB	O-CN-N1	-2.36	123.16	125.90
2	A	501	SAM	O4'-C4'-C3'	-2.16	100.79	105.15
5	B	502	DTB	N1-CN-N2	5.48	112.67	108.88
5	A	502	DTB	N1-CN-N2	5.91	112.96	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SAM	11	0
5	A	502	DTB	9	0
6	A	503	TRS	1	0
2	B	501	SAM	13	0
5	B	502	DTB	11	0

5.7 Other polymers

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	312/369 (84%)	0.07	7 (2%)	65	60	42, 83, 139, 169	6 (1%)
1	B	313/369 (84%)	0.24	19 (6%)	25	23	37, 89, 152, 190	6 (1%)
All	All	625/738 (84%)	0.16	26 (4%)	40	35	37, 85, 143, 190	12 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	TYR	5.3
1	B	98	MET	3.8
1	B	71	GLU	3.6
1	B	99	GLY	3.4
1	B	125	LEU	3.3
1	A	154	LEU	3.2
1	B	142	LEU	3.0
1	B	131	LEU	2.8
1	B	170	TYR	2.8
1	B	147	LEU	2.6
1	B	127	ALA	2.6
1	A	155	ASP	2.5
1	A	253	MET	2.5
1	B	129	MET	2.5
1	B	48	ILE	2.4
1	B	120	VAL	2.4
1	A	59	TYR	2.4
1	B	73	GLU	2.2
1	A	206	LEU	2.2
1	A	191	GLY	2.2
1	B	161	TYR	2.2
1	B	116	MET	2.2
1	B	134	LEU	2.1
1	B	96	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	7	TRP	2.1
1	B	100	ALA	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
6	TRS	A	503	8/8	0.80	0.48	4.16	147,147,147,147	0
5	DTB	A	502	15/15	0.95	0.49	2.96	47,47,47,47	4
5	DTB	B	502	15/15	0.93	0.39	1.56	61,61,61,61	4
2	SAM	B	501	27/27	0.92	0.38	0.94	84,88,146,146	0
2	SAM	A	501	27/27	0.92	0.33	0.52	68,84,130,130	0
4	FES	A	402	4/4	0.99	0.15	-0.79	35,35,35,35	0
4	FES	B	402	4/4	0.99	0.13	-1.18	43,43,43,43	0
3	SF4	B	401	8/8	0.99	0.11	-1.32	71,71,71,71	0
3	SF4	A	401	8/8	1.00	0.14	-1.64	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.