



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:27 AM GMT

PDB ID : 3IIQ  
Title : Crystallographic analysis of bacterial signal peptidase in ternary complex with Arylomycin A2 and a beta-sultam inhibitor  
Authors : Paetzel, M.  
Deposited on : 2009-08-03  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

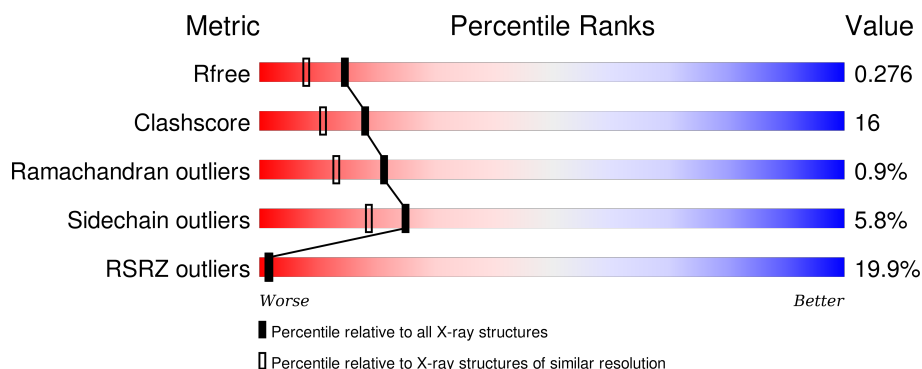
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	249	<div> <div>14%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	249	<div> <div>21%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>• •</div> <div>10%</div> </div> </div>
2	C	6	<div> <div>33%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
2	D	6	<div> <div></div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JZA	A	324	-	-	-	X
3	JZA	B	324	-	-	X	X
4	TRT	A	325	-	-	-	X
4	TRT	B	325	-	-	-	X
5	GOL	A	326	-	-	-	X
5	GOL	A	328	-	-	X	X
6	CCN	A	330	-	-	X	-
6	CCN	A	331	-	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3933 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 SIGNAL PEPTIDASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1726	1108	286	324	8			
1	B	224	Total	C	N	O	S	0	0	0
			1755	1121	295	331	8			

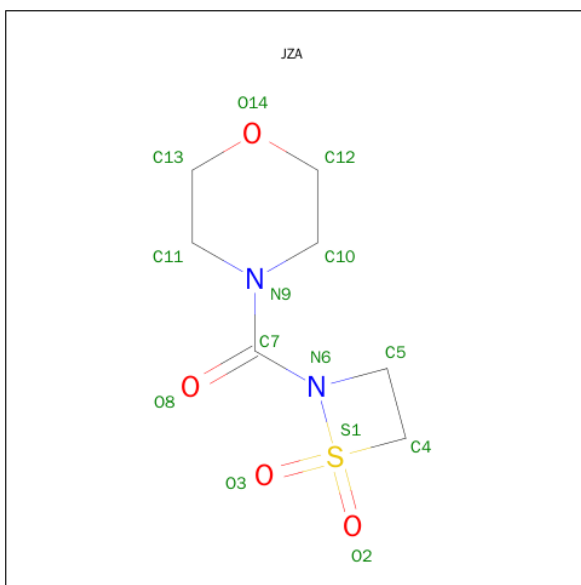
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MET	-	INITIATING METHIONINE	UNP P00803
B	75	MET	-	INITIATING METHIONINE	UNP P00803

- Molecule 2 is a protein called ARYLOMYCIN A2.

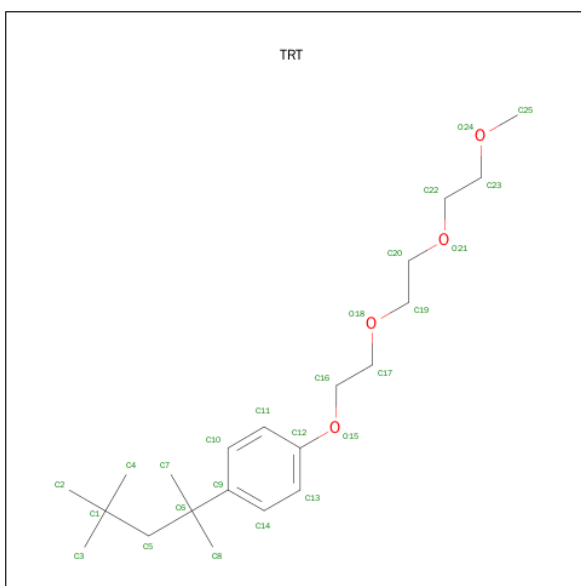
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			46	30	6	10			
2	D	6	Total	C	N	O	0	0	0
			46	30	6	10			

- Molecule 3 is 4-[(1,1-DIOXIDO-1,2-THIAZETIDIN-2-YL)CARBONYL]MORPHOLINE (three-letter code: JZA) (formula: C<sub>7</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	7	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			14	7	2	4	1		

- Molecule 4 is FRAGMENT OF TRITON X-100 (three-letter code: TRT) (formula:  $C_{21}H_{36}O_4$ ).



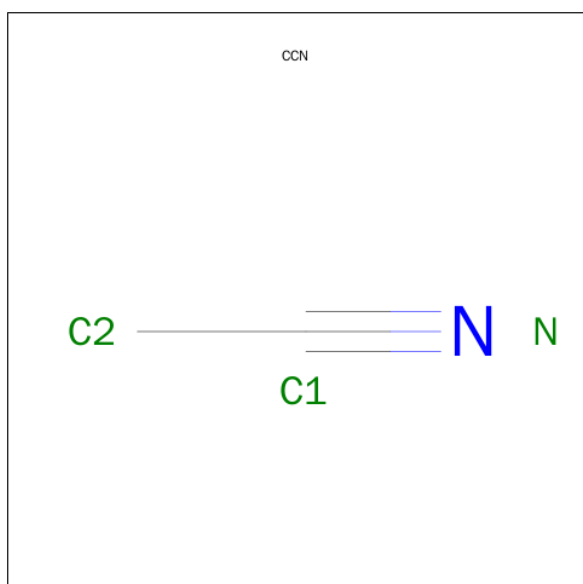
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



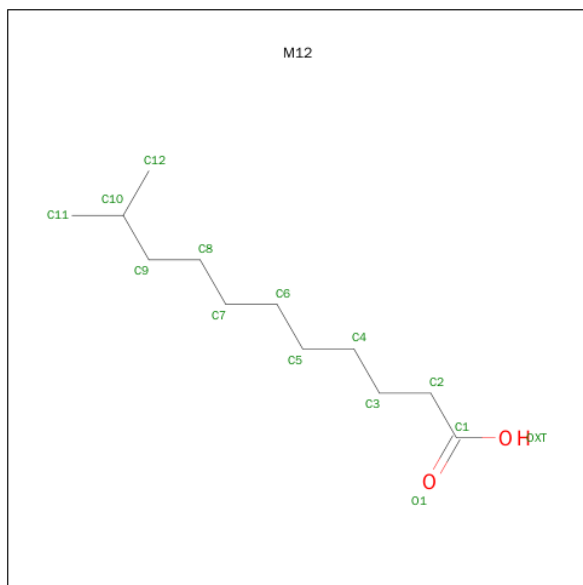
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETONITRILE (three-letter code: CCN) (formula:  $C_2H_3N$ ).



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

- Molecule 7 is 10-METHYLUNDECANOIC ACID (three-letter code: M12) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 13 12 1	0	0
7	D	1	Total C O 3 2 1	0	0

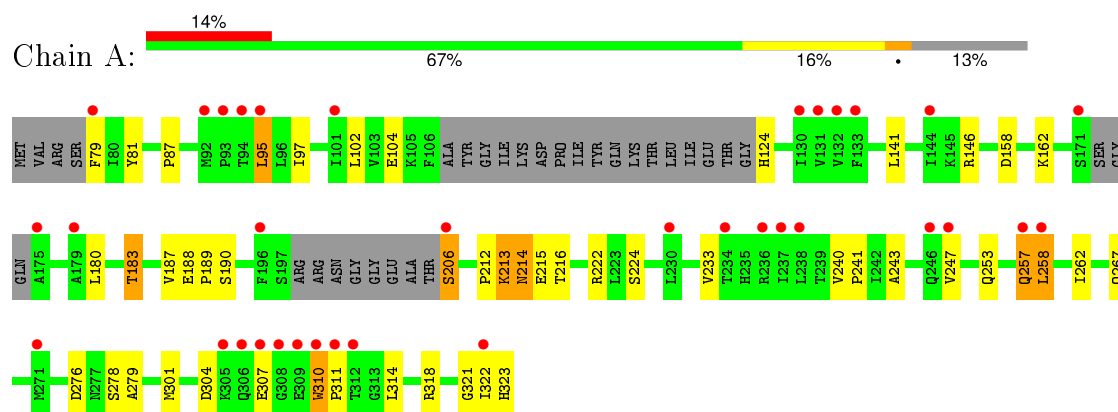
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	128	Total O 128 128	0	0
8	B	111	Total O 111 111	0	0
8	C	2	Total O 2 2	0	0
8	D	5	Total O 5 5	0	0

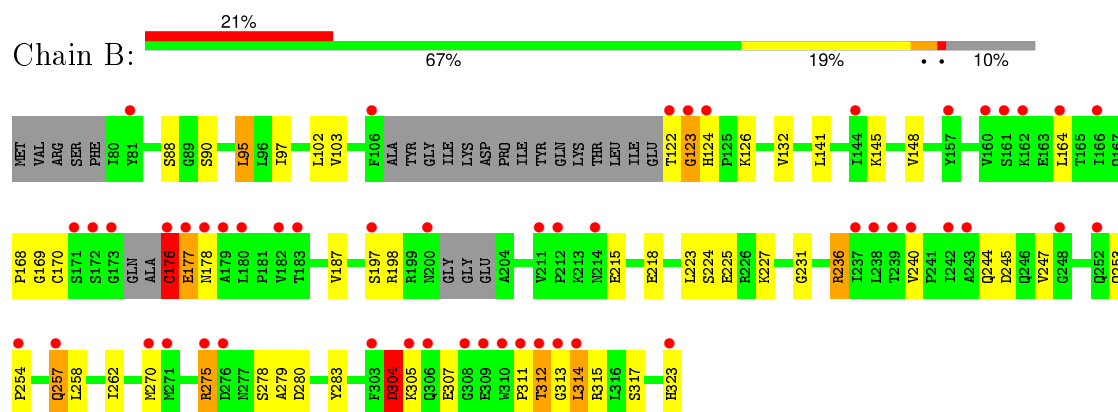
### 3 Residue-property plots

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.

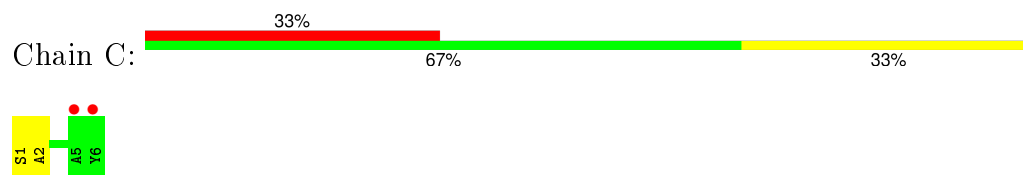
#### • Molecule 1: SIGNAL PEPTIDASE I



#### • Molecule 1: SIGNAL PEPTIDASE I



#### • Molecule 2: ARYLOMYCIN A2



#### • Molecule 2: ARYLOMYCIN A2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.01Å 70.01Å 259.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.40 – 2.00 42.98 – 2.04	Depositor EDS
% Data completeness (in resolution range)	95.1 (67.40-2.00) 95.1 (42.98-2.04)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.207 , 0.250 0.236 , 0.276	Depositor DCC
$R_{free}$ test set	2035 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 40272 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: GOL, DAL, 5PG, JZA, CCN, M12, DSE, TRT

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	1.17	5/1772 (0.3%)	0.96	5/2402 (0.2%)
1	B	1.29	13/1800 (0.7%)	0.96	5/2440 (0.2%)
2	C	1.90	0/21	2.16	0/24
2	D	1.58	0/21	1.78	0/24
All	All	1.24	18/3614 (0.5%)	0.97	10/4890 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
2	C	0	1
2	D	0	1
All	All	0	6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	GLU	CD-OE1	16.08	1.43	1.25
1	B	176	CYS	C-N	11.13	1.59	1.34
1	B	177	GLU	CG-CD	-9.56	1.37	1.51
1	B	177	GLU	C-O	9.21	1.40	1.23
1	A	216	THR	C-N	9.04	1.54	1.34
1	B	257	GLN	CD-NE2	8.60	1.54	1.32
1	A	206	SER	CB-OG	7.99	1.52	1.42
1	B	177	GLU	C-N	7.90	1.52	1.34
1	B	257	GLN	CD-OE1	7.11	1.39	1.24
1	B	170	CYS	C-N	6.58	1.49	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	ARG	CG-CD	-6.24	1.36	1.51
1	B	323	HIS	C-OXT	6.15	1.35	1.23
1	B	236	ARG	CZ-NH1	6.00	1.40	1.33
1	B	126	LYS	CE-NZ	5.89	1.63	1.49
1	B	170	CYS	C-O	5.76	1.34	1.23
1	A	213	LYS	CE-NZ	5.18	1.62	1.49
1	A	213	LYS	CD-CE	5.05	1.63	1.51
1	A	243	ALA	CA-CB	5.00	1.62	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	95	LEU	CB-CG-CD1	5.91	121.04	111.00
1	B	177	GLU	C-N-CA	-5.84	107.10	121.70
1	B	245	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	214	ASN	N-CA-CB	-5.62	100.49	110.60
1	A	310	TRP	C-N-CD	-5.61	108.27	120.60
1	A	95	LEU	CB-CG-CD2	5.22	119.87	111.00
1	A	222	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	146	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	B	304	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	TRP	Peptide
1	B	123	GLY	Peptide
1	B	176	CYS	Mainchain
1	B	198	ARG	Peptide
2	C	2	DAL	Mainchain
2	D	2	DAL	Mainchain

## 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	1726	0	1676	44	0
1	B	1755	0	1698	53	0
2	C	46	0	37	1	0
2	D	46	0	37	2	0
3	A	14	0	12	3	0
3	B	14	0	12	7	0
4	A	20	0	27	2	0
4	B	20	0	27	9	0
5	A	24	0	32	14	0
6	A	6	0	6	7	0
7	C	13	0	23	1	0
7	D	3	0	0	0	0
8	A	128	0	0	6	0
8	B	111	0	0	5	0
8	C	2	0	0	0	0
8	D	5	0	0	0	0
All	All	3933	0	3587	114	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 16.

All (114) 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:176:CYS:N	1:B:177:GLU:CG	1.75	1.46
1:B:168:PRO:HD2	1:B:178:ASN:O	1.30	1.23
1:B:176:CYS:N	1:B:177:GLU:HG2	0.86	1.18
4:B:325:TRT:H8C2	4:B:325:TRT:H3C3	1.34	1.07
1:B:123:GLY:HA2	1:B:124:HIS:CG	1.90	1.06
4:B:325:TRT:H3C3	4:B:325:TRT:C8	1.85	1.06
6:A:330:CCN:H21	6:A:331:CCN:H21	1.40	1.03
1:B:317:SER:HB3	8:B:2106:HOH:O	1.60	1.02
1:A:323:HIS:CD2	5:A:328:GOL:H32	2.01	0.95
1:A:183:THR:HG23	8:A:2044:HOH:O	1.64	0.95
1:A:253:GLN:HE22	1:A:262:ILE:H	1.13	0.94
1:B:314:LEU:N	1:B:314:LEU:CD1	2.30	0.94
1:B:312:THR:HG22	1:B:313:GLY:N	1.86	0.91
6:A:330:CCN:H21	6:A:331:CCN:C2	2.02	0.90
1:A:323:HIS:HD2	5:A:328:GOL:C3	1.85	0.90
1:A:323:HIS:HD2	5:A:328:GOL:H32	1.37	0.87
1:B:313:GLY:C	1:B:314:LEU:HD12	1.95	0.87
1:A:323:HIS:CD2	5:A:328:GOL:C3	2.58	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HA	8:A:2035:HOH:O	1.76	0.84
1:A:323:HIS:CD2	5:A:328:GOL:H12	2.14	0.82
1:B:314:LEU:N	1:B:314:LEU:HD12	1.95	0.82
1:B:123:GLY:HA2	1:B:124:HIS:CD2	2.16	0.80
1:B:278:SER:HA	3:B:324:JZA:H4	1.65	0.79
1:B:168:PRO:CD	1:B:178:ASN:O	2.24	0.79
1:A:323:HIS:HD2	5:A:328:GOL:H12	1.46	0.79
1:A:79:PHE:HA	8:A:2001:HOH:O	1.82	0.78
1:A:257:GLN:HB2	8:A:2053:HOH:O	1.86	0.76
1:A:323:HIS:HD2	5:A:328:GOL:C1	2.00	0.74
1:B:314:LEU:HD13	1:B:314:LEU:N	2.01	0.73
1:B:253:GLN:HE22	1:B:262:ILE:H	1.32	0.73
4:B:325:TRT:C3	4:B:325:TRT:C8	2.63	0.73
4:B:325:TRT:H8C2	4:B:325:TRT:C3	2.15	0.73
1:A:323:HIS:OXT	6:A:331:CCN:H22	1.88	0.72
1:A:278:SER:HA	3:A:324:JZA:H4	1.72	0.69
1:B:176:CYS:N	1:B:177:GLU:CB	2.55	0.68
6:A:330:CCN:C2	6:A:331:CCN:H21	2.21	0.67
1:B:187:VAL:CG1	1:B:224:SER:HB3	2.25	0.67
1:A:124:HIS:N	8:A:2011:HOH:O	2.27	0.67
3:B:324:JZA:H11A	2:D:6:TYR:HB3	1.76	0.67
1:B:123:GLY:HA2	1:B:124:HIS:ND1	2.08	0.66
1:A:323:HIS:CD2	5:A:328:GOL:C1	2.77	0.65
1:B:313:GLY:C	1:B:314:LEU:CD1	2.63	0.64
1:B:97:ILE:O	1:B:315:ARG:NH1	2.31	0.63
1:B:304:ASP:O	1:B:311:PRO:CB	2.47	0.62
1:B:176:CYS:HB2	1:B:177:GLU:HA	1.82	0.62
1:A:187:VAL:CG1	1:A:224:SER:HB3	2.31	0.61
4:B:325:TRT:H8C1	4:B:325:TRT:H3C3	1.77	0.60
5:A:328:GOL:O3	6:A:330:CCN:H22	2.01	0.60
1:A:253:GLN:HE22	1:A:262:ILE:N	1.93	0.60
1:B:145:LYS:HE3	1:B:280:ASP:HB3	1.84	0.60
1:B:148:VAL:HG11	1:B:164:LEU:HD13	1.83	0.59
1:A:189:PRO:HG2	1:A:213:LYS:HE3	1.85	0.58
1:B:123:GLY:CA	1:B:124:HIS:CG	2.78	0.58
1:B:279:ALA:H	3:B:324:JZA:C4	2.17	0.58
1:A:247:VAL:HG12	1:A:258:LEU:HG	1.86	0.57
1:A:323:HIS:CD2	5:A:328:GOL:H31	2.39	0.57
1:A:97:ILE:HD13	1:A:307:GLU:HB2	1.87	0.57
1:B:225:GLU:OE2	1:B:236:ARG:HD2	2.06	0.56
1:A:322:ILE:HA	6:A:330:CCN:H23	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:325:TRT:H8C1	4:B:325:TRT:H4C2	1.89	0.55
1:B:123:GLY:HA2	1:B:124:HIS:CE1	2.42	0.54
1:B:312:THR:CG2	1:B:313:GLY:N	2.55	0.54
1:B:223:LEU:HD22	1:B:240:VAL:HG22	1.90	0.54
1:A:81:TYR:CE2	1:A:104:GLU:HG2	2.43	0.54
1:B:304:ASP:O	1:B:311:PRO:CA	2.56	0.54
1:B:304:ASP:O	1:B:311:PRO:HB3	2.07	0.53
3:B:324:JZA:H11A	2:D:6:TYR:CB	2.39	0.53
1:B:223:LEU:CD2	1:B:240:VAL:HG22	2.39	0.53
1:B:307:GLU:HA	8:B:2004:HOH:O	2.08	0.53
1:A:279:ALA:H	3:A:324:JZA:H4A	1.72	0.52
1:A:253:GLN:NE2	1:A:262:ILE:H	1.94	0.52
1:A:301:MET:HE1	1:A:314:LEU:HD22	1.92	0.52
1:B:176:CYS:N	1:B:177:GLU:CA	2.73	0.52
1:B:187:VAL:HG13	1:B:224:SER:HB3	1.91	0.52
1:A:214:ASN:HD22	1:A:215:GLU:HG3	1.74	0.52
1:B:304:ASP:O	1:B:311:PRO:HA	2.10	0.51
1:A:190:SER:HB2	8:A:2072:HOH:O	2.09	0.51
4:A:325:TRT:H8C2	4:A:325:TRT:H2C3	1.92	0.51
1:B:315:ARG:NH2	8:B:2103:HOH:O	2.40	0.50
4:A:325:TRT:C14	4:A:325:TRT:H2C2	2.42	0.50
1:B:283:TYR:CE2	4:B:325:TRT:H3C1	2.47	0.49
1:A:187:VAL:HG13	1:A:224:SER:HB3	1.95	0.48
1:B:247:VAL:HG12	1:B:258:LEU:HD23	1.96	0.48
1:B:145:LYS:HB2	1:B:270:MET:HB3	1.96	0.47
5:A:327:GOL:H32	5:A:329:GOL:O1	2.14	0.47
1:A:322:ILE:CA	6:A:330:CCN:H23	2.44	0.47
1:A:247:VAL:HG11	1:A:258:LEU:HB3	1.96	0.47
1:A:323:HIS:HD2	5:A:328:GOL:C2	2.29	0.46
1:B:244:GLN:NE2	8:B:2077:HOH:O	2.49	0.46
1:A:279:ALA:H	3:A:324:JZA:C4	2.29	0.45
1:B:88:SER:HB3	3:B:324:JZA:H11	1.99	0.45
1:B:148:VAL:HG11	1:B:164:LEU:CD1	2.46	0.44
1:A:81:TYR:HB3	1:A:102:LEU:HD11	1.99	0.44
1:A:183:THR:HG21	8:B:2075:HOH:O	2.17	0.44
1:B:103:VAL:HG21	1:B:132:VAL:HG21	1.99	0.44
1:B:176:CYS:N	1:B:177:GLU:HG3	2.10	0.43
1:A:212:PRO:C	1:A:214:ASN:H	2.21	0.43
1:A:240:VAL:HG23	1:A:276:ASP:HB2	2.00	0.43
1:A:158:ASP:O	1:A:162:LYS:N	2.52	0.42
1:B:148:VAL:CG1	1:B:164:LEU:HD13	2.48	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:CB	3:B:324:JZA:H11	2.49	0.42
1:A:247:VAL:CG1	1:A:258:LEU:HB3	2.49	0.42
1:B:283:TYR:CZ	4:B:325:TRT:H3C1	2.55	0.42
1:B:169:GLY:O	1:B:176:CYS:O	2.38	0.42
1:B:253:GLN:HE22	1:B:262:ILE:N	2.09	0.42
1:B:218:GLU:H	1:B:218:GLU:CD	2.23	0.42
2:C:1:DSE:HN1	7:C:0:M12:H21C	1.51	0.42
1:A:318:ARG:HA	5:A:329:GOL:H2	2.02	0.41
1:B:90:SER:HB3	3:B:324:JZA:O2	2.20	0.41
1:B:227:LYS:HG2	1:B:236:ARG:HG2	2.01	0.41
1:A:214:ASN:ND2	1:A:215:GLU:HG3	2.34	0.41
4:B:325:TRT:H11	4:B:325:TRT:H161	1.94	0.41
1:A:321:GLY:C	5:A:328:GOL:H2	2.41	0.40
1:A:188:GLU:HB2	1:A:189:PRO:HD2	2.03	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	209/249 (84%)	203 (97%)	5 (2%)	1 (0%)	34	26
1	B	216/249 (87%)	205 (95%)	8 (4%)	3 (1%)	14	6
2	C	2/6 (33%)	2 (100%)	0	0	100	100
2	D	2/6 (33%)	2 (100%)	0	0	100	100
All	All	429/510 (84%)	412 (96%)	13 (3%)	4 (1%)	21	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	PRO

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	312	THR
1	B	254	PRO
1	B	231	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/214 (88%)	178 (94%)	11 (6%)	25	19
1	B	190/214 (89%)	179 (94%)	11 (6%)	25	19
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	381/430 (89%)	359 (94%)	22 (6%)	25	19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	PRO
1	A	95	LEU
1	A	141	LEU
1	A	180	LEU
1	A	183	THR
1	A	206	SER
1	A	233	VAL
1	A	257	GLN
1	A	258	LEU
1	A	267	GLN
1	A	304	ASP
1	B	95	LEU
1	B	102	LEU
1	B	122	THR
1	B	141	LEU
1	B	197	SER
1	B	215	GLU
1	B	257	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	275	ARG
1	B	304	ASP
1	B	305	LYS
1	B	314	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	214	ASN
1	A	244	GLN
1	A	253	GLN
1	A	257	GLN
1	A	267	GLN
1	A	291	ASN
1	A	323	HIS
1	B	85	GLN
1	B	124	HIS
1	B	235	HIS
1	B	244	GLN
1	B	252	GLN
1	B	253	GLN
1	B	291	ASN
1	B	323	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DSE	C	1	2,7	5,6,7	0.79	0	3,6,8	1.98	2 (66%)
2	DAL	C	2	2	3,4,5	2.32	1 (33%)	0,4,6	0.00	-
2	5PG	C	4	2	11,12,13	1.05	0	12,15,17	1.16	0
2	DSE	D	1	2,7	5,6,7	1.26	0	3,6,8	2.48	2 (66%)
2	DAL	D	2	2	3,4,5	2.35	1 (33%)	0,4,6	0.00	-
2	5PG	D	4	2	11,12,13	1.58	2 (18%)	12,15,17	1.13	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DSE	C	1	2,7	-	0/2/6/8	0/0/0/0
2	DAL	C	2	2	-	0/0/2/4	0/0/0/0
2	5PG	C	4	2	-	0/5/8/10	0/1/1/1
2	DSE	D	1	2,7	-	0/2/6/8	0/0/0/0
2	DAL	D	2	2	-	0/0/2/4	0/0/0/0
2	5PG	D	4	2	-	0/5/8/10	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	5PG	CN-N	2.46	1.53	1.46
2	D	4	5PG	CD1-CC1	3.06	1.44	1.38
2	C	2	DAL	O-C	3.80	1.37	1.19
2	D	2	DAL	O-C	3.99	1.38	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	DSE	OG-CB-CA	-2.94	104.36	111.04
2	D	1	DSE	O-C-CA	-2.91	117.76	125.44
2	C	1	DSE	OG-CB-CA	-2.57	105.20	111.04
2	C	1	DSE	O-C-CA	-2.04	120.06	125.44
2	D	4	5PG	CC2-CB-CC1	2.19	121.11	118.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	DSE	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	JZA	A	324	-	13,15,15	3.72	5 (38%)	10,22,22	1.41	1 (10%)
4	TRT	A	325	-	20,20,25	1.12	1 (5%)	28,28,33	0.65	0
5	GOL	A	326	-	5,5,5	0.17	0	5,5,5	0.49	0
5	GOL	A	327	-	5,5,5	0.43	0	5,5,5	1.32	0
5	GOL	A	328	-	5,5,5	0.81	0	5,5,5	1.05	0
5	GOL	A	329	-	5,5,5	0.49	0	5,5,5	0.95	0
6	CCN	A	330	-	2,2,2	1.10	0	1,1,1	0.32	0
6	CCN	A	331	-	2,2,2	1.65	1 (50%)	1,1,1	0.40	0
3	JZA	B	324	-	13,15,15	5.27	6 (46%)	10,22,22	1.56	2 (20%)
4	TRT	B	325	-	20,20,25	1.51	3 (15%)	28,28,33	1.14	2 (7%)
7	M12	C	0	2	12,12,13	1.12	0	11,12,14	0.65	0
7	M12	D	0	2	2,2,13	1.02	0	0,1,14	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JZA	A	324	-	-	0/4/28/28	0/1/2/2

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRT	A	325	-	-	0/18/18/23	0/1/1/1
5	GOL	A	326	-	-	0/4/4/4	0/0/0/0
5	GOL	A	327	-	-	0/4/4/4	0/0/0/0
5	GOL	A	328	-	-	0/4/4/4	0/0/0/0
5	GOL	A	329	-	-	0/4/4/4	0/0/0/0
6	CCN	A	330	-	-	0/0/0/0	0/0/0/0
6	CCN	A	331	-	-	0/0/0/0	0/0/0/0
3	JZA	B	324	-	-	0/4/28/28	0/1/2/2
4	TRT	B	325	-	-	0/18/18/23	0/1/1/1
7	M12	C	0	2	-	0/9/10/11	0/0/0/0
7	M12	D	0	2	-	0/0/0/11	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	324	JZA	C10-N9	2.05	1.50	1.47
6	A	331	CCN	C2-C1	2.18	1.61	1.44
4	B	325	TRT	O15-C16	2.21	1.51	1.43
3	A	324	JZA	C5-N6	2.29	1.51	1.48
4	B	325	TRT	O18-C17	2.66	1.53	1.42
4	A	325	TRT	C6-C9	2.97	1.58	1.53
3	A	324	JZA	C7-N6	3.38	1.50	1.40
4	B	325	TRT	C6-C9	3.46	1.59	1.53
3	B	324	JZA	C7-N6	3.52	1.50	1.40
3	B	324	JZA	C7-N9	6.65	1.51	1.36
3	A	324	JZA	O3-S1	6.81	1.51	1.43
3	A	324	JZA	C7-N9	6.97	1.52	1.36
3	A	324	JZA	O2-S1	7.38	1.52	1.43
3	B	324	JZA	O2-S1	7.53	1.52	1.43
3	B	324	JZA	O3-S1	8.08	1.52	1.43
3	B	324	JZA	C5-N6	12.88	1.62	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	324	JZA	C10-N9-C7	-2.42	110.86	120.99
3	B	324	JZA	O14-C13-C11	2.09	116.64	111.84
3	B	324	JZA	O14-C12-C10	2.19	116.86	111.84
4	B	325	TRT	O18-C17-C16	3.15	124.37	110.36
4	B	325	TRT	O15-C16-C17	3.48	120.55	108.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	324	JZA	3	0
4	A	325	TRT	2	0
5	A	327	GOL	1	0
5	A	328	GOL	12	0
5	A	329	GOL	2	0
6	A	330	CCN	6	0
6	A	331	CCN	4	0
3	B	324	JZA	7	0
4	B	325	TRT	9	0
7	C	0	M12	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	217/249 (87%)	1.19	35 (16%) 3 3	19, 35, 51, 71	0
1	B	224/249 (89%)	1.43	52 (23%) 1 1	20, 36, 69, 78	0
2	C	3/6 (50%)	2.05	2 (66%) 0 1	0, 0, 0, 33	0
2	D	3/6 (50%)	-0.10	0 100 100	34, 34, 37, 38	0
All	All	447/510 (87%)	1.30	89 (19%) 1 2	0, 35, 63, 78	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	TRP	10.9
1	B	176	CYS	8.7
1	B	178	ASN	7.9
1	B	122	THR	7.8
1	B	123	GLY	7.0
1	B	312	THR	6.5
1	A	79	PHE	6.0
1	B	200	ASN	5.8
1	B	313	GLY	5.8
1	B	310	TRP	5.6
1	A	306	GLN	5.5
1	B	323	HIS	5.5
1	A	308	GLY	5.1
1	B	81	TYR	5.0
1	B	179	ALA	5.0
1	B	183	THR	4.9
1	B	306	GLN	4.4
1	B	214	ASN	4.3
1	B	182	VAL	4.1
1	A	206	SER	4.0
1	B	164	LEU	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	309	GLU	3.8
1	B	308	GLY	3.8
1	B	314	LEU	3.8
1	A	312	THR	3.7
1	B	177	GLU	3.6
1	A	171	SER	3.6
1	B	106	PHE	3.6
1	A	130	ILE	3.5
1	B	172	SER	3.5
1	B	254	PRO	3.4
1	B	305	LYS	3.4
1	B	237	ILE	3.4
1	B	180	LEU	3.4
1	B	311	PRO	3.3
1	B	257	GLN	3.3
1	A	258	LEU	3.3
1	B	173	GLY	3.3
1	A	196	PHE	3.2
1	A	94	THR	3.1
1	A	95	LEU	3.1
1	B	211	VAL	3.1
1	B	161	SER	3.0
1	A	307	GLU	3.0
1	B	157	TYR	2.9
1	A	144	ILE	2.9
1	B	238	LEU	2.9
1	B	252	GLN	2.9
1	A	230	LEU	2.8
2	C	6	TYR	2.8
1	B	162	LYS	2.8
1	A	131	VAL	2.7
1	A	234	THR	2.7
1	A	257	GLN	2.7
1	B	303	PHE	2.6
1	A	101	ILE	2.6
1	A	311	PRO	2.5
1	B	212	PRO	2.5
1	A	322	ILE	2.5
1	A	237	ILE	2.5
1	B	242	ILE	2.5
1	A	132	VAL	2.5
1	B	166	ILE	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	5	ALA	2.4
1	B	309	GLU	2.4
1	B	144	ILE	2.4
1	B	271	MET	2.4
1	B	275	ARG	2.3
1	B	248	GLY	2.3
1	B	243	ALA	2.3
1	A	305	LYS	2.3
1	A	247	VAL	2.2
1	B	240	VAL	2.2
1	A	238	LEU	2.2
1	B	160	VAL	2.2
1	A	93	PRO	2.2
1	B	270	MET	2.2
1	B	171	SER	2.2
1	A	92	MET	2.2
1	B	124	HIS	2.2
1	A	246	GLN	2.2
1	A	175	ALA	2.2
1	A	236	ARG	2.1
1	A	271	MET	2.1
1	A	133	PHE	2.1
1	B	276	ASP	2.1
1	B	197	SER	2.1
1	B	239	THR	2.0
1	A	179	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DAL	D	2	5/6	0.92	0.15	-	42,43,46,52	5
2	DSE	C	1	7/8	0.93	0.13	-	42,49,56,57	5
2	DSE	D	1	7/8	0.80	0.33	-	59,62,66,69	5
2	5PG	D	4	12/13	0.96	0.10	-	31,33,37,39	0
2	DAL	C	2	5/6	0.94	0.11	-	33,37,39,39	5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	5PG	C	4	12/13	0.94	0.28	-	0,0,0,0	0

### 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( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	328	6/6	0.49	0.46	8.15	52,59,64,66	0
4	TRT	A	325	20/25	0.46	0.40	7.61	121,133,137,138	0
3	JZA	B	324	14/14	0.47	0.52	6.65	135,138,141,142	0
3	JZA	A	324	14/14	0.30	0.51	4.57	161,162,163,163	0
4	TRT	B	325	20/25	0.50	0.38	4.41	92,97,101,101	0
6	CCN	A	331	3/3	0.68	0.36	3.87	26,26,35,48	0
5	GOL	A	326	6/6	0.77	0.25	3.62	82,83,83,86	0
6	CCN	A	330	3/3	0.81	0.31	1.99	27,27,30,37	0
7	M12	C	0	13/14	0.60	0.26	-	60,77,83,85	3
5	GOL	A	327	6/6	0.78	0.27	-	83,86,88,88	0
7	M12	D	0	3/14	0.76	0.45	-	66,66,66,66	3
5	GOL	A	329	6/6	0.49	0.47	-	64,68,69,70	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.