



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2016 – 10:10 AM EDT

PDB ID : 5EY8  
Title : Structure of FadD32 from Mycobacterium smegmatis complexed to AMPC20  
Authors : Guillet, V.; Maveyraud, L.; Mourey, L.  
Deposited on : 2015-11-24  
Resolution : 3.50 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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) : rb-20027107

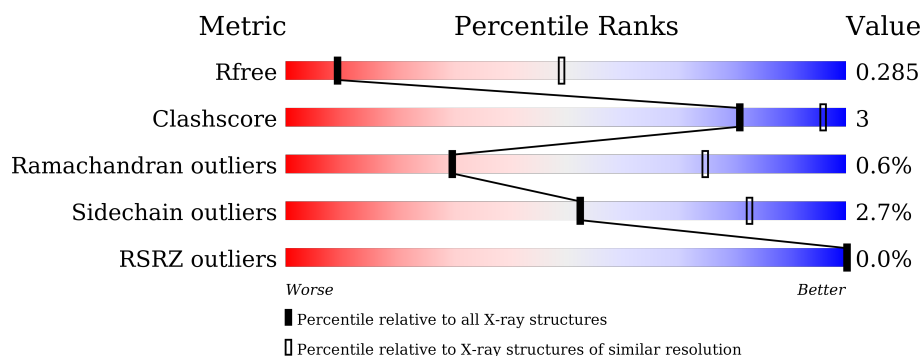
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	630	
1	B	630	
1	C	630	
1	D	630	
1	E	630	
1	F	630	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	630	 88%7%5%
1	H	630	 87%7%6%

## 2 Entry composition

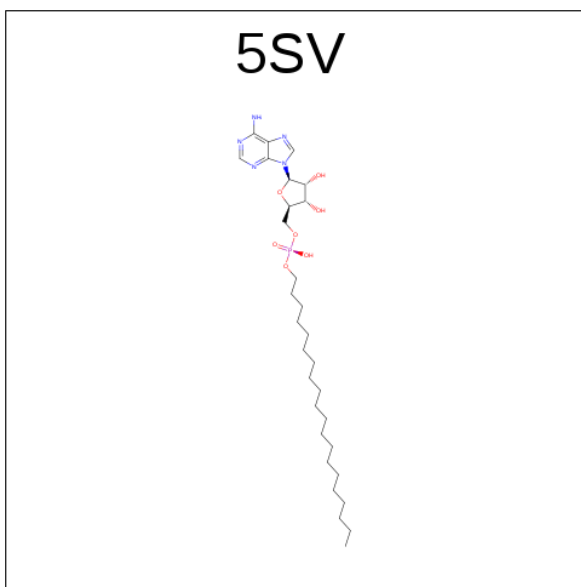
There are 3 unique types of molecules in this entry. The entry contains 33378 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4279	2719	744	809	7			
1	B	594	Total	C	N	O	S	0	0	0
			4129	2614	725	783	7			
1	C	605	Total	C	N	O	S	0	0	0
			4153	2626	726	794	7			
1	D	603	Total	C	N	O	S	0	0	0
			4194	2659	727	801	7			
1	E	592	Total	C	N	O	S	0	0	0
			4095	2598	714	776	7			
1	F	606	Total	C	N	O	S	0	0	0
			4303	2712	769	815	7			
1	G	597	Total	C	N	O	S	0	0	0
			4057	2572	697	781	7			
1	H	595	Total	C	N	O	S	0	0	0
			3871	2427	687	751	6			

- Molecule 2 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl icosyl hydrogen phosphate (three-letter code: 5SV) (formula: C<sub>30</sub>H<sub>54</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	23	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			35	22	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			36	23	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			39	26	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			36	23	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			34	21	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			34	21	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			35	22	5	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

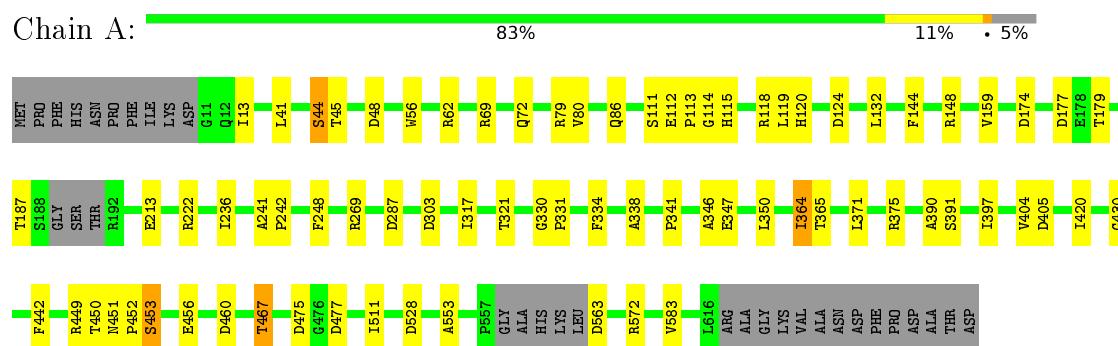


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

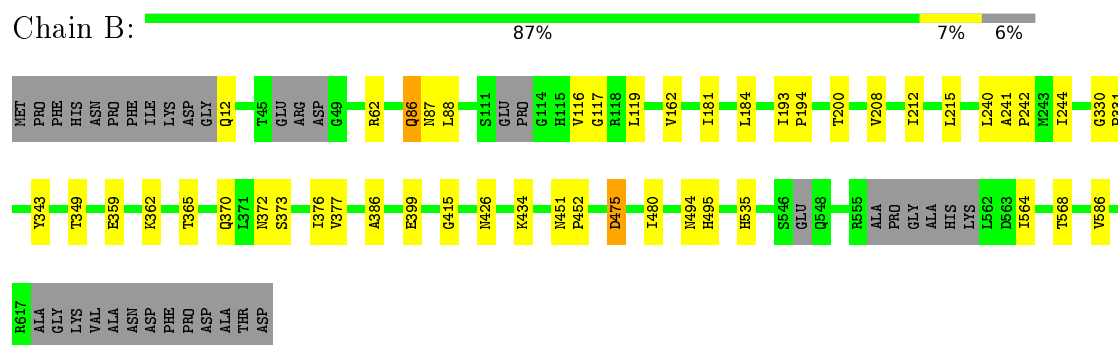
### 3 Residue-property plots

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.

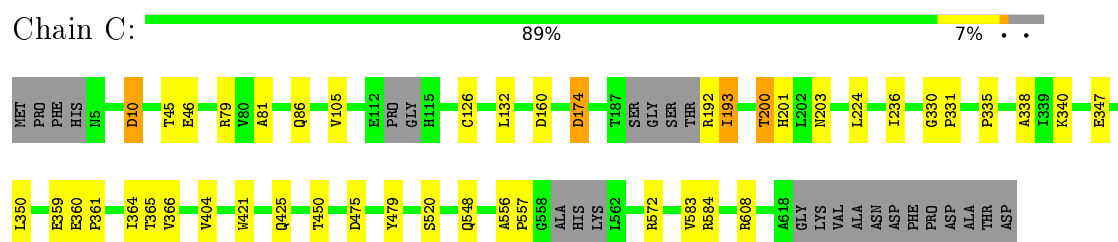
#### • Molecule 1: Acyl-CoA synthase



#### • Molecule 1: Acyl-CoA synthase

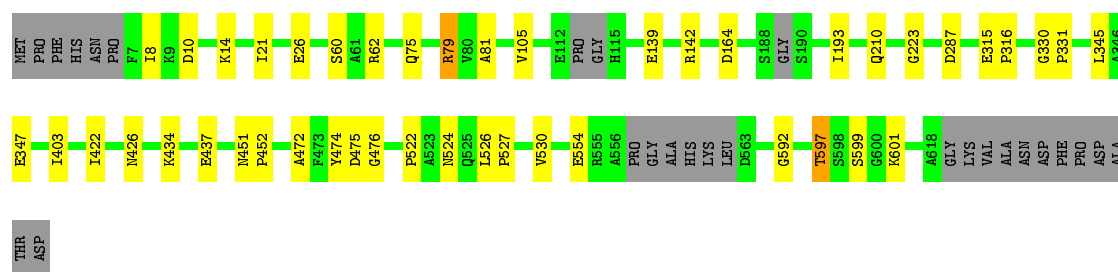


#### • Molecule 1: Acyl-CoA synthase



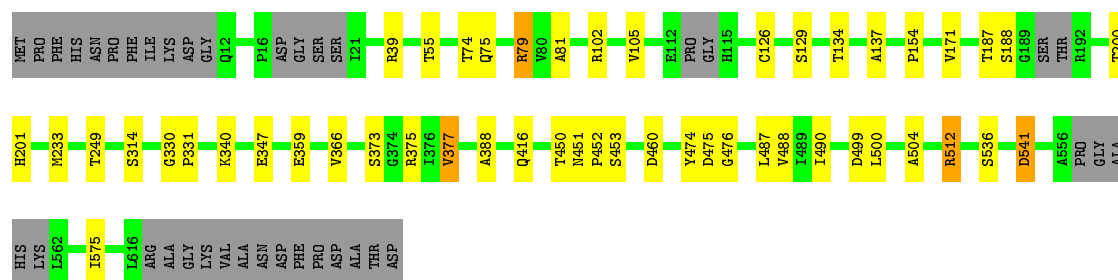
#### • Molecule 1: Acyl-CoA synthase





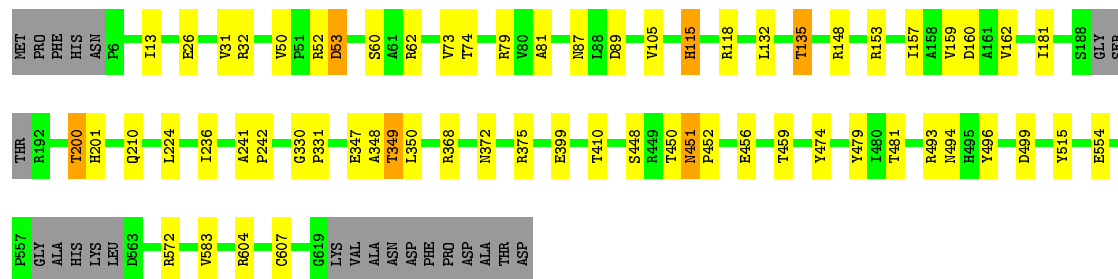
- Molecule 1: Acyl-CoA synthase

Chain E: 86% 7% 6%



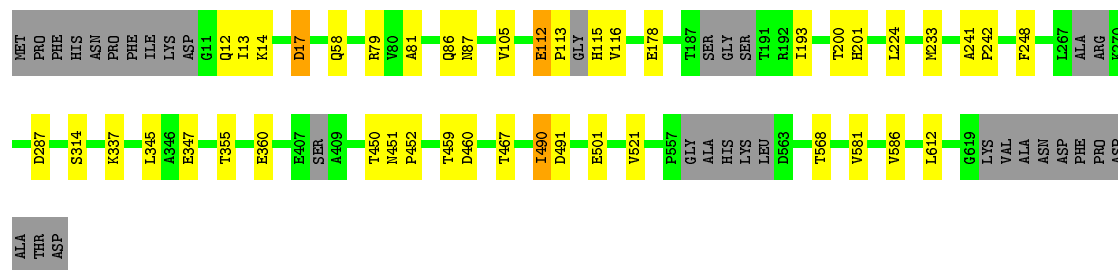
- Molecule 1: Acyl-CoA synthase

Chain F: 86% 9% 2%



- Molecule 1: Acyl-CoA synthase

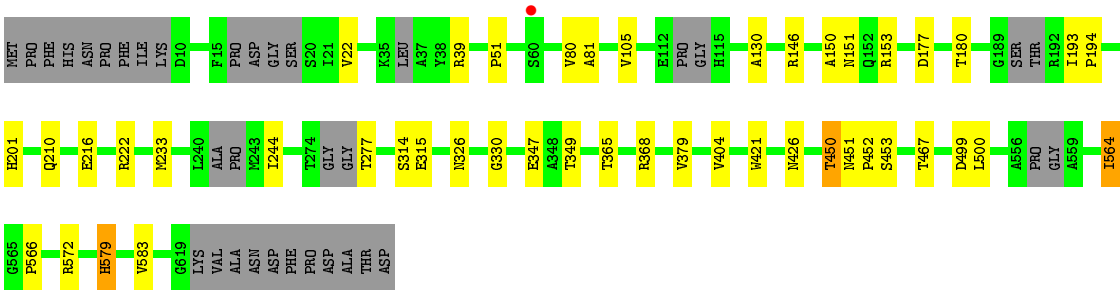
Chain G: 88% 7% 5%



- Molecule 1: Acyl-CoA synthase

Chain H: 87% 7% 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.04Å 164.04Å 231.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 3.50 50.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.44-3.50) 93.6 (50.62-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.23	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.223 , 0.286 0.222 , 0.285	Depositor DCC
$R_{free}$ test set	3628 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 72.6	EDS
Estimated twinning fraction	0.075 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 72012 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	33378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 5SV

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	0.30	0/4384	0.52	0/6025
1	B	0.29	0/4228	0.50	0/5814
1	C	0.28	0/4259	0.47	0/5867
1	D	0.28	0/4298	0.50	0/5913
1	E	0.28	0/4194	0.51	0/5770
1	F	0.28	0/4409	0.50	0/6054
1	G	0.27	0/4160	0.49	0/5736
1	H	0.26	0/3957	0.46	0/5452
All	All	0.28	0/33889	0.50	0/46631

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	B	0	1
1	E	0	2
1	G	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	SER	Peptide
1	E	373	SER	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	E	512	ARG	Peptide
1	G	116	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4279	0	3939	36	0
1	B	4129	0	3651	27	0
1	C	4153	0	3555	25	0
1	D	4194	0	3660	23	0
1	E	4095	0	3589	25	0
1	F	4303	0	3861	29	0
1	G	4057	0	3423	19	0
1	H	3871	0	3107	21	0
2	A	36	0	36	0	0
2	B	35	0	34	0	0
2	C	36	0	36	1	0
2	D	39	0	42	1	0
2	E	36	0	36	0	0
2	F	34	0	32	0	0
2	G	34	0	32	0	0
2	H	35	0	34	0	0
3	E	6	0	8	1	0
3	F	6	0	8	0	0
All	All	33378	0	29083	205	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 3.

All (205) 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:F:572:ARG:NH1	1:F:583:VAL:O	2.04	0.91
1:H:572:ARG:NH1	1:H:583:VAL:O	2.09	0.85
1:A:572:ARG:NH1	1:A:583:VAL:O	2.16	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:NH1	1:A:303:ASP:OD2	2.17	0.78
1:C:520:SER:O	1:C:608:ARG:NH1	2.17	0.78
1:D:223:GLY:HA3	2:D:701:5SV:H45	1.68	0.75
1:E:388:ALA:H	3:E:702:GOL:H11	1.50	0.74
1:H:450:THR:O	1:H:453:SER:OG	2.07	0.72
1:A:62:ARG:NH2	1:A:159:VAL:O	2.23	0.72
1:C:572:ARG:NH1	1:C:583:VAL:O	2.25	0.69
1:C:347:GLU:OE1	1:C:347:GLU:N	2.26	0.67
1:D:597:THR:OG1	1:D:601:LYS:O	2.12	0.67
1:D:139:GLU:OE1	1:D:142:ARG:NH1	2.28	0.66
1:E:74:THR:O	1:E:102:ARG:NH2	2.29	0.64
1:C:556:ALA:HB3	1:C:557:PRO:HD3	1.79	0.64
1:D:347:GLU:N	1:D:347:GLU:OE2	2.32	0.63
1:B:399:GLU:OE2	1:B:426:ASN:ND2	2.32	0.62
1:H:347:GLU:N	1:H:347:GLU:OE1	2.32	0.61
1:D:554:GLU:OE1	1:D:592:GLY:N	2.33	0.61
1:E:347:GLU:OE1	1:E:347:GLU:N	2.33	0.60
1:F:368:ARG:NH1	1:F:499:ASP:OD2	2.34	0.60
1:F:347:GLU:OE1	1:F:347:GLU:N	2.34	0.60
1:B:372:ASN:ND2	1:B:494:ASN:O	2.34	0.60
1:H:210:GLN:NE2	1:H:426:ASN:OD1	2.36	0.59
1:H:81:ALA:HA	1:H:105:VAL:HG13	1.86	0.58
1:G:347:GLU:OE1	1:G:347:GLU:N	2.37	0.58
1:C:340:LYS:NZ	1:C:359:GLU:O	2.37	0.57
1:G:490:ILE:HG23	1:G:491:ASP:H	1.68	0.57
1:A:347:GLU:N	1:A:347:GLU:OE1	2.38	0.57
1:H:564:ILE:C	1:H:566:PRO:HD2	2.25	0.57
1:F:115:HIS:NE2	1:F:118:ARG:HG3	2.21	0.56
1:G:112:GLU:CB	1:G:115:HIS:HA	2.37	0.54
1:B:87:ASN:OD1	1:B:88:LEU:N	2.40	0.54
1:A:177:ASP:OD1	1:A:179:THR:OG1	2.24	0.54
1:D:451:ASN:HB3	1:D:452:PRO:HD3	1.90	0.54
1:F:348:ALA:O	1:F:349:THR:HG22	2.08	0.54
1:D:81:ALA:HA	1:D:105:VAL:HG13	1.89	0.54
1:G:451:ASN:CB	1:G:452:PRO:HD3	2.38	0.54
1:F:53:ASP:N	1:F:53:ASP:OD1	2.41	0.53
1:D:10:ASP:OD1	1:D:10:ASP:N	2.40	0.53
1:E:81:ALA:HA	1:E:105:VAL:HG13	1.90	0.53
1:F:31:VAL:HG13	1:F:32:ARG:HG2	1.91	0.53
1:B:194:PRO:O	1:B:434:LYS:NZ	2.26	0.53
1:F:372:ASN:ND2	1:F:494:ASN:O	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ILE:HG22	1:C:365:THR:H	1.74	0.52
1:A:317:ILE:HG13	1:A:390:ALA:HB3	1.91	0.52
1:F:236:ILE:HD12	1:F:350:LEU:HB2	1.91	0.52
1:A:124:ASP:OD1	1:A:148:ARG:NH2	2.43	0.52
1:D:434:LYS:NZ	1:D:437:GLU:OE1	2.41	0.52
1:G:233:MET:SD	1:G:314:SER:HB3	2.50	0.52
1:A:563:ASP:OD1	1:A:563:ASP:N	2.43	0.51
1:A:120:HIS:CE1	1:A:144:PHE:CE1	2.98	0.51
1:A:453:SER:HB3	1:A:456:GLU:HG2	1.93	0.51
1:G:112:GLU:CB	1:G:113:PRO:CD	2.89	0.51
1:H:368:ARG:NH1	1:H:499:ASP:OD2	2.44	0.51
1:C:200:THR:OG1	1:C:201:HIS:N	2.43	0.51
1:C:330:GLY:N	1:C:331:PRO:HD2	2.25	0.51
1:A:80:VAL:CG1	1:A:132:LEU:HD13	2.41	0.50
1:F:62:ARG:NH2	1:F:159:VAL:O	2.43	0.50
1:F:330:GLY:N	1:F:331:PRO:HD2	2.26	0.50
1:E:39:ARG:HB3	1:E:249:THR:HG22	1.94	0.50
1:F:50:VAL:O	1:F:52:ARG:N	2.45	0.50
2:C:701:5SV:H2	2:C:701:5SV:H19	1.93	0.49
1:E:79:ARG:HD2	1:E:126:CYS:HB2	1.94	0.49
1:B:241:ALA:N	1:B:242:PRO:HD2	2.26	0.49
1:G:81:ALA:HA	1:G:105:VAL:HG13	1.93	0.49
1:G:112:GLU:CB	1:G:113:PRO:HD2	2.42	0.49
1:A:44:SER:OG	1:A:45:THR:N	2.46	0.49
1:E:79:ARG:NE	1:E:126:CYS:O	2.45	0.49
1:F:451:ASN:HB2	1:F:452:PRO:HD3	1.94	0.49
1:H:233:MET:SD	1:H:314:SER:OG	2.67	0.49
1:E:102:ARG:HD2	1:E:102:ARG:N	2.27	0.48
1:B:212:ILE:CD1	1:B:244:ILE:HD11	2.44	0.48
1:C:364:ILE:HG22	1:C:365:THR:N	2.29	0.48
1:G:17:ASP:OD1	1:G:17:ASP:N	2.45	0.48
1:D:330:GLY:N	1:D:331:PRO:HD2	2.28	0.48
1:F:148:ARG:O	1:F:153:ARG:NH1	2.47	0.47
1:H:150:ALA:HA	1:H:153:ARG:HD2	1.96	0.47
1:C:81:ALA:HA	1:C:105:VAL:HG13	1.95	0.47
1:E:187:THR:HG22	1:E:188:SER:N	2.29	0.47
1:E:541:ASP:N	1:E:541:ASP:OD1	2.47	0.47
1:H:404:VAL:HG21	1:H:421:TRP:CE2	2.49	0.47
1:D:62:ARG:NH1	1:D:164:ASP:OD1	2.47	0.47
1:B:86:GLN:O	1:B:87:ASN:CG	2.52	0.47
1:B:86:GLN:CG	1:B:87:ASN:H	2.28	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:CD1	1:A:341:PRO:HB3	2.45	0.47
1:C:192:ARG:O	1:C:193:ILE:HG22	2.14	0.47
1:E:451:ASN:CB	1:E:452:PRO:HD3	2.45	0.47
1:D:8:ILE:CB	1:D:14:LYS:H	2.27	0.47
1:C:556:ALA:CB	1:C:557:PRO:HD3	2.44	0.47
1:F:73:VAL:HG23	1:F:74:THR:HG23	1.96	0.47
1:B:376:ILE:N	1:B:415:GLY:O	2.39	0.46
1:C:174:ASP:N	1:C:174:ASP:OD1	2.43	0.46
1:C:556:ALA:HB3	1:C:557:PRO:CD	2.45	0.46
1:D:26:GLU:OE1	1:D:60:SER:OG	2.28	0.46
1:A:451:ASN:HB3	1:A:452:PRO:HD3	1.96	0.46
1:B:343:TYR:CD1	1:B:480:ILE:CD1	2.99	0.46
1:F:200:THR:OG1	1:F:201:HIS:N	2.49	0.46
1:B:451:ASN:CB	1:B:452:PRO:HD3	2.46	0.46
1:A:330:GLY:N	1:A:331:PRO:CD	2.79	0.45
1:E:200:THR:HG22	1:E:201:HIS:H	1.81	0.45
1:F:181:ILE:HA	1:F:200:THR:HA	1.97	0.45
1:D:527:PRO:HG2	1:D:530:VAL:HG23	1.97	0.45
1:H:500:LEU:HD23	1:H:579:HIS:CD2	2.51	0.45
1:D:522:PRO:C	1:D:524:ASN:H	2.20	0.45
1:E:187:THR:HG22	1:E:188:SER:H	1.82	0.45
1:F:132:LEU:HD23	1:F:157:ILE:CD1	2.47	0.45
1:C:236:ILE:HB	1:C:350:LEU:HD22	1.98	0.45
1:G:241:ALA:N	1:G:242:PRO:HD2	2.32	0.45
1:G:568:THR:HG23	1:G:586:VAL:CG1	2.47	0.45
1:C:364:ILE:HD11	1:C:479:TYR:OH	2.16	0.45
1:G:521:VAL:HG11	1:G:612:LEU:HD21	1.98	0.45
1:A:430:GLY:HA2	1:A:442:PHE:CD1	2.51	0.45
1:B:343:TYR:CG	1:B:480:ILE:CD1	3.00	0.45
1:C:45:THR:HG23	1:C:46:GLU:H	1.81	0.45
1:B:116:VAL:O	1:B:119:LEU:N	2.49	0.44
1:B:330:GLY:N	1:B:331:PRO:HD2	2.31	0.44
1:C:404:VAL:HG11	1:C:421:TRP:CE2	2.52	0.44
1:B:181:ILE:HD11	1:B:184:LEU:HD13	1.98	0.44
1:H:146:ARG:HA	1:H:153:ARG:HH21	1.82	0.44
1:A:112:GLU:O	1:A:114:GLY:N	2.50	0.44
1:B:208:VAL:HG13	1:B:240:LEU:HD12	1.98	0.44
1:E:488:VAL:O	1:E:488:VAL:HG12	2.18	0.44
1:H:451:ASN:CB	1:H:452:PRO:HD3	2.48	0.44
1:F:410:THR:HG22	1:F:448:SER:HB3	2.00	0.44
1:A:213:GLU:CB	1:A:397:ILE:HD12	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ILE:HG23	1:A:365:THR:N	2.32	0.44
1:A:80:VAL:HG13	1:A:132:LEU:CD1	2.48	0.44
1:F:241:ALA:HB3	1:F:242:PRO:HD3	2.00	0.44
1:H:177:ASP:HB3	1:H:180:THR:HG23	2.00	0.44
1:B:349:THR:OG1	1:B:426:ASN:O	2.31	0.43
1:E:504:ALA:HB2	1:E:575:ILE:HD11	2.00	0.43
1:F:604:ARG:O	1:F:607:CYS:N	2.51	0.43
1:A:80:VAL:CG1	1:A:132:LEU:CD1	2.96	0.43
1:G:200:THR:HG22	1:G:201:HIS:H	1.84	0.43
1:B:343:TYR:CG	1:B:480:ILE:HD11	2.54	0.43
1:G:241:ALA:CB	1:G:248:PHE:HB2	2.48	0.43
1:A:334:PHE:CZ	1:A:338:ALA:HB3	2.53	0.43
1:E:499:ASP:OD1	1:E:500:LEU:N	2.51	0.43
1:B:116:VAL:HG13	1:B:117:GLY:N	2.33	0.43
1:B:494:ASN:O	1:B:495:HIS:ND1	2.52	0.43
1:E:474:TYR:O	1:E:476:GLY:N	2.52	0.43
1:A:241:ALA:HB2	1:A:248:PHE:HB2	2.01	0.43
1:F:135:THR:OG1	1:F:160:ASP:OD2	2.37	0.43
1:G:345:LEU:HD11	1:G:467:THR:HB	2.00	0.43
1:B:86:GLN:HG3	1:B:87:ASN:H	1.84	0.42
1:F:515:TYR:CB	1:F:554:GLU:HB2	2.49	0.42
1:H:193:ILE:HG13	1:H:194:PRO:HD2	2.01	0.42
1:A:391:SER:HB2	1:A:477:ASP:HB3	2.00	0.42
1:B:365:THR:CG2	1:B:386:ALA:HB1	2.49	0.42
1:D:315:GLU:HB2	1:D:316:PRO:HD2	2.00	0.42
1:E:129:SER:C	1:E:154:PRO:HB3	2.39	0.42
1:H:365:THR:OG1	1:H:379:VAL:O	2.30	0.42
1:E:233:MET:SD	1:E:314:SER:HB3	2.60	0.42
1:G:178:GLU:O	1:G:200:THR:HG21	2.20	0.42
1:B:370:GLN:HG2	1:B:377:VAL:HG22	2.02	0.42
1:C:132:LEU:HD12	1:C:132:LEU:N	2.35	0.42
1:G:490:ILE:HG21	1:G:581:VAL:HG11	2.02	0.42
1:A:187:THR:HG21	1:A:346:ALA:CB	2.50	0.42
1:C:548:GLN:HB3	1:C:584:ARG:HG3	2.00	0.42
1:F:81:ALA:HA	1:F:105:VAL:HG13	2.01	0.42
1:B:362:LYS:NZ	1:B:475:ASP:OD2	2.49	0.42
1:D:403:ILE:HG21	1:D:472:ALA:HA	2.02	0.42
1:F:26:GLU:OE1	1:F:60:SER:OG	2.36	0.42
1:G:12:GLN:CB	1:G:14:LYS:H	2.33	0.42
1:C:203:ASN:ND2	1:C:425:GLN:O	2.53	0.42
1:B:181:ILE:HA	1:B:200:THR:HA	2.02	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:HD2	1:C:126:CYS:HB2	2.02	0.41
1:E:200:THR:HG22	1:E:201:HIS:N	2.35	0.41
1:H:222:ARG:HG2	1:H:277:THR:HG22	2.01	0.41
1:A:287:ASP:OD2	1:A:321:THR:OG1	2.32	0.41
1:A:404:VAL:HG12	1:A:405:ASP:N	2.35	0.41
1:A:56:TRP:CH2	1:A:242:PRO:HA	2.55	0.41
1:A:236:ILE:HD12	1:A:350:LEU:HB2	2.02	0.41
1:D:210:GLN:OE1	1:D:426:ASN:ND2	2.53	0.41
1:E:340:LYS:NZ	1:E:359:GLU:O	2.53	0.41
1:F:474:TYR:HB3	1:F:479:TYR:CE1	2.55	0.41
1:A:69:ARG:O	1:A:72:GLN:HG2	2.21	0.41
1:C:160:ASP:OD1	1:C:160:ASP:N	2.54	0.41
1:D:79:ARG:HB2	1:D:79:ARG:HH11	1.85	0.41
1:F:87:ASN:OD1	1:F:89:ASP:N	2.53	0.41
1:D:75:GLN:HA	1:H:151:ASN:HB3	2.03	0.41
1:A:420:ILE:HB	1:A:467:THR:HG21	2.02	0.41
1:C:360:GLU:HG2	1:C:361:PRO:HD2	2.03	0.41
1:D:474:TYR:O	1:D:476:GLY:N	2.53	0.41
1:E:375:ARG:HA	1:E:416:GLN:HA	2.02	0.41
1:D:345:LEU:N	1:D:345:LEU:HD23	2.36	0.41
1:A:317:ILE:CG1	1:A:390:ALA:HB3	2.50	0.41
1:C:335:PRO:HG2	1:C:338:ALA:HB2	2.03	0.41
1:D:345:LEU:HD21	1:D:422:ILE:HD13	2.03	0.41
1:E:366:VAL:HG13	1:E:377:VAL:H	1.85	0.41
1:H:326:ASN:O	1:H:330:GLY:N	2.54	0.41
1:B:62:ARG:NH2	1:B:162:VAL:O	2.49	0.41
1:F:210:GLN:NE2	1:F:399:GLU:OE2	2.53	0.41
1:G:337:LYS:HA	1:G:360:GLU:HG3	2.03	0.41
1:A:132:LEU:HD12	1:A:132:LEU:N	2.35	0.40
1:B:568:THR:HG23	1:B:586:VAL:CG1	2.52	0.40
1:A:511:ILE:HG23	1:A:553:ALA:HB1	2.03	0.40
1:F:481:THR:HG21	1:F:496:TYR:CZ	2.57	0.40
1:H:80:VAL:HG12	1:H:130:ALA:HB3	2.03	0.40
1:A:41:LEU:HD12	1:A:41:LEU:N	2.37	0.40
1:A:114:GLY:O	1:A:115:HIS:CB	2.70	0.40
1:E:134:THR:HG23	1:E:137:ALA:H	1.87	0.40
1:E:330:GLY:N	1:E:331:PRO:CD	2.85	0.40
1:H:39:ARG:HH11	1:H:51:PRO:HB3	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	592/630 (94%)	568 (96%)	19 (3%)	5 (1%)	24	70
1	B	584/630 (93%)	559 (96%)	21 (4%)	4 (1%)	26	72
1	C	597/630 (95%)	581 (97%)	14 (2%)	2 (0%)	46	84
1	D	595/630 (94%)	572 (96%)	20 (3%)	3 (0%)	34	78
1	E	582/630 (92%)	557 (96%)	21 (4%)	4 (1%)	26	72
1	F	600/630 (95%)	572 (95%)	27 (4%)	1 (0%)	52	88
1	G	585/630 (93%)	565 (97%)	17 (3%)	3 (0%)	34	78
1	H	579/630 (92%)	550 (95%)	25 (4%)	4 (1%)	26	72
All	All	4714/5040 (94%)	4524 (96%)	164 (4%)	26 (1%)	30	75

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	475	ASP
1	E	475	ASP
1	G	13	ILE
1	H	244	ILE
1	A	44	SER
1	A	475	ASP
1	B	564	ILE
1	A	453	SER
1	E	453	SER
1	E	512	ARG
1	F	115	HIS
1	B	86	GLN
1	B	475	ASP
1	H	22	VAL
1	A	113	PRO
1	C	10	ASP
1	D	526	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	536	SER
1	G	112	GLU
1	B	193	ILE
1	H	349	THR
1	A	13	ILE
1	C	193	ILE
1	G	193	ILE
1	D	21	ILE
1	H	564	ILE

### 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	395/501 (79%)	379 (96%)	16 (4%)	37	74
1	B	352/501 (70%)	348 (99%)	4 (1%)	80	92
1	C	343/501 (68%)	335 (98%)	8 (2%)	58	85
1	D	355/501 (71%)	350 (99%)	5 (1%)	74	91
1	E	345/501 (69%)	335 (97%)	10 (3%)	50	81
1	F	380/501 (76%)	366 (96%)	14 (4%)	41	76
1	G	326/501 (65%)	313 (96%)	13 (4%)	38	75
1	H	277/501 (55%)	271 (98%)	6 (2%)	60	85
All	All	2773/4008 (69%)	2697 (97%)	76 (3%)	52	83

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	79	ARG
1	A	86	GLN
1	A	111	SER
1	A	118	ARG
1	A	119	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	174	ASP
1	A	222	ARG
1	A	364	ILE
1	A	371	LEU
1	A	375	ARG
1	A	449	ARG
1	A	450	THR
1	A	460	ASP
1	A	467	THR
1	A	528	ASP
1	B	12	GLN
1	B	215	LEU
1	B	359	GLU
1	B	535	HIS
1	C	10	ASP
1	C	86	GLN
1	C	174	ASP
1	C	200	THR
1	C	224	LEU
1	C	366	VAL
1	C	450	THR
1	C	475	ASP
1	D	79	ARG
1	D	193	ILE
1	D	287	ASP
1	D	597	THR
1	D	599	SER
1	E	55	THR
1	E	75	GLN
1	E	79	ARG
1	E	171	VAL
1	E	377	VAL
1	E	450	THR
1	E	460	ASP
1	E	487	LEU
1	E	490	ILE
1	E	541	ASP
1	F	13	ILE
1	F	53	ASP
1	F	79	ARG
1	F	135	THR
1	F	162	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	200	THR
1	F	224	LEU
1	F	349	THR
1	F	375	ARG
1	F	450	THR
1	F	451	ASN
1	F	456	GLU
1	F	459	THR
1	F	493	ARG
1	G	17	ASP
1	G	58	GLN
1	G	79	ARG
1	G	86	GLN
1	G	87	ASN
1	G	224	LEU
1	G	287	ASP
1	G	355	THR
1	G	450	THR
1	G	459	THR
1	G	460	ASP
1	G	490	ILE
1	G	501	GLU
1	H	201	HIS
1	H	216	GLU
1	H	315	GLU
1	H	450	THR
1	H	467	THR
1	H	579	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	207	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	5SV	A	701	-	35,38,45	1.06	3 (8%)	34,51,58	1.21	4 (11%)
2	5SV	B	701	-	34,37,45	1.03	2 (5%)	33,50,58	1.10	2 (6%)
2	5SV	C	701	-	35,38,45	1.06	2 (5%)	34,51,58	1.29	4 (11%)
2	5SV	D	701	-	38,41,45	1.08	3 (7%)	37,54,58	1.12	1 (2%)
2	5SV	E	701	-	35,38,45	1.10	4 (11%)	34,51,58	1.12	4 (11%)
3	GOL	E	702	-	5,5,5	0.40	0	5,5,5	0.26	0
2	5SV	F	701	-	33,36,45	1.03	2 (6%)	32,49,58	1.08	2 (6%)
3	GOL	F	702	-	5,5,5	0.34	0	5,5,5	0.29	0
2	5SV	G	701	-	33,36,45	1.15	3 (9%)	32,49,58	1.17	3 (9%)
2	5SV	H	701	-	34,37,45	1.05	3 (8%)	33,50,58	1.14	5 (15%)

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	5SV	A	701	-	-	0/21/41/48	0/3/3/3
2	5SV	B	701	-	-	0/20/40/48	0/3/3/3
2	5SV	C	701	-	-	0/21/41/48	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5SV	D	701	-	-	0/24/44/48	0/3/3/3
2	5SV	E	701	-	-	0/21/41/48	0/3/3/3
3	GOL	E	702	-	-	0/4/4/4	0/0/0/0
2	5SV	F	701	-	-	0/19/39/48	0/3/3/3
3	GOL	F	702	-	-	0/4/4/4	0/0/0/0
2	5SV	G	701	-	-	0/19/39/48	0/3/3/3
2	5SV	H	701	-	-	0/20/40/48	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	5SV	P-O2P	-2.17	1.45	1.55
2	F	701	5SV	O4'-C4'	-2.09	1.40	1.45
2	E	701	5SV	O2'-C2'	-2.01	1.38	1.43
2	E	701	5SV	C2'-C1'	2.01	1.56	1.53
2	A	701	5SV	P-O1P	2.01	1.58	1.51
2	D	701	5SV	C2-N3	2.09	1.35	1.32
2	F	701	5SV	P-O1P	2.12	1.59	1.51
2	H	701	5SV	P-O1P	2.16	1.59	1.51
2	B	701	5SV	P-O1P	2.18	1.59	1.51
2	H	701	5SV	C2-N3	2.23	1.36	1.32
2	E	701	5SV	P-O1P	2.23	1.59	1.51
2	C	701	5SV	C2'-C1'	2.24	1.57	1.53
2	B	701	5SV	C2-N3	2.26	1.36	1.32
2	D	701	5SV	P-O1P	2.30	1.59	1.51
2	G	701	5SV	P-O1P	2.38	1.60	1.51
2	C	701	5SV	C2-N3	2.42	1.36	1.32
2	D	701	5SV	C2'-C1'	2.42	1.57	1.53
2	E	701	5SV	C2-N3	2.44	1.36	1.32
2	G	701	5SV	C2'-C1'	2.47	1.57	1.53
2	H	701	5SV	C2'-C1'	2.50	1.57	1.53
2	G	701	5SV	C2-N3	2.63	1.36	1.32
2	A	701	5SV	C2-N3	2.65	1.36	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	5SV	C1'-N9-C4	-3.63	122.75	126.81
2	G	701	5SV	C1'-N9-C4	-2.91	123.56	126.81
2	A	701	5SV	O3P-P-O1P	-2.58	98.66	109.21
2	B	701	5SV	O5'-P-O1P	-2.57	98.68	109.21
2	E	701	5SV	C1'-N9-C4	-2.45	124.07	126.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	5SV	O3P-P-O1P	-2.44	99.22	109.21
2	F	701	5SV	O3P-P-O1P	-2.44	99.22	109.21
2	E	701	5SV	O3P-P-O1P	-2.36	99.54	109.21
2	B	701	5SV	O3P-P-O1P	-2.33	99.66	109.21
2	H	701	5SV	O3P-P-O1P	-2.31	99.74	109.21
2	H	701	5SV	C1'-N9-C4	-2.31	124.22	126.81
2	E	701	5SV	O5'-P-O1P	-2.26	99.97	109.21
2	F	701	5SV	C1'-N9-C4	-2.24	124.31	126.81
2	H	701	5SV	O5'-P-O1P	-2.23	100.06	109.21
2	D	701	5SV	O5'-P-O1P	-2.18	100.28	109.21
2	C	701	5SV	O5'-P-O1P	-2.16	100.37	109.21
2	G	701	5SV	O5'-P-O1P	-2.15	100.42	109.21
2	A	701	5SV	C1'-N9-C4	-2.14	124.41	126.81
2	A	701	5SV	O3'-C3'-C4'	-2.14	104.61	111.01
2	G	701	5SV	O3P-P-O1P	-2.08	100.69	109.21
2	H	701	5SV	O3'-C3'-C4'	-2.01	105.02	111.01
2	C	701	5SV	O4'-C4'-C3'	2.06	109.35	105.16
2	E	701	5SV	N3-C2-N1	2.10	130.52	128.87
2	H	701	5SV	N3-C2-N1	2.11	130.53	128.87
2	A	701	5SV	C4'-O4'-C1'	2.42	112.21	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	5SV	1	0
2	D	701	5SV	1	0
3	E	702	GOL	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	598/630 (94%)	-0.46	0	100	100	32, 48, 94, 160	0
1	B	594/630 (94%)	-0.43	0	100	100	38, 57, 105, 196	0
1	C	605/630 (96%)	-0.42	0	100	100	38, 58, 99, 181	0
1	D	603/630 (95%)	-0.48	0	100	100	35, 54, 97, 171	0
1	E	592/630 (93%)	-0.36	0	100	100	37, 63, 115, 183	0
1	F	606/630 (96%)	-0.45	0	100	100	33, 53, 101, 173	0
1	G	597/630 (94%)	-0.39	0	100	100	37, 64, 113, 187	0
1	H	595/630 (94%)	-0.39	1 (0%)	95	93	38, 74, 123, 170	0
All	All	4790/5040 (95%)	-0.42	1 (0%)	100	100	32, 58, 109, 196	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	SER	2.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	5SV	D	701	39/43	0.97	0.30	1.23	35,42,49,50	0
2	5SV	E	701	36/43	0.97	0.29	1.02	37,38,44,50	0
2	5SV	F	701	34/43	0.97	0.26	0.58	33,34,44,45	0
2	5SV	G	701	34/43	0.96	0.30	0.57	39,47,53,70	0
2	5SV	A	701	36/43	0.96	0.26	0.31	32,32,36,56	0
2	5SV	C	701	36/43	0.96	0.26	0.11	38,44,79,89	0
2	5SV	B	701	35/43	0.96	0.25	0.06	38,38,39,68	0
2	5SV	H	701	35/43	0.97	0.26	-0.12	37,38,57,60	0
3	GOL	E	702	6/6	0.82	0.26	-0.33	40,40,40,74	0
3	GOL	F	702	6/6	0.90	0.20	-0.37	35,35,37,40	0

## 6.5 Other polymers

There are no such residues in this entry.