



# Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2017 – 10:49 AM EDT

PDB ID : 5WYA  
Title : Structure of amino acid racemase, 2.65 Å  
Authors : Sakuraba, H.; Mutaguchi, Y.; Hayashi, J.; Ohshima, T.  
Deposited on : 2017-01-11  
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029077

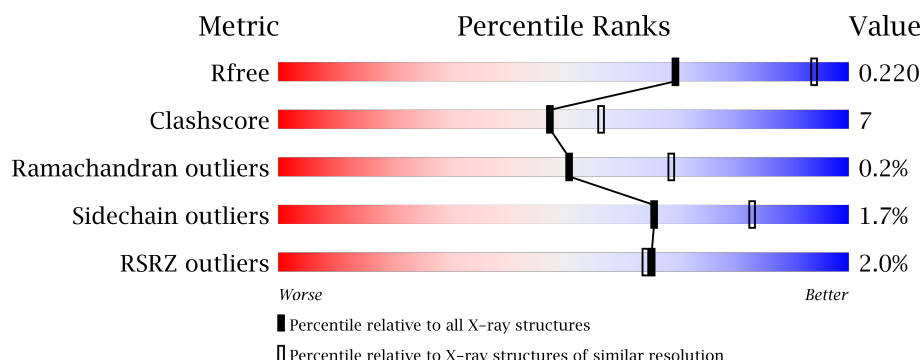
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	450	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	B	450	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	C	450	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	D	450	<div> <div>80%</div> <div>17%</div> <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	DMS	A	1003	-	-	-	X
3	DMS	B	1003	-	-	-	X
3	DMS	C	2004	-	-	-	X

## 2 Entry composition [i](#)

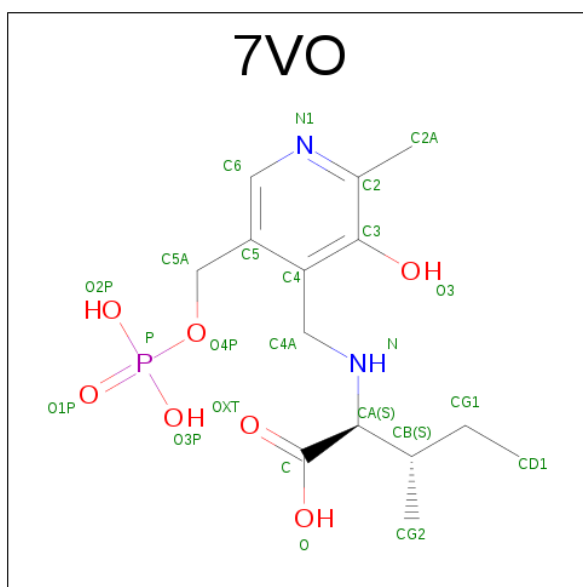
There are 4 unique types of molecules in this entry. The entry contains 14376 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isoleucine 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3397	2165	570	646	16			
1	B	440	Total	C	N	O	S	0	0	0
			3401	2167	571	647	16			
1	C	440	Total	C	N	O	S	0	0	0
			3401	2167	571	647	16			
1	D	439	Total	C	N	O	S	0	0	0
			3397	2165	570	646	16			

- Molecule 2 is (2S,3S)-3-methyl-2-[[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylamino]pentanoic acid (three-letter code: 7VO) (formula: C<sub>14</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>P).



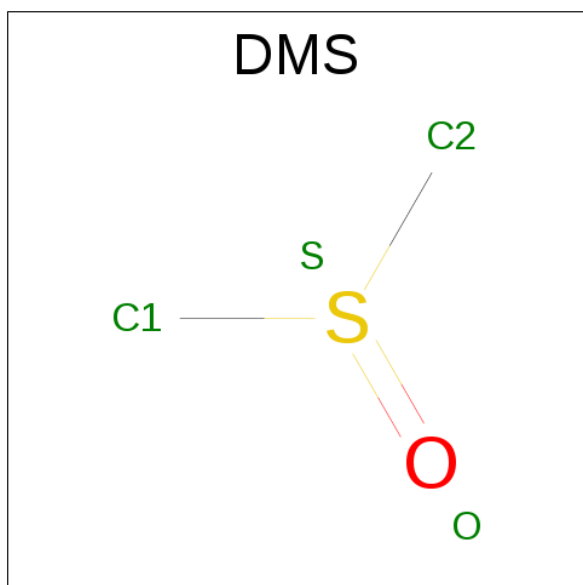
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	14	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			24	14	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			24	14	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			24	14	2	7	1		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

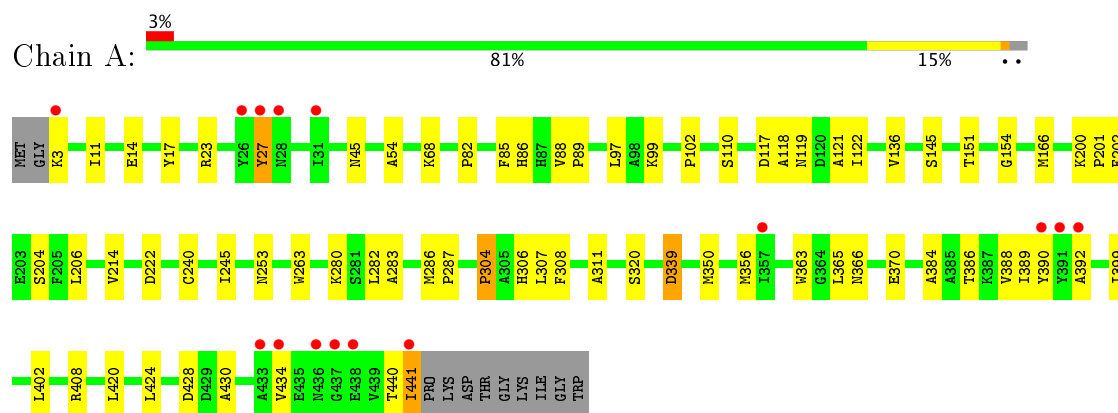
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	158	Total	O	0	0
			158	158		
4	C	183	Total	O	0	0
			183	183		
4	D	167	Total	O	0	0
			167	167		

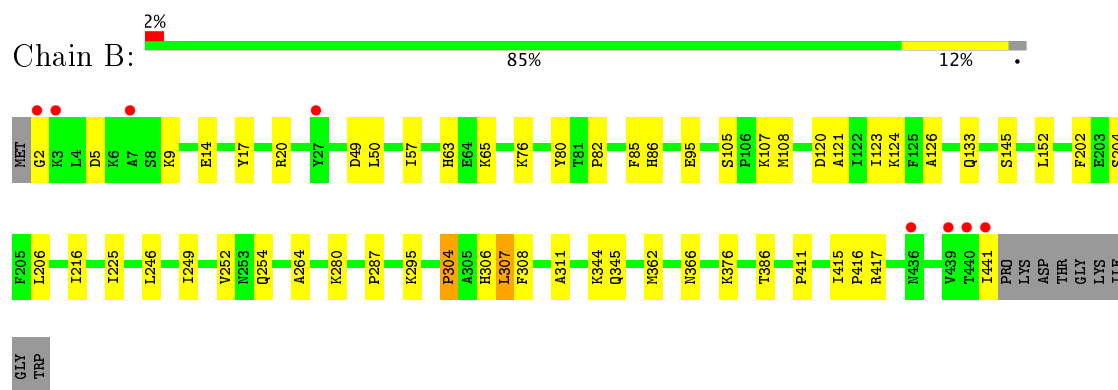
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

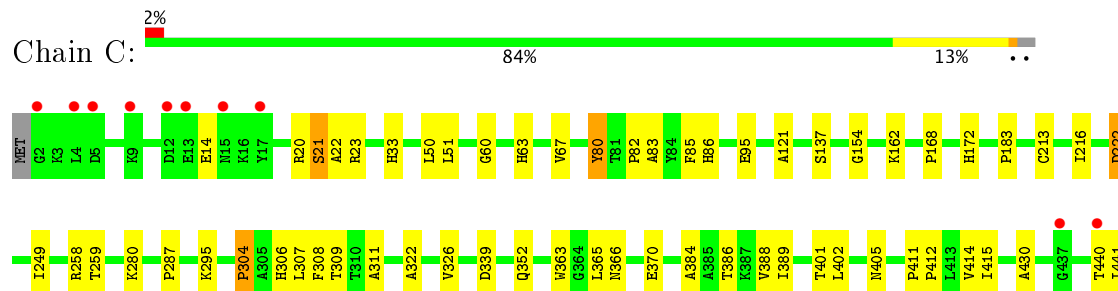
#### • Molecule 1: Isoleucine 2-epimerase



#### • Molecule 1: Isoleucine 2-epimerase



#### • Molecule 1: Isoleucine 2-epimerase



PRO  
LYS  
ASP  
THR  
GLY  
LYS  
ILE  
GLY  
TRP

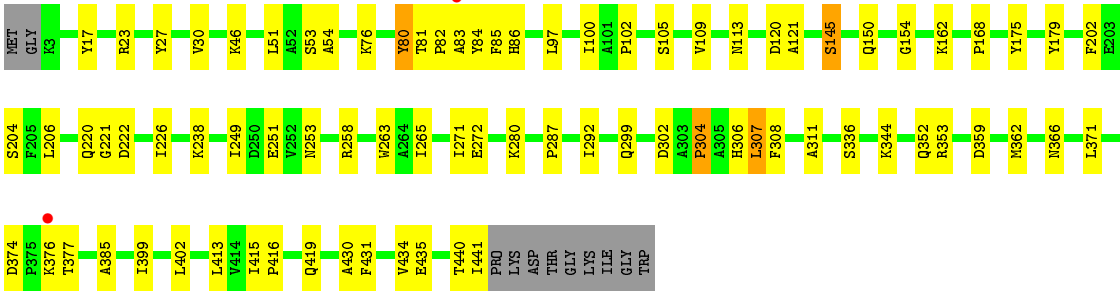
● Molecule 1: Isoleucine 2-epimerase

Chain D: 

80%

17%

••





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.09Å 160.68Å 186.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 48.68 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.65) 99.5 (48.68-2.65)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.175 , 0.222 0.182 , 0.220	Depositor DCC
$R_{free}$ test set	2752 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: DMS, 7VO

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	0.63	0/3475	0.71	0/4712
1	B	0.64	0/3479	0.73	2/4717 (0.0%)
1	C	0.68	0/3479	0.73	0/4717
1	D	0.67	0/3475	0.73	1/4712 (0.0%)
All	All	0.66	0/13908	0.73	3/18858 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	417	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	353	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3397	0	3360	61	0
1	B	3401	0	3363	49	0
1	C	3401	0	3363	51	0
1	D	3397	0	3360	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	24	0	0	1	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	3	0
3	A	16	0	24	0	0
3	B	12	0	18	1	0
3	C	12	0	18	0	0
3	D	4	0	6	1	0
4	A	132	0	0	3	0
4	B	158	0	0	8	0
4	C	183	0	0	10	0
4	D	167	0	0	8	0
All	All	14376	0	13512	191	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 7.

All (191) 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:356:MET:CE	1:A:384:ALA:HB1	1.87	1.03
4:C:2103:HOH:O	1:D:76:LYS:HE3	1.74	0.88
1:B:376:LYS:HD2	4:B:1106:HOH:O	1.78	0.81
3:B:1004:DMS:H23	4:C:2224:HOH:O	1.81	0.79
1:B:57:ILE:HD12	4:B:1183:HOH:O	1.81	0.79
1:B:306:HIS:HB3	4:B:1150:HOH:O	1.81	0.78
1:A:304:PRO:HB3	1:A:307:LEU:HD21	1.68	0.76
1:C:82:PRO:HA	1:C:85:PHE:O	1.86	0.74
1:A:82:PRO:HA	1:A:85:PHE:O	1.88	0.73
1:A:389:ILE:HG22	1:A:399:ILE:HG23	1.69	0.73
1:A:356:MET:HE3	1:A:384:ALA:HB1	1.72	0.72
1:B:386:THR:HG21	1:B:441:ILE:HD12	1.72	0.71
1:A:86:HIS:ND1	1:B:14:GLU:OE1	2.25	0.70
1:D:162:LYS:HE2	4:D:1239:HOH:O	1.92	0.69
1:B:124:LYS:NZ	1:B:306:HIS:HD2	1.89	0.69
1:D:258:ARG:HD2	1:D:366:ASN:HB2	1.72	0.69
1:C:304:PRO:HB3	1:C:307:LEU:HD21	1.76	0.68
1:B:133:GLN:HG2	4:B:1152:HOH:O	1.94	0.68
1:B:82:PRO:HA	1:B:85:PHE:O	1.95	0.67
1:C:308:PHE:HB2	1:C:311:ALA:HB2	1.77	0.67
1:A:356:MET:HE1	1:A:384:ALA:HB1	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:NH1	1:D:299:GLN:O	2.21	0.67
1:D:416:PRO:HA	4:D:1128:HOH:O	1.95	0.66
1:B:121:ALA:HB2	1:B:306:HIS:CE1	2.30	0.66
1:A:283:ALA:HB1	1:A:286:MET:HB2	1.77	0.66
1:B:5:ASP:O	1:B:9:LYS:HD3	1.95	0.66
1:A:14:GLU:OE1	1:B:86:HIS:ND1	2.29	0.66
1:A:154:GLY:O	1:D:204:SER:HB2	1.96	0.65
1:C:384:ALA:O	1:C:388:VAL:HG23	1.97	0.65
1:A:441:ILE:HG12	4:A:1225:HOH:O	1.97	0.64
1:C:20:ARG:NH2	1:D:302:ASP:OD1	2.30	0.64
1:B:20:ARG:HA	4:B:1210:HOH:O	1.97	0.64
1:B:254:GLN:OE1	1:B:366:ASN:ND2	2.30	0.63
1:B:225:ILE:HG22	1:B:225:ILE:O	2.00	0.60
1:D:258:ARG:CD	1:D:366:ASN:HB2	2.31	0.60
1:A:253:ASN:HD22	1:A:280:LYS:NZ	2.00	0.60
1:C:21:SER:HB2	4:D:1211:HOH:O	2.02	0.60
1:D:46:LYS:HE2	3:D:1002:DMS:C1	2.32	0.60
1:A:350:MET:HE2	1:A:428:ASP:HA	1.83	0.59
1:A:27:TYR:CE1	1:B:85:PHE:CE1	2.91	0.59
1:D:238:LYS:NZ	4:D:1102:HOH:O	2.35	0.58
1:D:308:PHE:HB2	1:D:311:ALA:HB2	1.86	0.57
1:A:3:LYS:O	1:A:45:ASN:ND2	2.39	0.56
1:B:386:THR:HG21	1:B:441:ILE:CD1	2.35	0.56
1:D:121:ALA:HB2	1:D:306:HIS:NE2	2.21	0.56
1:D:352:GLN:HG2	4:D:1224:HOH:O	2.05	0.56
1:D:109:VAL:HG22	1:D:292:ILE:HG12	1.87	0.55
1:A:308:PHE:HB2	1:A:311:ALA:HB2	1.88	0.55
1:C:287:PRO:HB2	1:D:287:PRO:HB2	1.88	0.55
1:A:23:ARG:CZ	1:B:86:HIS:CE1	2.90	0.55
1:D:202:PHE:HA	1:D:206:LEU:O	2.07	0.55
1:A:287:PRO:HB2	1:B:287:PRO:HB2	1.89	0.54
1:A:402:LEU:HD21	1:A:408:ARG:HD2	1.90	0.54
1:D:441:ILE:HD12	1:D:441:ILE:N	2.23	0.54
1:C:22:ALA:O	1:D:83:ALA:HA	2.07	0.54
1:A:384:ALA:O	1:A:388:VAL:HG23	2.07	0.54
1:B:304:PRO:HB2	1:B:307:LEU:HD11	1.90	0.53
1:A:23:ARG:NH1	1:B:86:HIS:CE1	2.77	0.52
1:A:283:ALA:CB	1:A:286:MET:HB2	2.40	0.52
1:D:416:PRO:HD2	1:D:419:GLN:OE1	2.09	0.52
1:C:23:ARG:HA	1:D:83:ALA:O	2.10	0.51
1:D:221:GLY:O	1:D:402:LEU:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:THR:O	1:A:390:TYR:HD2	1.94	0.51
1:A:240:CYS:HB3	1:A:245:ILE:O	2.11	0.51
1:D:81:THR:HG23	1:D:84:TYR:H	1.76	0.50
1:A:102:PRO:HD3	1:A:263:TRP:CD1	2.47	0.50
1:A:363:TRP:O	1:A:366:ASN:HB3	2.11	0.50
1:A:200:LYS:N	1:A:201:PRO:HD2	2.28	0.49
1:A:350:MET:CE	1:A:428:ASP:HA	2.42	0.49
1:A:204:SER:HB2	1:D:154:GLY:O	2.13	0.49
1:B:124:LYS:HZ2	1:B:306:HIS:HD2	1.61	0.49
1:C:352:GLN:NE2	4:C:2104:HOH:O	2.36	0.48
1:D:344:LYS:HB2	1:D:362:MET:HG2	1.96	0.48
1:B:308:PHE:HB2	1:B:311:ALA:HB2	1.94	0.48
1:C:95:GLU:HG3	1:D:17:TYR:CE2	2.48	0.48
1:A:68:LYS:HG3	4:A:1128:HOH:O	2.12	0.48
1:D:308:PHE:HB2	1:D:311:ALA:CB	2.43	0.48
1:B:204:SER:HB2	1:C:154:GLY:O	2.14	0.48
1:C:33:HIS:HB2	1:D:76:LYS:O	2.14	0.48
1:C:308:PHE:HB2	1:C:311:ALA:CB	2.43	0.48
1:C:83:ALA:O	1:D:23:ARG:HA	2.14	0.48
1:C:306:HIS:HE1	4:C:2185:HOH:O	1.97	0.47
1:A:356:MET:HE3	1:A:384:ALA:CB	2.43	0.47
1:B:254:GLN:HB3	1:B:264:ALA:HB2	1.94	0.47
1:C:137:SER:O	1:C:172:HIS:HA	2.14	0.47
1:D:82:PRO:HA	1:D:85:PHE:O	2.13	0.47
1:A:54:ALA:HB1	2:A:1001:7VO:O	2.14	0.47
1:A:350:MET:HE3	1:A:428:ASP:N	2.30	0.47
1:D:336:SER:HB2	1:D:413:LEU:HD22	1.97	0.47
1:C:287:PRO:HB3	1:D:113:ASN:ND2	2.30	0.47
1:A:97:LEU:HD21	1:A:282:LEU:HD11	1.97	0.46
1:A:118:ALA:O	1:A:121:ALA:HB3	2.15	0.46
1:A:136:VAL:HB	1:A:214:VAL:HG22	1.96	0.46
1:D:249:ILE:HD12	1:D:251:GLU:HG2	1.97	0.46
1:D:430:ALA:O	1:D:434:VAL:HG23	2.16	0.46
1:B:2:GLY:HA2	4:B:1250:HOH:O	2.16	0.46
1:B:50:LEU:HA	1:B:411:PRO:HB3	1.98	0.46
1:C:258:ARG:CD	1:C:366:ASN:HB2	2.46	0.46
1:D:280:LYS:HE3	2:D:1001:7VO:C4A	2.46	0.45
1:B:306:HIS:HE1	4:B:1218:HOH:O	1.98	0.45
1:C:388:VAL:HG13	1:C:430:ALA:HB1	1.98	0.45
1:C:389:ILE:HD13	1:C:401:THR:HG23	1.98	0.45
1:B:307:LEU:HA	4:B:1201:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:THR:HG21	1:D:280:LYS:HG2	1.97	0.45
1:C:304:PRO:CB	1:C:307:LEU:HD21	2.45	0.45
1:A:27:TYR:CE1	1:B:85:PHE:HE1	2.34	0.45
1:A:430:ALA:O	1:A:434:VAL:HG23	2.17	0.45
1:C:60:GLY:HA2	1:C:412:PRO:HB3	1.99	0.45
1:C:50:LEU:HD23	1:C:411:PRO:HB3	1.98	0.44
1:C:63:HIS:O	1:C:67:VAL:HG23	2.17	0.44
1:A:17:TYR:CE2	1:B:95:GLU:HG3	2.52	0.44
1:C:183:PRO:HA	4:C:2273:HOH:O	2.17	0.44
1:C:386:THR:O	1:C:389:ILE:HG12	2.18	0.44
1:A:99:LYS:HE3	1:B:17:TYR:CE1	2.53	0.44
1:D:175:TYR:CE2	1:D:220:GLN:HG3	2.53	0.44
1:D:80:TYR:CE1	1:D:85:PHE:HD2	2.35	0.44
1:A:308:PHE:CE1	1:B:145:SER:HB3	2.52	0.44
1:C:168:PRO:HG3	1:D:168:PRO:HG3	1.99	0.44
1:D:304:PRO:HB3	1:D:307:LEU:HD21	2.00	0.44
1:D:179:TYR:CD1	1:D:359:ASP:HB2	2.53	0.44
1:B:252:VAL:HG12	1:B:280:LYS:HD2	2.00	0.44
1:A:350:MET:CE	1:A:428:ASP:CA	2.96	0.44
1:B:304:PRO:HB3	1:B:307:LEU:HD21	2.00	0.44
1:A:356:MET:CE	1:A:384:ALA:CB	2.78	0.44
1:C:259:THR:HA	1:C:363:TRP:O	2.18	0.44
1:B:123:ILE:HD11	1:B:152:LEU:HD11	1.99	0.43
1:D:415:ILE:HA	1:D:416:PRO:HD3	1.83	0.43
1:D:280:LYS:NZ	2:D:1001:7VO:C4A	2.81	0.43
1:D:431:PHE:O	1:D:435:GLU:HG3	2.19	0.43
1:D:105:SER:HG	1:D:272:GLU:CD	2.21	0.43
1:C:440:THR:HG23	4:C:2180:HOH:O	2.18	0.43
1:A:27:TYR:CE1	1:B:85:PHE:CZ	3.06	0.43
1:C:162:LYS:HE2	4:C:2262:HOH:O	2.19	0.43
1:D:280:LYS:CE	2:D:1001:7VO:C4A	2.95	0.43
1:C:280:LYS:O	4:C:2101:HOH:O	2.21	0.43
1:B:76:LYS:HB3	1:B:76:LYS:HE2	1.82	0.43
1:A:420:LEU:O	1:A:424:LEU:HG	2.19	0.42
1:A:88:VAL:HB	1:A:89:PRO:HD3	2.02	0.42
1:D:374:ASP:HB3	1:D:377:THR:OG1	2.19	0.42
1:D:371:LEU:HD12	1:D:385:ALA:HA	2.01	0.42
1:C:295:LYS:NZ	4:C:2112:HOH:O	2.52	0.42
1:C:388:VAL:HG13	1:C:430:ALA:CB	2.50	0.42
1:C:23:ARG:CZ	1:D:86:HIS:CE1	3.03	0.42
1:D:416:PRO:CA	4:D:1128:HOH:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:CZ	1:B:86:HIS:ND1	2.83	0.42
1:D:53:SER:O	1:D:54:ALA:HB3	2.20	0.42
1:A:119:ASN:HD22	1:A:122:ILE:HD12	1.85	0.42
1:A:402:LEU:HG	1:A:408:ARG:HB2	2.02	0.42
1:B:108:MET:HG3	1:B:295:LYS:HG2	2.01	0.42
1:B:216:ILE:O	1:B:249:ILE:HA	2.19	0.42
1:B:63:HIS:HE1	1:B:65:LYS:HG3	1.85	0.42
1:D:145:SER:HA	1:D:150:GLN:OE1	2.19	0.42
1:D:253:ASN:HD22	1:D:280:LYS:NZ	2.17	0.42
1:A:151:THR:OG1	1:A:166:MET:HB3	2.20	0.42
1:C:86:HIS:HB2	1:D:30:VAL:HG22	2.02	0.42
1:A:121:ALA:HB2	1:A:306:HIS:CE1	2.55	0.42
1:A:202:PHE:HA	1:A:206:LEU:O	2.20	0.42
1:B:415:ILE:HA	1:B:416:PRO:HD2	1.84	0.41
1:A:11:ILE:HG12	1:B:86:HIS:CD2	2.55	0.41
1:A:17:TYR:CD2	1:B:95:GLU:HG3	2.55	0.41
1:D:97:LEU:HD23	1:D:100:ILE:HD11	2.01	0.41
1:A:117:ASP:HB2	1:A:308:PHE:CZ	2.55	0.41
1:A:304:PRO:CB	1:A:307:LEU:HD21	2.45	0.41
1:B:126:ALA:HA	1:B:246:LEU:HD12	2.03	0.41
1:C:370:GLU:HG3	1:C:405:ASN:ND2	2.35	0.41
1:C:51:LEU:HD23	1:D:85:PHE:HE2	1.86	0.41
1:C:85:PHE:HE2	1:D:51:LEU:HD23	1.85	0.41
1:C:23:ARG:HG3	1:D:83:ALA:O	2.21	0.41
1:A:339:ASP:HB3	1:A:365:LEU:HD21	2.01	0.41
1:C:322:ALA:O	1:C:326:VAL:HG23	2.21	0.41
1:A:306:HIS:HE1	4:A:1213:HOH:O	2.03	0.41
1:B:415:ILE:HG23	1:B:415:ILE:O	2.20	0.41
1:C:216:ILE:O	1:C:249:ILE:HA	2.20	0.41
1:D:27:TYR:OH	1:D:399:ILE:O	2.35	0.41
1:C:121:ALA:HB2	1:C:306:HIS:CE1	2.55	0.41
1:A:389:ILE:O	1:A:392:ALA:HB3	2.21	0.41
1:C:80:TYR:CE1	1:C:85:PHE:HD2	2.39	0.41
1:D:253:ASN:HD22	1:D:280:LYS:HZ3	1.68	0.41
1:B:344:LYS:HB2	1:B:362:MET:HG2	2.02	0.41
1:C:22:ALA:HB1	4:C:2136:HOH:O	2.21	0.41
1:C:339:ASP:HB3	1:C:365:LEU:HD21	2.03	0.41
1:A:282:LEU:O	1:A:320:SER:HA	2.21	0.40
1:A:402:LEU:HD11	1:A:408:ARG:HG3	2.04	0.40
1:B:202:PHE:HA	1:B:206:LEU:O	2.20	0.40
1:C:222:ASP:HA	1:C:402:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:SER:O	1:B:107:LYS:HG3	2.22	0.40
1:C:14:GLU:HA	4:D:1152:HOH:O	2.20	0.40
1:D:102:PRO:HD3	1:D:263:TRP:CD1	2.56	0.40
1:D:226:ILE:HD12	4:D:1206:HOH:O	2.20	0.40
1:C:414:VAL:O	1:C:415:ILE:C	2.58	0.40
1:D:265:ILE:HD11	1:D:271:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/450 (97%)	416 (95%)	20 (5%)	1 (0%)	51	69
1	B	438/450 (97%)	421 (96%)	16 (4%)	1 (0%)	51	69
1	C	438/450 (97%)	421 (96%)	16 (4%)	1 (0%)	51	69
1	D	437/450 (97%)	421 (96%)	15 (3%)	1 (0%)	51	69
All	All	1750/1800 (97%)	1679 (96%)	67 (4%)	4 (0%)	51	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	PRO
1	B	304	PRO
1	C	304	PRO
1	D	304	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	363/371 (98%)	355 (98%)	8 (2%)	57	77
1	B	363/371 (98%)	359 (99%)	4 (1%)	78	90
1	C	363/371 (98%)	358 (99%)	5 (1%)	71	86
1	D	363/371 (98%)	356 (98%)	7 (2%)	62	80
All	All	1452/1484 (98%)	1428 (98%)	24 (2%)	66	83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	110	SER
1	A	145	SER
1	A	222	ASP
1	A	339	ASP
1	A	370	GLU
1	A	440	THR
1	A	441	ILE
1	B	80	TYR
1	B	120	ASP
1	B	307	LEU
1	B	345	GLN
1	C	21	SER
1	C	80	TYR
1	C	213	CYS
1	C	222	ASP
1	C	441	ILE
1	D	80	TYR
1	D	120	ASP
1	D	145	SER
1	D	222	ASP
1	D	307	LEU
1	D	376	LYS
1	D	440	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	196	ASN
1	A	267	GLN
1	A	306	HIS
1	B	45	ASN
1	B	119	ASN
1	B	133	GLN
1	B	243	HIS
1	B	306	HIS
1	C	15	ASN
1	C	119	ASN
1	C	133	GLN
1	C	243	HIS
1	D	79	HIS
1	D	86	HIS
1	D	113	ASN
1	D	119	ASN
1	D	133	GLN
1	D	243	HIS
1	D	299	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 ⓘ

15 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	7VO	A	1001	-	21,24,24	3.24	6 (28%)	26,34,34	2.27	12 (46%)
3	DMS	A	1002	-	3,3,3	0.49	0	3,3,3	0.99	0
3	DMS	A	1003	-	3,3,3	0.45	0	3,3,3	0.74	0
3	DMS	A	1004	-	3,3,3	0.49	0	3,3,3	0.67	0
3	DMS	A	1005	-	3,3,3	0.24	0	3,3,3	0.53	0
2	7VO	B	1001	-	21,24,24	2.58	7 (33%)	26,34,34	1.99	9 (34%)
3	DMS	B	1002	-	3,3,3	0.44	0	3,3,3	1.10	0
3	DMS	B	1003	-	3,3,3	0.31	0	3,3,3	0.78	0
3	DMS	B	1004	-	3,3,3	0.53	0	3,3,3	1.05	0
3	DMS	C	2001	-	3,3,3	0.64	0	3,3,3	1.24	0
2	7VO	C	2002	-	21,24,24	2.96	6 (28%)	26,34,34	1.75	6 (23%)
3	DMS	C	2003	-	3,3,3	0.42	0	3,3,3	1.04	0
3	DMS	C	2004	-	3,3,3	0.34	0	3,3,3	0.63	0
2	7VO	D	1001	-	21,24,24	2.56	6 (28%)	26,34,34	1.74	7 (26%)
3	DMS	D	1002	-	3,3,3	0.36	0	3,3,3	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7VO	A	1001	-	-	0/17/21/21	0/1/1/1
3	DMS	A	1002	-	-	0/0/0/0	0/0/0/0
3	DMS	A	1003	-	-	0/0/0/0	0/0/0/0
3	DMS	A	1004	-	-	0/0/0/0	0/0/0/0
3	DMS	A	1005	-	-	0/0/0/0	0/0/0/0
2	7VO	B	1001	-	-	0/17/21/21	0/1/1/1
3	DMS	B	1002	-	-	0/0/0/0	0/0/0/0
3	DMS	B	1003	-	-	0/0/0/0	0/0/0/0
3	DMS	B	1004	-	-	0/0/0/0	0/0/0/0
3	DMS	C	2001	-	-	0/0/0/0	0/0/0/0
2	7VO	C	2002	-	-	0/17/21/21	0/1/1/1
3	DMS	C	2003	-	-	0/0/0/0	0/0/0/0
3	DMS	C	2004	-	-	0/0/0/0	0/0/0/0
2	7VO	D	1001	-	-	0/17/21/21	0/1/1/1
3	DMS	D	1002	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	7VO	C4A-C4	-10.74	1.39	1.51
2	C	2002	7VO	C4A-C4	-8.79	1.41	1.51
2	D	1001	7VO	C4A-C4	-8.13	1.42	1.51
2	B	1001	7VO	C4A-C4	-7.43	1.43	1.51
2	A	1001	7VO	C2A-C2	-6.89	1.37	1.50
2	C	2002	7VO	C2A-C2	-6.20	1.39	1.50
2	B	1001	7VO	C2A-C2	-5.84	1.39	1.50
2	D	1001	7VO	C2A-C2	-5.35	1.40	1.50
2	C	2002	7VO	C5A-C5	-4.17	1.39	1.50
2	A	1001	7VO	C5A-C5	-3.91	1.40	1.50
2	C	2002	7VO	C3-C2	-3.91	1.38	1.40
2	D	1001	7VO	C5A-C5	-3.12	1.42	1.50
2	B	1001	7VO	C5A-C5	-3.01	1.42	1.50
2	A	1001	7VO	C3-C2	-2.40	1.39	1.40
2	C	2002	7VO	P-O2P	-2.29	1.45	1.54
2	A	1001	7VO	P-O3P	-2.25	1.45	1.54
2	D	1001	7VO	P-O2P	-2.17	1.45	1.54
2	B	1001	7VO	P-O3P	-2.04	1.46	1.54
2	B	1001	7VO	CG2-CB	2.12	1.58	1.53
2	B	1001	7VO	C5-C4	2.47	1.43	1.40
2	D	1001	7VO	C3-C2	2.56	1.42	1.40
2	B	1001	7VO	C2-N1	3.03	1.40	1.33
2	D	1001	7VO	C2-N1	3.10	1.40	1.33
2	C	2002	7VO	C2-N1	3.31	1.40	1.33
2	A	1001	7VO	C2-N1	3.43	1.41	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	7VO	O3P-P-O4P	-4.39	95.04	106.73
2	B	1001	7VO	O3P-P-O4P	-4.37	95.10	106.73
2	C	2002	7VO	O3P-P-O4P	-3.73	96.82	106.73
2	B	1001	7VO	O2P-P-O4P	-3.60	97.14	106.73
2	A	1001	7VO	C4A-N-CA	-3.05	109.56	113.78
2	B	1001	7VO	O4P-P-O1P	-2.84	98.50	106.47
2	C	2002	7VO	C4A-N-CA	-2.84	109.85	113.78
2	C	2002	7VO	O2P-P-O4P	-2.71	99.52	106.73
2	A	1001	7VO	C4A-C4-C3	-2.65	116.73	119.65
2	D	1001	7VO	O4P-P-O1P	-2.61	99.15	106.47
2	B	1001	7VO	C3-C4-C5	-2.55	116.20	118.71
2	B	1001	7VO	C5A-C5-C6	-2.41	115.18	119.33
2	A	1001	7VO	C5-C6-N1	-2.26	120.04	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	7VO	O2P-P-O4P	-2.15	101.02	106.73
2	A	1001	7VO	O2P-P-O4P	-2.13	101.06	106.73
2	A	1001	7VO	O4P-P-O1P	-2.10	100.58	106.47
2	B	1001	7VO	C3-C2-N1	-2.04	118.08	120.75
2	C	2002	7VO	C3-C2-N1	-2.01	118.11	120.75
2	D	1001	7VO	C6-C5-C4	2.11	119.70	118.13
2	A	1001	7VO	O2P-P-O1P	2.16	118.96	110.50
2	A	1001	7VO	C6-C5-C4	2.20	119.77	118.13
2	C	2002	7VO	O3P-P-O2P	2.44	117.47	107.61
2	A	1001	7VO	O3P-P-O2P	2.49	117.65	107.61
2	D	1001	7VO	O3P-P-O1P	2.64	120.81	110.50
2	B	1001	7VO	O2P-P-O1P	2.68	120.97	110.50
2	B	1001	7VO	O3P-P-O2P	2.69	118.46	107.61
2	D	1001	7VO	C4-C4A-N	2.83	119.57	111.78
2	D	1001	7VO	O4P-C5A-C5	3.06	115.46	109.32
2	B	1001	7VO	C4A-C4-C5	3.14	122.63	119.75
2	A	1001	7VO	C4-C4A-N	3.49	121.38	111.78
2	C	2002	7VO	C4-C4A-N	3.62	121.76	111.78
2	D	1001	7VO	C4A-C4-C5	3.77	123.20	119.75
2	A	1001	7VO	O4P-C5A-C5	4.28	117.92	109.32
2	A	1001	7VO	C4A-C4-C5	4.47	123.85	119.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	7VO	1	0
3	B	1004	DMS	1	0
2	D	1001	7VO	3	0
3	D	1002	DMS	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	439/450 (97%)	-0.14	15 (3%) 46 44	22, 39, 68, 100	0
1	B	440/450 (97%)	-0.41	8 (1%) 69 68	20, 34, 58, 88	0
1	C	440/450 (97%)	-0.45	10 (2%) 61 59	17, 33, 61, 105	0
1	D	439/450 (97%)	-0.46	2 (0%) 90 91	20, 36, 56, 81	0
All	All	1758/1800 (97%)	-0.36	35 (1%) 65 64	17, 35, 63, 105	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	GLY	5.4
1	C	9	LYS	4.2
1	B	441	ILE	4.0
1	A	441	ILE	3.9
1	C	4	LEU	3.4
1	C	12	ASP	3.4
1	C	13	GLU	3.4
1	C	440	THR	3.3
1	C	5	ASP	3.2
1	C	17	TYR	3.1
1	A	391	TYR	3.0
1	A	438	GLU	2.8
1	C	15	ASN	2.8
1	A	3	LYS	2.8
1	A	26	TYR	2.7
1	A	437	GLY	2.7
1	A	390	TYR	2.6
1	B	436	ASN	2.6
1	D	83	ALA	2.6
1	B	440	THR	2.5
1	B	3	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	436	ASN	2.4
1	B	2	GLY	2.4
1	B	439	VAL	2.4
1	C	437	GLY	2.3
1	A	357	ILE	2.3
1	A	27	TYR	2.3
1	B	27	TYR	2.2
1	B	7	ALA	2.2
1	A	31	ILE	2.1
1	A	392	ALA	2.1
1	A	433	ALA	2.1
1	A	434	VAL	2.1
1	D	376	LYS	2.1
1	A	28	ASN	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DMS	B	1003	4/4	0.95	0.34	16.48	41,45,47,48	0
3	DMS	C	2004	4/4	0.96	0.19	4.75	44,45,49,49	0
3	DMS	A	1003	4/4	0.95	0.19	2.21	56,61,65,68	0
3	DMS	A	1002	4/4	0.95	0.16	1.97	48,49,50,52	0
3	DMS	A	1005	4/4	0.97	0.27	1.85	36,37,37,38	0
3	DMS	B	1004	4/4	0.93	0.21	1.81	56,58,64,74	0
3	DMS	A	1004	4/4	0.98	0.16	0.78	56,66,69,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	7VO	D	1001	24/24	0.96	0.15	0.32	30,36,47,49	0
2	7VO	A	1001	24/24	0.97	0.16	0.18	35,45,62,63	0
3	DMS	C	2003	4/4	0.97	0.15	0.13	50,56,56,59	0
2	7VO	B	1001	24/24	0.97	0.15	-0.02	30,37,58,65	0
3	DMS	B	1002	4/4	0.99	0.12	-0.40	36,40,42,48	0
2	7VO	C	2002	24/24	0.98	0.10	-0.83	29,33,49,56	0
3	DMS	C	2001	4/4	0.97	0.11	-1.82	46,47,47,49	0
3	DMS	D	1002	4/4	0.96	0.44	-	46,48,50,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.