



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:01 AM GMT

PDB ID : 2Z73  
Title : Crystal structure of squid rhodopsin  
Authors : Murakami, M.; Kouyama, T.  
Deposited on : 2007-08-13  
Resolution : 2.50 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.

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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 (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

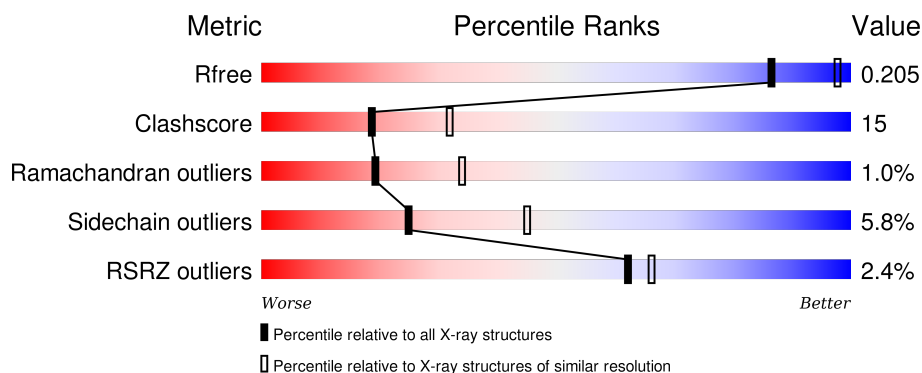
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	448	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>27%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	448	<div> <div>52%</div> <div>22%</div> <div>•</div> <div>23%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	A	1005	-	-	-	X
2	BOG	B	1005	-	-	-	X
4	RET	B	1000	-	-	-	X
5	PLM	A	1001	-	-	-	X
5	PLM	A	1002	-	-	-	X
5	PLM	B	1001	-	-	-	X
5	PLM	B	1002	-	-	-	X
6	TWT	A	1003	-	-	-	X
6	TWT	B	1003	-	-	-	X

## 2 Entry composition [i](#)

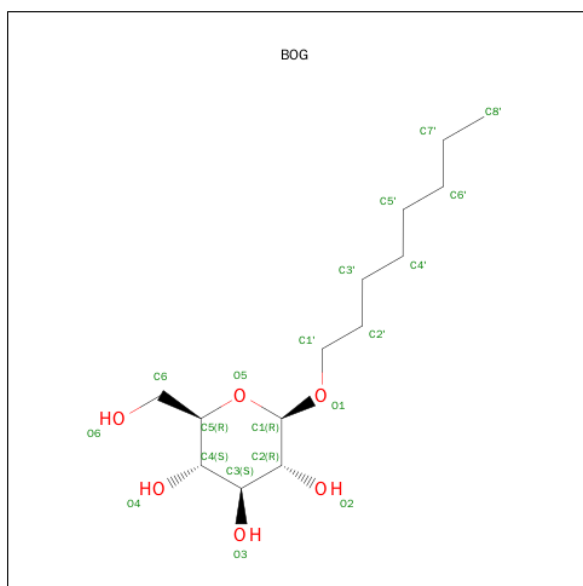
There are 8 unique types of molecules in this entry. The entry contains 5835 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2780	1838	443	473	26			
1	B	347	Total	C	N	O	S	0	0	0
			2762	1828	440	468	26			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



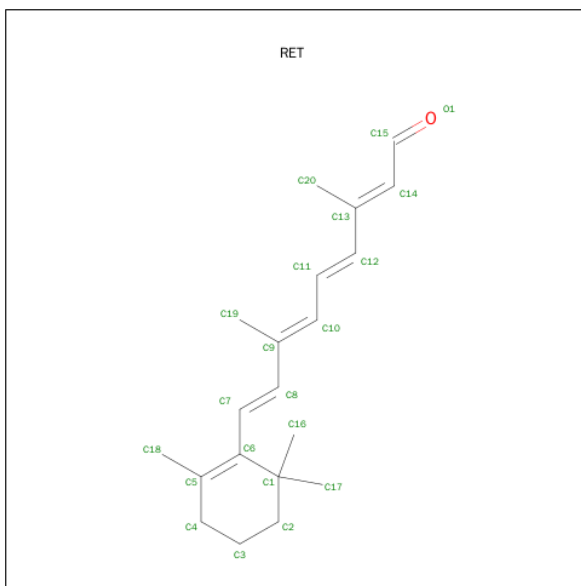
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



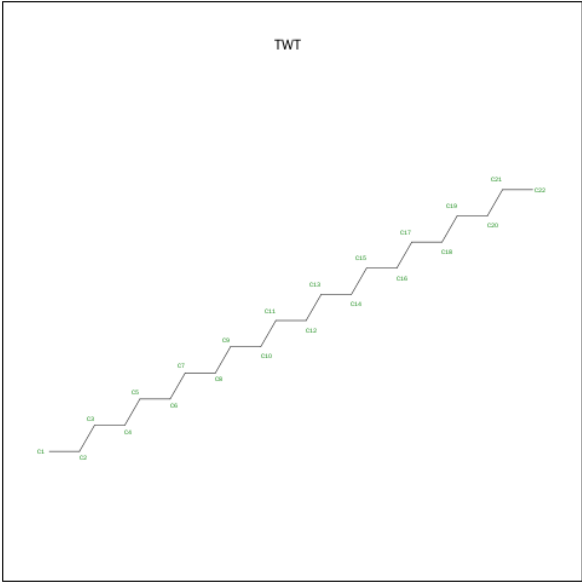
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			20	20		
4	B	1	Total	C	0	0
			20	20		

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



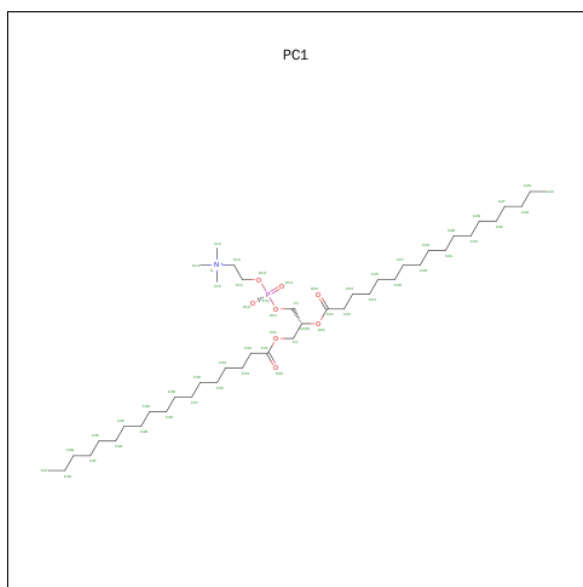
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	16	1		
5	A	1	Total	C	O	0	0
			17	16	1		
5	B	1	Total	C	O	0	0
			17	16	1		
5	B	1	Total	C	O	0	0
			17	16	1		

- Molecule 6 is DOCOSANE (three-letter code: TWT) (formula: C<sub>22</sub>H<sub>46</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 22 22	0	0
6	B	1	Total C 22 22	0	0

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O P 39 30 8 1	0	0

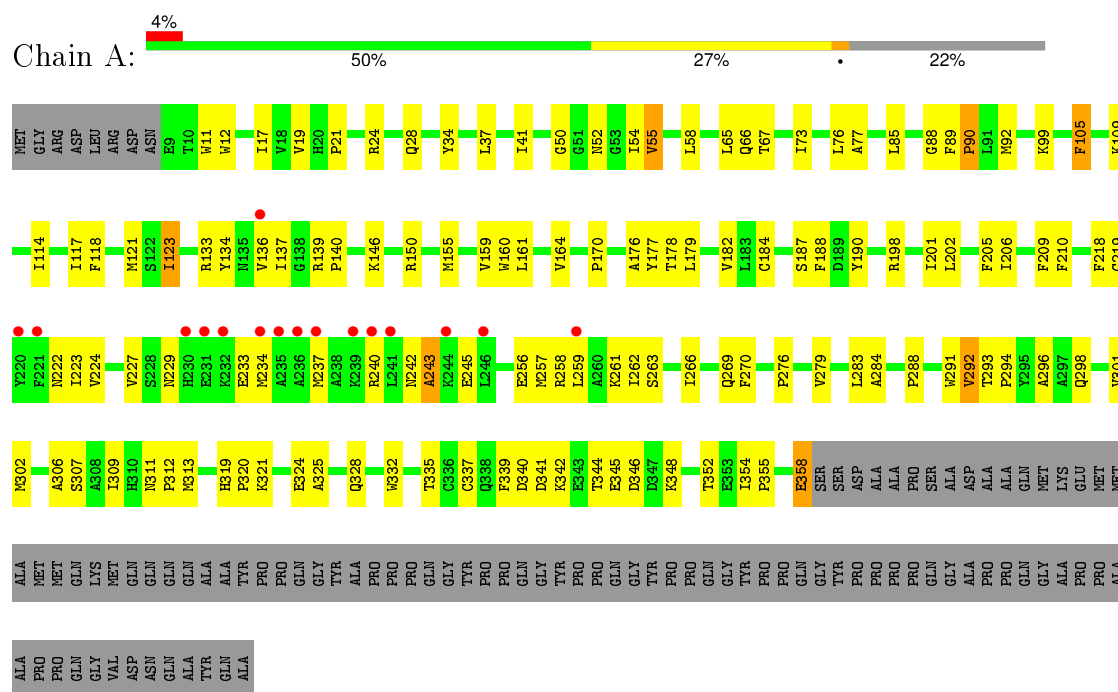
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	28	Total O 28 28	0	0
8	B	29	Total O 29 29	0	0

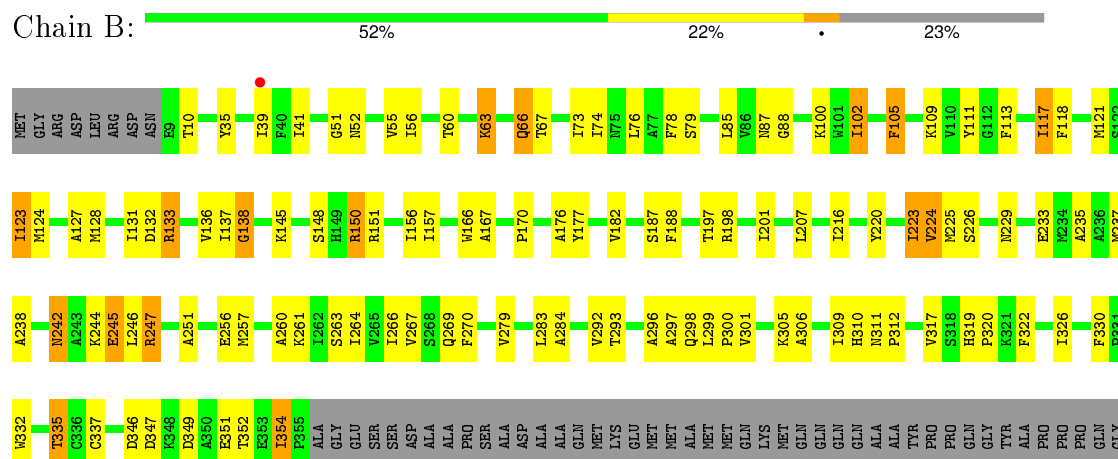
### 3 Residue-property plots

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: Rhodopsin



#### • Molecule 1: Rhodopsin





TYR	PRO	PRO	GLN	GLY	TYR	PRO	PRO	PRO	GLN	GLY	TYR	PRO	PRO	PRO	GLN	GLY	ALA	ALA	ALA	ALA	ALA	GLN	GLY	VAL	ASP	ASN	GLN	ALA	ALA	TYR	GLN	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.55Å 122.55Å 158.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 57.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (15.00-2.50) 93.3 (57.16-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.188 , 0.206 0.186 , 0.205	Depositor DCC
$R_{free}$ test set	2162 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 73.7	EDS
Estimated twinning fraction	0.107 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 43511 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: PC1, RET, SO4, TWT, PLM, BOG

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	0.38	0/2865	0.57	0/3889
1	B	0.38	0/2847	0.57	0/3865
All	All	0.38	0/5712	0.57	0/7754

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2780	0	2765	90	0
1	B	2762	0	2751	86	0
2	A	20	0	28	4	0
2	B	20	0	28	2	0
3	B	5	0	0	0	0
4	A	20	0	27	2	0
4	B	20	0	27	2	0
5	A	34	0	62	1	0
5	B	34	0	62	1	0
6	A	22	0	46	0	0
6	B	22	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	39	0	49	1	0
8	A	28	0	0	4	0
8	B	29	0	0	1	0
All	All	5835	0	5891	180	0

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

All (180) 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:150:ARG:H	1:B:150:ARG:HD2	1.28	0.96
1:B:354:ILE:H	1:B:354:ILE:HD13	1.30	0.94
1:A:21:PRO:HA	1:A:24:ARG:HD3	1.52	0.92
1:A:284:ALA:HB2	1:A:292:VAL:HG21	1.54	0.89
1:B:148:SER:HB2	1:B:150:ARG:HH21	1.43	0.83
1:B:113:PHE:O	1:B:117:ILE:HG23	1.83	0.77
1:B:67:THR:HG21	2:B:1005:BOG:H5	1.67	0.76
1:B:102:ILE:HD13	1:B:102:ILE:H	1.53	0.73
1:A:298:GLN:O	1:A:301:VAL:HG12	1.87	0.72
1:A:137:ILE:HD11	1:A:256:GLU:HB2	1.72	0.71
1:A:117:ILE:HD11	1:A:164:VAL:HG22	1.73	0.70
1:A:218:PHE:O	1:A:222:ASN:HB2	1.90	0.70
1:A:21:PRO:CA	1:A:24:ARG:HD3	2.24	0.67
1:B:298:GLN:O	1:B:301:VAL:HG12	1.93	0.66
1:A:306:ALA:O	1:A:309:ILE:HG12	1.96	0.65
1:B:136:VAL:HG23	1:B:137:ILE:HG12	1.77	0.65
1:A:320:PRO:HG2	8:A:521:HOH:O	1.98	0.64
1:A:67:THR:HB	8:A:520:HOH:O	1.97	0.64
1:B:41:ILE:HG13	1:B:88:GLY:HA2	1.79	0.63
1:A:133:ARG:NH2	1:A:136:VAL:HG11	2.13	0.62
1:B:354:ILE:H	1:B:354:ILE:CD1	2.08	0.62
1:A:340:ASP:OD2	1:A:342:LYS:HB2	2.00	0.62
1:B:319:HIS:HB3	1:B:322:PHE:HB3	1.80	0.62
1:A:65:LEU:HD21	1:A:321:LYS:HB3	1.83	0.61
1:B:306:ALA:O	1:B:309:ILE:HG12	2.00	0.60
1:A:259:LEU:HD13	1:A:262:ILE:HD12	1.84	0.59
1:B:138:GLY:HA2	1:B:223:ILE:HA	1.84	0.59
1:B:87:ASN:HA	1:B:111:TYR:CE1	2.38	0.59
1:B:237:MET:O	1:B:242:ASN:HB2	2.04	0.58
1:A:355:PRO:HG2	1:A:358:GLU:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:THR:O	1:B:201:ILE:HG13	2.02	0.58
1:B:123:ILE:HG12	1:B:270:PHE:CZ	2.40	0.57
1:A:37:LEU:HD22	1:A:302:MET:HE2	1.87	0.57
1:B:52:ASN:HA	1:B:55:VAL:CG1	2.35	0.57
1:B:311:ASN:HB2	1:B:312:PRO:HD3	1.85	0.57
1:A:155:MET:O	1:A:159:VAL:HG23	2.05	0.56
1:A:19:VAL:O	1:A:24:ARG:HD2	2.06	0.56
1:A:73:ILE:HD11	2:A:1005:BOG:H7'2	1.87	0.56
1:B:242:ASN:HD22	1:B:245:GLU:HG3	1.70	0.56
1:A:12:TRP:CD2	1:A:24:ARG:HG2	2.42	0.55
1:B:73:ILE:HD11	2:B:1005:BOG:H7'2	1.89	0.55
1:B:257:MET:HG3	1:B:261:LYS:NZ	2.22	0.54
1:B:117:ILE:HG22	1:B:167:ALA:HB3	1.87	0.54
1:A:240:ARG:NE	1:A:240:ARG:HA	2.23	0.54
1:B:117:ILE:HD11	1:B:118:PHE:CZ	2.43	0.54
1:A:67:THR:HG21	2:A:1005:BOG:H5	1.89	0.54
1:B:238:ALA:HA	1:B:246:LEU:HD13	1.90	0.53
1:B:137:ILE:HD11	1:B:256:GLU:HB3	1.91	0.53
1:B:117:ILE:HD11	1:B:118:PHE:CE1	2.44	0.53
1:B:299:LEU:HB2	1:B:300:PRO:HD3	1.91	0.52
1:A:311:ASN:HB2	1:A:312:PRO:HD3	1.92	0.52
1:A:348:LYS:O	1:A:352:THR:HG23	2.10	0.52
1:B:322:PHE:CE2	1:B:326:ILE:HD11	2.45	0.52
1:B:198:ARG:HG2	7:B:1004:PC1:H341	1.91	0.52
1:B:56:ILE:HD11	1:B:78:PHE:HA	1.90	0.52
1:A:243:ALA:HB3	1:A:245:GLU:HG2	1.91	0.51
1:A:41:ILE:HG13	1:A:88:GLY:HA2	1.91	0.51
1:B:347:ASP:O	1:B:351:GLU:HG2	2.11	0.51
1:B:284:ALA:HB2	1:B:292:VAL:HG21	1.93	0.51
1:A:182:VAL:HG22	1:A:298:GLN:OE1	2.11	0.51
1:A:345:GLU:HA	1:A:348:LYS:HD2	1.92	0.51
1:B:197:THR:HG22	1:B:201:ILE:HD11	1.93	0.51
1:A:134:TYR:O	1:A:139:ARG:HG3	2.11	0.51
1:A:332:TRP:O	1:A:335:THR:HG23	2.11	0.51
1:A:257:MET:HE3	1:A:261:LYS:HG3	1.93	0.51
1:A:139:ARG:HB3	1:A:140:PRO:HD2	1.92	0.50
1:A:17:ILE:HG12	1:A:105:PHE:CD2	2.45	0.50
1:A:160:TRP:O	1:A:164:VAL:HG23	2.11	0.50
1:A:11:TRP:CD2	1:A:28:GLN:HB2	2.46	0.50
1:B:301:VAL:O	1:B:305:LYS:HG3	2.11	0.50
1:B:117:ILE:HG22	1:B:167:ALA:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HA	1:A:117:ILE:HG22	1.93	0.50
1:A:133:ARG:HA	1:A:133:ARG:NE	2.26	0.50
1:B:124:MET:O	1:B:128:MET:HG2	2.12	0.50
1:B:136:VAL:HG11	8:B:528:HOH:O	2.11	0.49
1:B:79:SER:HB2	1:B:121:MET:CE	2.43	0.49
1:B:166:TRP:CZ2	1:B:207:LEU:HG	2.47	0.49
1:A:325:ALA:HA	1:A:328:GLN:HE21	1.77	0.49
1:A:342:LYS:HA	1:A:345:GLU:HG3	1.94	0.49
1:B:60:THR:HG22	1:B:74:ILE:HD13	1.95	0.49
1:A:233:GLU:HG2	1:A:237:MET:HE3	1.94	0.48
1:A:52:ASN:O	1:A:55:VAL:HG13	2.13	0.48
1:B:260:ALA:O	1:B:264:ILE:HG13	2.14	0.48
1:A:258:ARG:O	1:A:262:ILE:HG13	2.14	0.48
1:B:63:LYS:HA	1:B:66:GLN:NE2	2.29	0.48
1:B:317:VAL:HG22	5:B:1002:PLM:O2	2.14	0.47
1:B:150:ARG:CD	1:B:150:ARG:H	2.08	0.47
1:B:52:ASN:HA	1:B:55:VAL:HG12	1.96	0.47
1:B:235:ALA:C	1:B:237:MET:H	2.18	0.47
1:B:79:SER:HB2	1:B:121:MET:HE3	1.96	0.47
1:A:224:VAL:O	1:A:227:VAL:HG23	2.15	0.47
1:B:117:ILE:HG13	1:B:118:PHE:N	2.30	0.47
1:B:35:TYR:O	1:B:39:ILE:HG12	2.15	0.47
1:A:293:THR:HB	1:A:294:PRO:HD2	1.96	0.47
4:B:1000:RET:H10	4:B:1000:RET:H202	1.96	0.47
1:A:324:GLU:HG3	1:A:339:PHE:CZ	2.50	0.47
1:A:114:ILE:O	1:A:117:ILE:HG22	2.14	0.46
1:A:121:MET:HG3	1:A:159:VAL:HG12	1.96	0.46
1:A:206:ILE:HA	1:A:210:PHE:CD2	2.50	0.46
1:A:34:TYR:CD1	1:A:99:LYS:HG2	2.50	0.46
1:A:123:ILE:HG12	1:A:270:PHE:CZ	2.50	0.46
1:A:176:ALA:O	1:A:188:PHE:HA	2.15	0.46
1:B:269:GLN:NE2	1:B:310:HIS:HD2	2.12	0.46
1:A:344:THR:O	1:A:348:LYS:HG3	2.15	0.46
1:B:145:LYS:HD3	1:B:151:ARG:NH2	2.30	0.46
1:B:269:GLN:HE21	1:B:310:HIS:HD2	1.62	0.46
1:A:283:LEU:HD23	1:A:291:TRP:HE3	1.80	0.46
1:B:247:ARG:O	1:B:251:ALA:HB2	2.16	0.46
1:A:276:PRO:HB2	8:A:510:HOH:O	2.15	0.46
1:A:146:LYS:HE2	2:A:1005:BOG:H61	1.96	0.45
1:B:133:ARG:NH2	1:B:136:VAL:HG21	2.31	0.45
1:B:244:LYS:HD3	1:B:247:ARG:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASN:ND2	1:B:245:GLU:HG3	2.31	0.45
1:A:177:TYR:HA	1:A:187:SER:O	2.17	0.45
1:B:132:ASP:OD1	1:B:133:ARG:NH1	2.49	0.45
1:A:257:MET:HG3	1:A:261:LYS:HZ3	1.81	0.45
1:A:137:ILE:HD11	1:A:256:GLU:CB	2.44	0.45
1:A:354:ILE:O	1:A:354:ILE:HG13	2.16	0.45
1:A:219:CYS:O	1:A:223:ILE:HG13	2.17	0.45
1:B:223:ILE:O	1:B:224:VAL:C	2.53	0.45
1:A:233:GLU:O	1:A:237:MET:HG2	2.17	0.45
1:A:52:ASN:HA	1:A:55:VAL:CG1	2.47	0.45
1:B:150:ARG:HD2	1:B:150:ARG:N	2.11	0.44
1:B:170:PRO:HB3	1:B:176:ALA:HA	1.98	0.44
1:B:293:THR:H	1:B:296:ALA:HB3	1.81	0.44
1:A:65:LEU:CD2	1:A:321:LYS:HB3	2.45	0.44
1:B:127:ALA:O	1:B:131:ILE:HG13	2.17	0.44
4:B:1000:RET:H10	4:B:1000:RET:C20	2.47	0.44
1:A:279:VAL:O	1:A:283:LEU:HD13	2.17	0.44
1:A:190:TYR:HA	1:A:201:ILE:HD11	1.99	0.44
1:B:326:ILE:O	1:B:330:PHE:N	2.50	0.44
1:B:177:TYR:HA	1:B:187:SER:O	2.17	0.44
1:A:12:TRP:CE3	1:A:24:ARG:HG2	2.53	0.44
1:A:284:ALA:CB	1:A:292:VAL:HG21	2.36	0.44
4:A:1000:RET:C20	4:A:1000:RET:H10	2.48	0.44
1:A:269:GLN:NE2	1:A:307:SER:OG	2.38	0.43
1:A:161:LEU:HD13	1:A:161:LEU:HA	1.81	0.43
1:A:92:MET:HG3	1:A:184:CYS:O	2.18	0.43
1:B:317:VAL:O	1:B:317:VAL:HG12	2.18	0.43
1:A:313:MET:SD	5:A:1002:PLM:H72	2.59	0.43
1:A:170:PRO:HB3	1:A:176:ALA:CA	2.49	0.43
1:B:100:LYS:HE2	1:B:100:LYS:HB2	1.69	0.43
1:B:182:VAL:HG22	1:B:298:GLN:OE1	2.19	0.43
1:B:176:ALA:O	1:B:188:PHE:HA	2.19	0.43
1:A:198:ARG:O	1:A:202:LEU:HG	2.19	0.43
1:B:279:VAL:O	1:B:283:LEU:HD13	2.19	0.42
1:A:50:GLY:O	1:A:54:ILE:HG13	2.18	0.42
1:B:332:TRP:O	1:B:335:THR:HG23	2.18	0.42
1:A:206:ILE:HA	1:A:210:PHE:HD2	1.83	0.42
1:A:259:LEU:HD12	2:A:1005:BOG:H6'1	2.01	0.42
1:B:51:GLY:O	1:B:55:VAL:HG12	2.19	0.42
1:B:257:MET:HG3	1:B:261:LYS:HZ1	1.84	0.42
1:A:170:PRO:HB2	1:A:177:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:SER:O	1:A:266:ILE:HG12	2.20	0.42
1:B:266:ILE:HG13	1:B:267:VAL:N	2.34	0.42
1:A:117:ILE:HG23	1:A:118:PHE:CD1	2.55	0.42
1:A:77:ALA:HA	8:A:508:HOH:O	2.19	0.42
1:B:156:ILE:HG13	1:B:157:ILE:N	2.34	0.42
4:A:1000:RET:H202	4:A:1000:RET:H10	2.01	0.42
1:B:257:MET:O	1:B:261:LYS:HG3	2.19	0.42
1:B:297:ALA:O	1:B:300:PRO:HD2	2.20	0.42
1:B:354:ILE:HG12	1:B:354:ILE:O	2.20	0.42
1:B:229:ASN:O	1:B:233:GLU:HG3	2.19	0.42
1:B:137:ILE:HD11	1:B:256:GLU:CB	2.49	0.41
1:A:288:PRO:HB2	1:A:291:TRP:CD2	2.55	0.41
1:A:293:THR:N	1:A:296:ALA:HB3	2.35	0.41
1:A:319:HIS:HA	1:A:320:PRO:HD2	1.91	0.41
1:B:296:ALA:O	1:B:300:PRO:HG2	2.20	0.41
1:A:229:ASN:HD22	1:A:229:ASN:N	2.18	0.41
1:B:220:TYR:O	1:B:224:VAL:HG23	2.20	0.41
1:A:105:PHE:O	1:A:109:LYS:HG3	2.21	0.41
1:A:328:GLN:HE21	1:A:328:GLN:HB2	1.78	0.41
1:B:105:PHE:O	1:B:109:LYS:HG3	2.20	0.41
1:A:205:PHE:O	1:A:209:PHE:HB3	2.20	0.41
1:B:263:SER:O	1:B:266:ILE:HG12	2.21	0.41
1:A:341:ASP:OD2	1:A:341:ASP:N	2.54	0.41
1:B:319:HIS:HA	1:B:320:PRO:HD2	1.97	0.40
1:B:216:ILE:HG23	1:B:220:TYR:CE2	2.55	0.40
1:A:178:THR:OG1	1:A:179:LEU:N	2.54	0.40
1:A:89:PHE:HA	1:A:90:PRO:HA	1.89	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	348/448 (78%)	316 (91%)	30 (9%)	2 (1%)	30	50
1	B	345/448 (77%)	318 (92%)	22 (6%)	5 (1%)	14	24
All	All	693/896 (77%)	634 (92%)	52 (8%)	7 (1%)	19	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ALA
1	B	226	SER
1	B	138	GLY
1	B	352	THR
1	B	223	ILE
1	A	292	VAL
1	B	224	VAL

### 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	296/369 (80%)	282 (95%)	14 (5%)	32	56
1	B	295/369 (80%)	275 (93%)	20 (7%)	20	36
All	All	591/738 (80%)	557 (94%)	34 (6%)	25	45

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	58	LEU
1	A	66	GLN
1	A	76	LEU
1	A	85	LEU
1	A	90	PRO
1	A	105	PHE
1	A	123	ILE
1	A	150	ARG

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Mol	Chain	Res	Type
1	A	234	MET
1	A	242	ASN
1	A	337	CYS
1	A	346	ASP
1	A	358	GLU
1	B	10	THR
1	B	63	LYS
1	B	66	GLN
1	B	76	LEU
1	B	85	LEU
1	B	102	ILE
1	B	105	PHE
1	B	117	ILE
1	B	123	ILE
1	B	133	ARG
1	B	150	ARG
1	B	225	MET
1	B	242	ASN
1	B	245	GLU
1	B	247	ARG
1	B	335	THR
1	B	337	CYS
1	B	346	ASP
1	B	349	ASP
1	B	354	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	229	ASN
1	A	242	ASN
1	A	254	ASN
1	A	269	GLN
1	A	328	GLN
1	B	70	ASN
1	B	222	ASN
1	B	242	ASN
1	B	269	GLN
1	B	328	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 ⓘ

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$
4	RET	A	1000	1	19,20,21	1.56	4 (21%)	27,27,28	1.69	7 (25%)
5	PLM	A	1001	-	16,16,17	0.42	0	14,15,17	0.62	0
5	PLM	A	1002	1	16,16,17	0.42	0	14,15,17	0.65	0
6	TWT	A	1003	-	21,21,21	0.29	0	20,20,20	1.63	4 (20%)
2	BOG	A	1005	-	20,20,20	1.81	7 (35%)	25,25,25	2.86	11 (44%)
4	RET	B	1000	1	19,20,21	1.53	4 (21%)	27,27,28	1.68	6 (22%)
5	PLM	B	1001	-	16,16,17	0.42	0	14,15,17	0.63	0
5	PLM	B	1002	1	16,16,17	0.46	0	14,15,17	0.63	0
6	TWT	B	1003	-	21,21,21	0.26	0	20,20,20	1.71	6 (30%)
7	PC1	B	1004	-	38,38,53	1.57	2 (5%)	39,43,61	0.96	1 (2%)
2	BOG	B	1005	-	20,20,20	1.81	7 (35%)	25,25,25	2.89	11 (44%)
3	SO4	B	1006	-	4,4,4	0.23	0	6,6,6	0.13	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
4	RET	A	1000	1	-	0/13/30/31	0/1/1/1
5	PLM	A	1001	-	-	0/13/14/15	0/0/0/0
5	PLM	A	1002	1	-	0/13/14/15	0/0/0/0
6	TWT	A	1003	-	-	0/19/19/19	0/0/0/0
2	BOG	A	1005	-	-	0/11/31/31	0/1/1/1
4	RET	B	1000	1	-	0/13/30/31	0/1/1/1
5	PLM	B	1001	-	-	0/13/14/15	0/0/0/0
5	PLM	B	1002	1	-	0/13/14/15	0/0/0/0
6	TWT	B	1003	-	-	0/19/19/19	0/0/0/0
7	PC1	B	1004	-	-	0/42/42/57	0/0/0/0
2	BOG	B	1005	-	-	0/11/31/31	0/1/1/1
3	SO4	B	1006	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1005	BOG	C4-C5	-2.77	1.47	1.53
2	A	1005	BOG	C4-C5	-2.66	1.47	1.53
2	A	1005	BOG	C3-C2	-2.22	1.46	1.52
2	B	1005	BOG	C3-C2	-2.15	1.46	1.52
2	B	1005	BOG	O1-C1	-2.11	1.36	1.40
2	A	1005	BOG	C6-C5	2.03	1.59	1.51
4	A	1000	RET	C5-C6	2.12	1.37	1.34
4	B	1000	RET	C8-C7	2.16	1.39	1.33
2	A	1005	BOG	O2-C2	2.26	1.48	1.43
2	B	1005	BOG	O2-C2	2.31	1.48	1.43
2	B	1005	BOG	C4-C3	2.42	1.58	1.52
2	A	1005	BOG	C4-C3	2.43	1.58	1.52
2	B	1005	BOG	O6-C6	2.48	1.53	1.42
2	A	1005	BOG	O6-C6	2.49	1.53	1.42
4	B	1000	RET	C12-C13	2.59	1.51	1.45
4	A	1000	RET	C8-C7	2.66	1.40	1.33
4	A	1000	RET	C12-C13	2.69	1.51	1.45
4	B	1000	RET	C5-C6	2.78	1.38	1.34
4	B	1000	RET	C1-C6	3.29	1.58	1.53
4	A	1000	RET	C1-C6	3.49	1.58	1.53
2	B	1005	BOG	O5-C1	3.80	1.51	1.41
2	A	1005	BOG	O5-C1	3.80	1.51	1.41
7	B	1004	PC1	O31-C31	4.27	1.46	1.33
7	B	1004	PC1	O21-C21	6.95	1.55	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1005	BOG	C1'-O1-C1	-8.24	99.54	113.94
2	A	1005	BOG	C1'-O1-C1	-7.96	100.03	113.94
2	A	1005	BOG	O1-C1-C2	-5.84	100.66	108.04
2	B	1005	BOG	O1-C1-C2	-5.73	100.81	108.04
2	B	1005	BOG	C1-C2-C3	-4.63	100.85	109.97
2	A	1005	BOG	C1-C2-C3	-4.56	100.98	109.97
2	A	1005	BOG	O5-C5-C4	-4.23	101.74	109.68
2	B	1005	BOG	O5-C5-C4	-4.12	101.95	109.68
2	A	1005	BOG	O3-C3-C2	-3.91	101.53	110.34
4	B	1000	RET	C8-C9-C10	-3.85	112.78	118.98
2	B	1005	BOG	O3-C3-C2	-3.84	101.69	110.34
4	A	1000	RET	C8-C9-C10	-3.72	112.99	118.98
6	B	1003	TWT	C14-C13-C12	-3.43	96.80	114.53
6	A	1003	TWT	C14-C13-C12	-3.31	97.45	114.53
6	B	1003	TWT	C16-C15-C14	-3.24	97.80	114.53
6	A	1003	TWT	C16-C15-C14	-3.05	98.76	114.53
6	B	1003	TWT	C12-C11-C10	-2.96	99.26	114.53
6	A	1003	TWT	C12-C11-C10	-2.92	99.47	114.53
6	B	1003	TWT	C18-C17-C16	-2.85	99.80	114.53
2	B	1005	BOG	C4'-C3'-C2'	-2.70	100.59	114.53
2	A	1005	BOG	C4'-C3'-C2'	-2.69	100.62	114.53
2	B	1005	BOG	O4-C4-C5	-2.63	102.26	109.24
2	A	1005	BOG	C6'-C5'-C4'	-2.60	101.09	114.53
2	A	1005	BOG	C3'-C2'-C1'	-2.60	101.86	113.47
6	A	1003	TWT	C18-C17-C16	-2.59	101.15	114.53
2	B	1005	BOG	C3'-C2'-C1'	-2.59	101.91	113.47
2	A	1005	BOG	O4-C4-C5	-2.54	102.51	109.24
2	B	1005	BOG	C6'-C5'-C4'	-2.51	101.55	114.53
2	A	1005	BOG	O1-C1'-C2'	-2.26	100.88	109.88
2	B	1005	BOG	O1-C1'-C2'	-2.20	101.12	109.88
2	B	1005	BOG	C5'-C4'-C3'	-2.15	103.41	114.53
6	B	1003	TWT	C20-C19-C18	-2.14	103.46	114.53
2	A	1005	BOG	C5'-C4'-C3'	-2.08	103.79	114.53
6	B	1003	TWT	C10-C9-C8	-2.03	104.02	114.53
4	A	1000	RET	C2-C1-C6	2.13	113.73	110.36
4	A	1000	RET	C19-C9-C10	2.26	126.24	122.90
4	B	1000	RET	C19-C9-C10	2.40	126.45	122.90
4	A	1000	RET	C18-C5-C6	2.75	127.30	124.61
4	B	1000	RET	C11-C12-C13	2.76	134.44	126.32
4	A	1000	RET	C11-C10-C9	2.85	131.31	127.20
4	B	1000	RET	C18-C5-C6	2.88	127.43	124.61
4	A	1000	RET	C11-C12-C13	2.90	134.87	126.32
7	B	1004	PC1	O21-C21-C22	3.09	118.24	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1000	RET	C11-C10-C9	3.20	131.82	127.20
4	B	1000	RET	C7-C8-C9	3.36	131.34	126.22
4	A	1000	RET	C7-C8-C9	3.86	132.10	126.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	RET	2	0
5	A	1002	PLM	1	0
2	A	1005	BOG	4	0
4	B	1000	RET	2	0
5	B	1002	PLM	1	0
7	B	1004	PC1	1	0
2	B	1005	BOG	2	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	350/448 (78%)	0.22	16 (4%) 36 41	35, 55, 118, 140	0
1	B	347/448 (77%)	0.04	1 (0%) 94 95	32, 49, 98, 121	0
All	All	697/896 (77%)	0.13	17 (2%) 62 66	32, 52, 108, 140	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	5.6
1	A	239	LYS	5.3
1	A	237	MET	4.7
1	A	234	MET	4.3
1	A	236	ALA	3.7
1	A	241	LEU	3.7
1	A	221	PHE	3.2
1	A	240	ARG	3.1
1	A	220	TYR	2.9
1	A	244	LYS	2.8
1	A	259	LEU	2.7
1	A	230	HIS	2.7
1	A	235	ALA	2.6
1	A	232	LYS	2.5
1	B	39	ILE	2.5
1	A	231	GLU	2.5
1	A	136	VAL	2.4

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

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( $\text{\AA}^2$ )	Q<0.9
5	PLM	B	1002	17/18	0.74	0.73	30.51	104,108,111,111	0
6	TWT	B	1003	22/22	0.89	0.73	22.99	63,80,87,88	0
6	TWT	A	1003	22/22	0.86	0.69	10.40	57,93,102,102	0
5	PLM	A	1001	17/18	0.82	0.30	8.13	62,67,70,70	0
5	PLM	A	1002	17/18	0.89	0.32	7.18	96,102,110,110	0
5	PLM	B	1001	17/18	0.82	0.38	6.89	53,70,74,74	0
2	BOG	B	1005	20/20	0.87	0.44	5.79	68,113,119,121	0
2	BOG	A	1005	20/20	0.92	0.39	4.38	54,100,107,107	0
4	RET	B	1000	20/21	0.97	0.23	3.99	33,38,40,44	0
4	RET	A	1000	20/21	0.96	0.23	1.94	39,52,58,59	0
7	PC1	B	1004	39/54	0.89	0.18	1.77	42,67,120,120	0
3	SO4	B	1006	5/5	0.96	0.12	-1.05	96,96,96,97	0

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

There are no such residues in this entry.