



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:05 PM GMT

PDB ID : 1NFQ  
Title : Rv2002 gene product from Mycobacterium tuberculosis  
Authors : Yang, J.K.; Park, M.S.; Waldo, G.S.; Suh, S.W.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2002-12-15  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

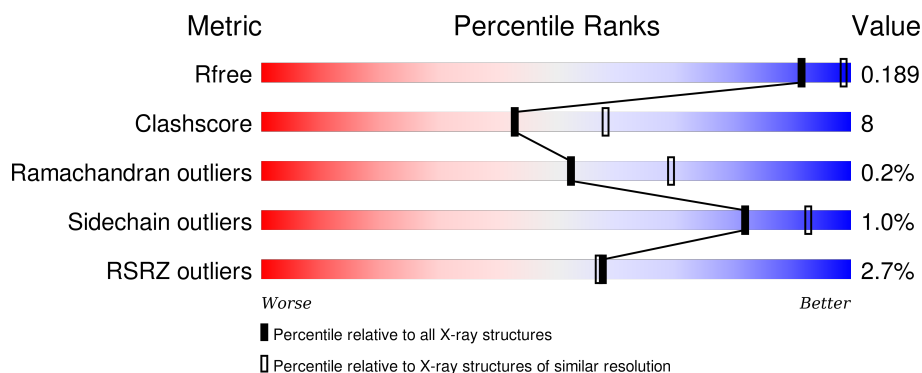
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	260	<div> <div>4%</div> <div>81% 13% 6%</div> </div>
1	B	260	<div> <div>%</div> <div>81% 13% 6%</div> </div>
1	C	260	<div> <div>2%</div> <div>81% 13% 6%</div> </div>
1	D	260	<div> <div>3%</div> <div>79% 15% 6%</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
3	AOI	A	401	X	-	-	X
3	AOI	B	1401	X	-	-	X
3	AOI	C	2401	X	-	-	X
3	AOI	D	3401	X	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7618 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.

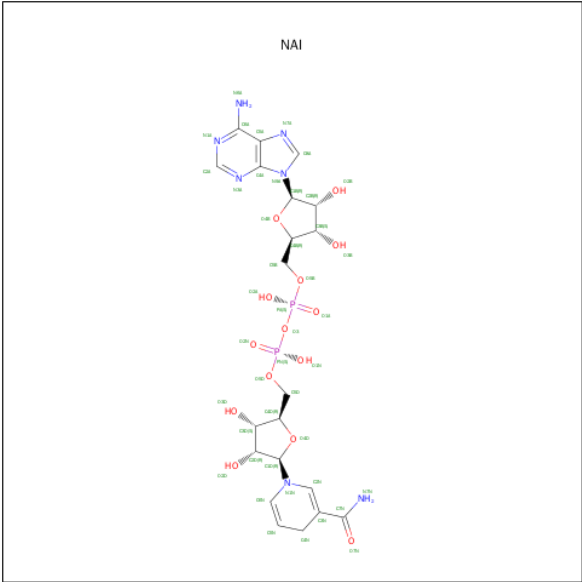
- Molecule 1 is a protein called Putative oxidoreductase Rv2002.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			
1	B	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			
1	C	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			
1	D	244	Total	C	N	O	S	0	0	0
			1780	1122	310	342	6			

There are 12 discrepancies between the modelled and reference sequences:

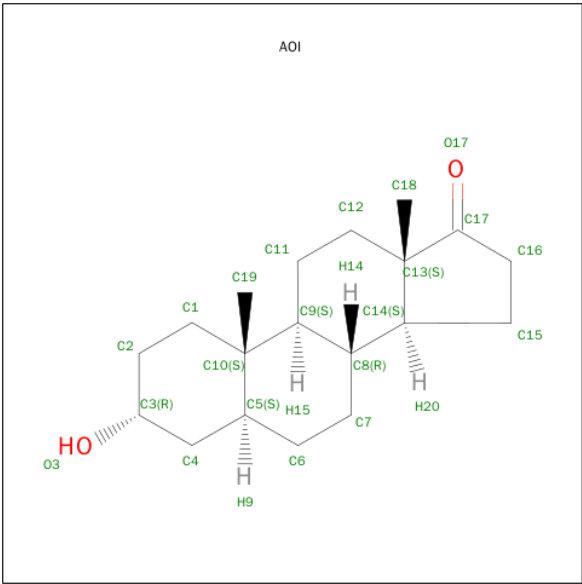
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	THR	ILE	ENGINEERED	UNP P69167
A	47	MET	VAL	ENGINEERED	UNP P69167
A	69	LYS	THR	ENGINEERED	UNP P69167
B	6	THR	ILE	ENGINEERED	UNP P69167
B	47	MET	VAL	ENGINEERED	UNP P69167
B	69	LYS	THR	ENGINEERED	UNP P69167
C	6	THR	ILE	ENGINEERED	UNP P69167
C	47	MET	VAL	ENGINEERED	UNP P69167
C	69	LYS	THR	ENGINEERED	UNP P69167
D	6	THR	ILE	ENGINEERED	UNP P69167
D	47	MET	VAL	ENGINEERED	UNP P69167
D	69	LYS	THR	ENGINEERED	UNP P69167

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ANDROSTERONE (three-letter code: AOI) (formula: C<sub>19</sub>H<sub>30</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		
3	C	1	Total	C	O	0	0
			21	19	2		
3	D	1	Total	C	O	0	0
			21	19	2		

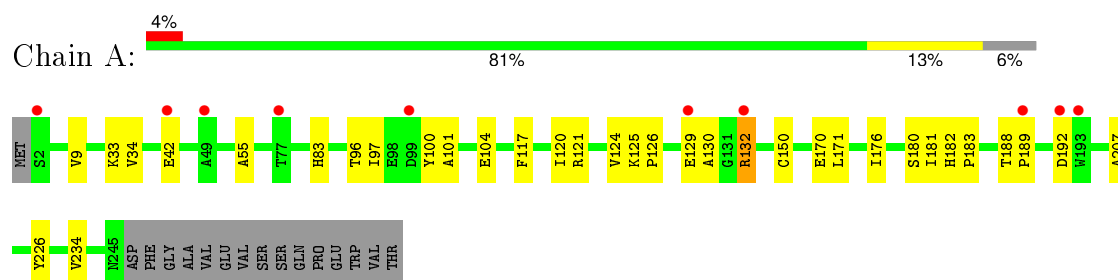
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	70	Total	O	0	0
			70	70		
4	C	61	Total	O	0	0
			61	61		
4	D	48	Total	O	0	0
			48	48		

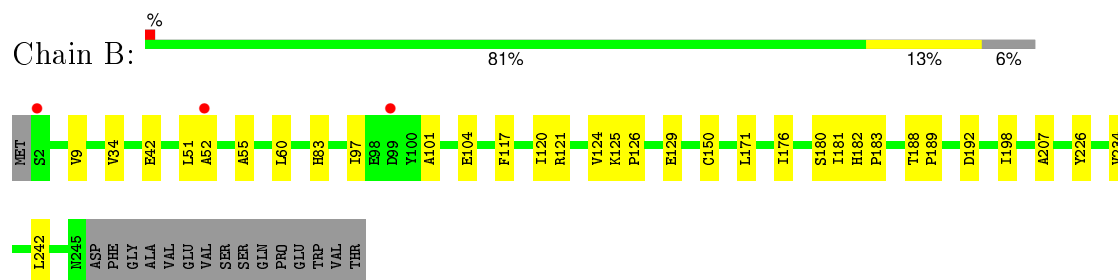
### 3 Residue-property plots

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.

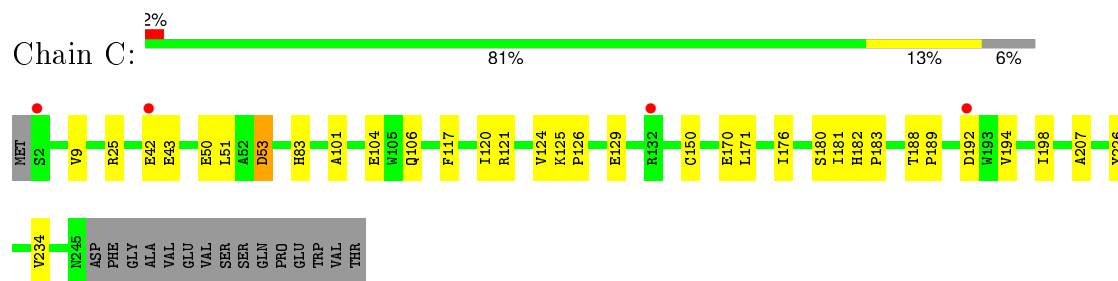
#### • Molecule 1: Putative oxidoreductase Rv2002



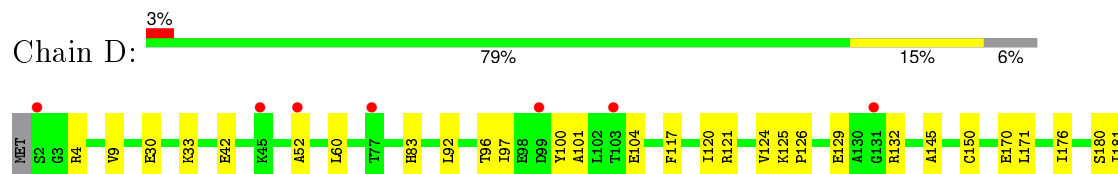
#### • Molecule 1: Putative oxidoreductase Rv2002

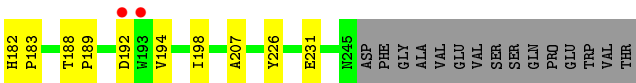


#### • Molecule 1: Putative oxidoreductase Rv2002



#### • Molecule 1: Putative oxidoreductase Rv2002







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.16Å 122.16Å 141.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.40 19.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (19.91-2.40) 96.2 (19.91-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.162 , 0.189 0.162 , 0.189	Depositor DCC
$R_{free}$ test set	3918 reflections (10.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.0	EDS
Estimated twinning fraction	0.036 for -h,k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40348 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: NAI, AOI

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	0.34	0/1809	0.61	0/2460
1	B	0.33	0/1809	0.60	0/2460
1	C	0.41	1/1809 (0.1%)	0.68	2/2460 (0.1%)
1	D	0.31	0/1809	0.59	0/2460
All	All	0.35	1/7236 (0.0%)	0.62	2/9840 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	ASP	CB-CG	6.42	1.65	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	ASP	CB-CG-OD1	11.72	128.85	118.30
1	C	53	ASP	CB-CG-OD2	-5.33	113.51	118.30

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	1780	0	1791	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1780	0	1791	25	0
1	C	1780	0	1791	28	0
1	D	1780	0	1791	34	0
2	A	44	0	27	1	0
2	B	44	0	27	2	0
2	C	44	0	27	1	0
2	D	44	0	27	2	0
3	A	21	0	28	4	0
3	B	21	0	28	4	0
3	C	21	0	28	6	0
3	D	21	0	28	8	0
4	A	59	0	0	0	0
4	B	70	0	0	1	0
4	C	61	0	0	1	0
4	D	48	0	0	1	0
All	All	7618	0	7384	121	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 8.

All (121) 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)
3:A:401:AOI:C11	3:A:401:AOI:C9	1.75	1.63
3:D:3401:AOI:C11	3:D:3401:AOI:C9	1.74	1.57
3:B:1401:AOI:C9	3:B:1401:AOI:C11	1.75	1.57
3:C:2401:AOI:C11	3:C:2401:AOI:C9	1.75	1.54
1:C:9:VAL:H	1:C:83:HIS:HD2	1.14	0.89
1:D:9:VAL:H	1:D:83:HIS:HD2	1.14	0.89
1:A:9:VAL:H	1:A:83:HIS:HD2	1.18	0.87
1:B:9:VAL:H	1:B:83:HIS:HD2	1.18	0.86
1:B:42:GLU:H	1:B:42:GLU:CD	1.88	0.76
1:C:42:GLU:CD	1:C:42:GLU:H	1.89	0.76
1:A:42:GLU:CD	1:A:42:GLU:H	1.90	0.74
1:D:42:GLU:H	1:D:42:GLU:CD	1.88	0.74
1:D:9:VAL:H	1:D:83:HIS:CD2	2.05	0.69
3:D:3401:AOI:C9	3:D:3401:AOI:C12	2.72	0.68
1:D:9:VAL:N	1:D:83:HIS:HD2	1.91	0.67
1:C:9:VAL:N	1:C:83:HIS:HD2	1.91	0.67
1:C:9:VAL:H	1:C:83:HIS:CD2	2.05	0.67
3:B:1401:AOI:C12	3:B:1401:AOI:C9	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2401:AOI:C12	3:C:2401:AOI:C9	2.72	0.66
1:A:132:ARG:HG3	1:A:132:ARG:HH11	1.61	0.66
1:C:181:ILE:HG22	1:C:183:PRO:HD3	1.77	0.66
1:D:181:ILE:HG22	1:D:183:PRO:HD3	1.78	0.65
1:A:181:ILE:HG22	1:A:183:PRO:HD3	1.78	0.65
1:A:9:VAL:H	1:A:83:HIS:CD2	2.09	0.65
3:A:401:AOI:C9	3:A:401:AOI:C12	2.72	0.64
1:B:9:VAL:H	1:B:83:HIS:CD2	2.09	0.64
1:B:181:ILE:HG22	1:B:183:PRO:HD3	1.77	0.64
1:B:9:VAL:N	1:B:83:HIS:HD2	1.95	0.62
1:D:132:ARG:HB3	1:D:132:ARG:HH11	1.64	0.62
1:D:132:ARG:HB3	1:D:132:ARG:NH1	2.17	0.59
1:B:117:PHE:CE2	1:B:121:ARG:HD2	2.39	0.58
1:D:188:THR:HB	1:D:189:PRO:HD2	1.85	0.57
3:A:401:AOI:C11	3:A:401:AOI:C8	2.82	0.57
1:A:9:VAL:N	1:A:83:HIS:HD2	1.95	0.57
3:D:3401:AOI:C11	3:D:3401:AOI:C8	2.82	0.57
1:A:132:ARG:NH1	1:A:132:ARG:HG3	2.20	0.57
1:C:188:THR:HB	1:C:189:PRO:HD2	1.86	0.57
1:C:117:PHE:CE2	1:C:121:ARG:HD2	2.40	0.56
1:C:120:ILE:O	1:C:124:VAL:HG13	2.05	0.56
1:A:188:THR:HB	1:A:189:PRO:HD2	1.86	0.56
1:B:188:THR:HB	1:B:189:PRO:HD2	1.86	0.56
1:D:120:ILE:O	1:D:124:VAL:HG13	2.05	0.56
3:C:2401:AOI:C11	3:C:2401:AOI:C8	2.81	0.56
1:D:117:PHE:CE2	1:D:121:ARG:HD2	2.41	0.56
1:A:120:ILE:O	1:A:124:VAL:HG13	2.06	0.56
1:B:120:ILE:O	1:B:124:VAL:HG13	2.06	0.55
1:A:117:PHE:CE2	1:A:121:ARG:HD2	2.41	0.55
3:B:1401:AOI:C11	3:B:1401:AOI:C8	2.82	0.54
1:C:226:TYR:CE2	1:D:207:ALA:HB2	2.43	0.54
1:A:226:TYR:CE2	1:B:207:ALA:HB2	2.43	0.53
1:A:207:ALA:HB2	1:B:226:TYR:CE2	2.43	0.53
1:D:183:PRO:HG2	2:D:3300:NAI:C5N	2.39	0.52
1:C:207:ALA:HB2	1:D:226:TYR:CE2	2.45	0.51
1:D:4:ARG:HG3	1:D:30:GLU:OE1	2.10	0.51
1:A:183:PRO:HG2	2:A:300:NAI:C5N	2.41	0.51
1:C:43:GLU:HG2	4:C:662:HOH:O	2.11	0.50
1:A:207:ALA:HB2	1:B:226:TYR:CD2	2.48	0.48
1:C:226:TYR:CD2	1:D:207:ALA:HB2	2.48	0.48
1:A:226:TYR:CD2	1:B:207:ALA:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LYS:HB3	1:B:126:PRO:CD	2.44	0.48
1:A:170:GLU:OE2	1:D:97:ILE:HG13	2.14	0.48
1:A:34:VAL:O	1:A:55:ALA:HA	2.14	0.48
1:B:183:PRO:HG2	2:B:1300:NAI:C5N	2.44	0.48
1:D:101:ALA:HB3	1:D:104:GLU:HG3	1.96	0.48
1:D:198:ILE:HG12	3:D:3401:AOI:H17	1.96	0.47
1:C:207:ALA:HB2	1:D:226:TYR:CD2	2.49	0.47
1:A:97:ILE:HG13	1:D:170:GLU:OE2	2.13	0.47
1:C:198:ILE:HG12	3:C:2401:AOI:H17	1.96	0.47
1:A:101:ALA:HB3	1:A:104:GLU:HG3	1.96	0.47
1:C:180:SER:OG	1:C:182:HIS:HE1	1.96	0.47
1:C:101:ALA:HB3	1:C:104:GLU:HG3	1.97	0.47
1:C:25:ARG:NH2	1:C:50:GLU:OE2	2.47	0.47
1:C:125:LYS:HB3	1:C:126:PRO:CD	2.45	0.47
1:B:101:ALA:HB3	1:B:104:GLU:HG3	1.97	0.47
1:A:130:ALA:CB	1:A:132:ARG:HH22	2.28	0.47
1:A:132:ARG:O	1:A:132:ARG:CZ	2.63	0.46
1:A:125:LYS:O	1:A:129:GLU:HG3	2.15	0.46
1:D:189:PRO:HA	1:D:192:ASP:OD2	2.15	0.46
1:A:125:LYS:HB3	1:A:126:PRO:CD	2.45	0.46
1:D:180:SER:OG	1:D:182:HIS:HE1	1.99	0.46
1:A:180:SER:OG	1:A:182:HIS:HE1	1.98	0.46
1:A:189:PRO:HA	1:A:192:ASP:OD2	2.16	0.46
1:D:125:LYS:HB3	1:D:126:PRO:CD	2.45	0.46
1:B:180:SER:OG	1:B:182:HIS:HE1	1.99	0.45
1:D:125:LYS:O	1:D:129:GLU:HG3	2.17	0.45
1:C:125:LYS:O	1:C:129:GLU:HG3	2.16	0.44
1:B:125:LYS:O	1:B:129:GLU:HG3	2.17	0.44
3:D:3401:AOI:C11	3:D:3401:AOI:C10	2.89	0.44
1:D:60:LEU:O	2:D:3300:NAI:H2A	2.18	0.44
1:C:189:PRO:HA	1:C:192:ASP:OD2	2.17	0.44
1:B:60:LEU:O	2:B:1300:NAI:H2A	2.18	0.44
1:B:189:PRO:HA	1:B:192:ASP:OD2	2.16	0.44
1:A:96:THR:O	1:A:100:TYR:HB2	2.18	0.43
1:C:183:PRO:HG2	2:C:2300:NAI:C5N	2.48	0.43
1:C:51:LEU:HD23	1:C:51:LEU:HA	1.84	0.43
4:B:551:HOH:O	1:C:106:GLN:NE2	2.45	0.43
1:D:194:VAL:HG21	3:D:3401:AOI:C19	2.49	0.43
1:D:96:THR:O	1:D:100:TYR:HB2	2.19	0.43
1:A:130:ALA:HB1	1:A:132:ARG:HH12	1.83	0.42
1:B:242:LEU:CD2	1:D:145:ALA:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HB3	1:A:176:ILE:HB	2.00	0.42
1:C:234:VAL:HG13	1:C:234:VAL:O	2.20	0.42
1:D:171:LEU:HB3	1:D:176:ILE:HB	2.00	0.42
1:D:33:LYS:HD3	1:D:33:LYS:HA	1.83	0.42
3:A:401:AOI:C11	3:A:401:AOI:C10	2.90	0.41
1:B:198:ILE:HG12	3:B:1401:AOI:H17	2.02	0.41
1:D:231:GLU:HG3	4:D:526:HOH:O	2.19	0.41
1:B:234:VAL:O	1:B:234:VAL:HG13	2.19	0.41
1:D:132:ARG:HH11	1:D:132:ARG:CB	2.29	0.41
1:B:97:ILE:HG13	1:C:170:GLU:OE2	2.20	0.41
1:C:194:VAL:HG21	3:C:2401:AOI:C19	2.49	0.41
1:C:194:VAL:HG11	3:C:2401:AOI:H30	2.02	0.41
1:A:234:VAL:HG13	1:A:234:VAL:O	2.21	0.41
1:D:92:LEU:HD21	3:D:3401:AOI:H11	2.02	0.41
1:B:171:LEU:HB3	1:B:176:ILE:HB	2.02	0.41
1:C:171:LEU:HB3	1:C:176:ILE:HB	2.01	0.41
1:D:194:VAL:HG11	3:D:3401:AOI:H30	2.02	0.41
1:A:132:ARG:O	1:A:132:ARG:NH2	2.54	0.41
1:A:33:LYS:HD3	1:A:33:LYS:HA	1.83	0.41
1:B:34:VAL:O	1:B:55:ALA:HA	2.21	0.40
1:A:130:ALA:HB1	1:A:132:ARG:HH22	1.87	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	242/260 (93%)	232 (96%)	10 (4%)	0	100	100
1	B	242/260 (93%)	232 (96%)	9 (4%)	1 (0%)	39	56
1	C	242/260 (93%)	232 (96%)	10 (4%)	0	100	100
1	D	242/260 (93%)	229 (95%)	12 (5%)	1 (0%)	39	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	968/1040 (93%)	925 (96%)	41 (4%)	2 (0%)	52 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	ALA
1	D	52	ALA

### 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	182/196 (93%)	180 (99%)	2 (1%)	80 92
1	B	182/196 (93%)	180 (99%)	2 (1%)	80 92
1	C	182/196 (93%)	180 (99%)	2 (1%)	80 92
1	D	182/196 (93%)	181 (100%)	1 (0%)	92 97
All	All	728/784 (93%)	721 (99%)	7 (1%)	82 93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ARG
1	A	150	CYS
1	B	51	LEU
1	B	150	CYS
1	C	53	ASP
1	C	150	CYS
1	D	150	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS

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Mol	Chain	Res	Type
1	A	83	HIS
1	A	182	HIS
1	A	244	HIS
1	B	83	HIS
1	B	88	ASN
1	B	182	HIS
1	B	200	GLN
1	B	244	HIS
1	C	59	HIS
1	C	83	HIS
1	C	88	ASN
1	C	182	HIS
1	C	200	GLN
1	C	244	HIS
1	D	83	HIS
1	D	88	ASN
1	D	182	HIS
1	D	244	HIS

### 5.3.3 RNA [i](#)

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](#)

8 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	NAI	A	300	-	38,48,48	1.33	4 (10%)	48,73,73	1.07	5 (10%)
3	AOI	A	401	-	24,24,24	6.55	21 (87%)	39,39,39	4.85	26 (66%)
2	NAI	B	1300	-	38,48,48	1.31	4 (10%)	48,73,73	1.12	5 (10%)
3	AOI	B	1401	-	24,24,24	6.53	21 (87%)	39,39,39	4.86	26 (66%)
2	NAI	C	2300	-	38,48,48	1.35	4 (10%)	48,73,73	1.08	4 (8%)
3	AOI	C	2401	-	24,24,24	6.53	21 (87%)	39,39,39	4.87	26 (66%)
2	NAI	D	3300	-	38,48,48	1.31	4 (10%)	48,73,73	1.03	3 (6%)
3	AOI	D	3401	-	24,24,24	6.53	21 (87%)	39,39,39	4.84	26 (66%)

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	NAI	A	300	-	-	0/25/72/72	0/5/5/5
3	AOI	A	401	-	2/2/8/8	0/0/58/58	0/4/4/4
2	NAI	B	1300	-	-	0/25/72/72	0/5/5/5
3	AOI	B	1401	-	2/2/8/8	0/0/58/58	0/4/4/4
2	NAI	C	2300	-	-	0/25/72/72	0/5/5/5
3	AOI	C	2401	-	2/2/8/8	0/0/58/58	0/4/4/4
2	NAI	D	3300	-	-	0/25/72/72	0/5/5/5
3	AOI	D	3401	-	2/2/8/8	0/0/58/58	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2401	AOI	C4-C3	-3.78	1.44	1.51
3	A	401	AOI	C4-C3	-3.74	1.44	1.51
3	B	1401	AOI	C4-C3	-3.73	1.44	1.51
3	D	3401	AOI	C4-C3	-3.72	1.44	1.51
2	C	2300	NAI	O4B-C1B	-3.33	1.37	1.41
2	B	1300	NAI	O4B-C1B	-2.87	1.37	1.41
2	D	3300	NAI	O4B-C1B	-2.80	1.37	1.41
2	A	300	NAI	O4B-C1B	-2.78	1.37	1.41
3	B	1401	AOI	C13-C14	-2.14	1.50	1.54
3	A	401	AOI	C13-C14	-2.14	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2401	AOI	C13-C14	-2.06	1.50	1.54
3	D	3401	AOI	C13-C14	-2.00	1.50	1.54
3	C	2401	AOI	C4-C5	2.08	1.57	1.53
2	A	300	NAI	C6N-N1N	2.09	1.43	1.37
2	C	2300	NAI	C6N-N1N	2.09	1.43	1.37
2	B	1300	NAI	C6N-N1N	2.11	1.43	1.37
2	D	3300	NAI	C6N-N1N	2.12	1.43	1.37
3	D	3401	AOI	C4-C5	2.16	1.57	1.53
2	A	300	NAI	C2A-N1A	2.22	1.38	1.33
2	D	3300	NAI	C2A-N1A	2.24	1.38	1.33
3	A	401	AOI	C4-C5	2.26	1.57	1.53
3	B	1401	AOI	C4-C5	2.26	1.57	1.53
2	B	1300	NAI	C2A-N1A	2.30	1.38	1.33
2	C	2300	NAI	C2A-N1A	2.31	1.38	1.33
3	B	1401	AOI	C10-C5	3.23	1.60	1.55
3	A	401	AOI	C10-C5	3.32	1.61	1.55
3	C	2401	AOI	C10-C5	3.33	1.61	1.55
3	D	3401	AOI	C10-C5	3.34	1.61	1.55
3	A	401	AOI	C13-C17	3.69	1.57	1.52
3	C	2401	AOI	C13-C17	3.72	1.57	1.52
3	B	1401	AOI	C13-C17	3.78	1.57	1.52
3	D	3401	AOI	C13-C17	3.79	1.57	1.52
3	C	2401	AOI	C2-C3	4.54	1.64	1.51
3	D	3401	AOI	C2-C3	4.56	1.64	1.51
3	B	1401	AOI	C2-C3	4.60	1.64	1.51
3	A	401	AOI	C2-C3	4.66	1.64	1.51
3	D	3401	AOI	C1-C10	4.74	1.63	1.54
3	B	1401	AOI	C1-C10	4.75	1.63	1.54
3	C	2401	AOI	C1-C10	4.78	1.63	1.54
3	A	401	AOI	C1-C10	4.89	1.63	1.54
3	D	3401	AOI	C19-C10	4.95	1.63	1.54
3	B	1401	AOI	C19-C10	5.03	1.63	1.54
3	C	2401	AOI	C19-C10	5.09	1.63	1.54
3	A	401	AOI	C19-C10	5.16	1.64	1.54
3	B	1401	AOI	C7-C6	5.18	1.66	1.52
3	D	3401	AOI	C7-C6	5.20	1.66	1.52
3	A	401	AOI	C7-C6	5.24	1.66	1.52
3	C	2401	AOI	C7-C6	5.30	1.66	1.52
3	A	401	AOI	C8-C14	5.33	1.64	1.53
3	B	1401	AOI	C8-C14	5.34	1.64	1.53
3	C	2401	AOI	C8-C14	5.38	1.64	1.53
3	D	3401	AOI	C8-C14	5.40	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3300	NAI	C2N-C3N	5.66	1.48	1.34
2	B	1300	NAI	C2N-C3N	5.73	1.48	1.34
2	C	2300	NAI	C2N-C3N	5.75	1.48	1.34
2	A	300	NAI	C2N-C3N	5.82	1.49	1.34
3	C	2401	AOI	C15-C16	5.85	1.67	1.53
3	A	401	AOI	C15-C16	5.86	1.67	1.53
3	B	1401	AOI	C15-C16	5.86	1.67	1.53
3	D	3401	AOI	C15-C16	5.87	1.67	1.53
3	A	401	AOI	C12-C11	6.09	1.66	1.53
3	B	1401	AOI	C12-C11	6.09	1.66	1.53
3	C	2401	AOI	C12-C11	6.13	1.67	1.53
3	D	3401	AOI	C12-C11	6.21	1.67	1.53
3	A	401	AOI	C18-C13	7.07	1.67	1.54
3	B	1401	AOI	C18-C13	7.10	1.67	1.54
3	D	3401	AOI	C18-C13	7.10	1.67	1.54
3	C	2401	AOI	C18-C13	7.12	1.67	1.54
3	B	1401	AOI	C15-C14	7.46	1.71	1.54
3	A	401	AOI	C15-C14	7.53	1.71	1.54
3	D	3401	AOI	C15-C14	7.56	1.71	1.54
3	C	2401	AOI	C15-C14	7.57	1.71	1.54
3	C	2401	AOI	C12-C13	7.77	1.68	1.54
3	D	3401	AOI	C10-C9	7.83	1.71	1.56
3	B	1401	AOI	C10-C9	7.83	1.71	1.56
3	A	401	AOI	C12-C13	7.86	1.68	1.54
3	C	2401	AOI	C10-C9	7.89	1.71	1.56
3	B	1401	AOI	C12-C13	7.92	1.68	1.54
3	D	3401	AOI	C12-C13	7.93	1.68	1.54
3	A	401	AOI	C10-C9	7.94	1.71	1.56
3	D	3401	AOI	C1-C2	7.97	1.71	1.53
3	C	2401	AOI	C1-C2	7.98	1.71	1.53
3	A	401	AOI	C1-C2	8.03	1.71	1.53
3	B	1401	AOI	C1-C2	8.07	1.71	1.53
3	B	1401	AOI	C16-C17	8.75	1.66	1.51
3	C	2401	AOI	C16-C17	8.75	1.66	1.51
3	A	401	AOI	C16-C17	8.80	1.66	1.51
3	D	3401	AOI	C16-C17	8.80	1.66	1.51
3	A	401	AOI	C8-C9	10.39	1.74	1.53
3	B	1401	AOI	C8-C9	10.43	1.74	1.53
3	D	3401	AOI	C8-C9	10.43	1.74	1.53
3	C	2401	AOI	C8-C9	10.49	1.74	1.53
3	D	3401	AOI	C11-C9	11.92	1.74	1.53
3	C	2401	AOI	C11-C9	11.93	1.75	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1401	AOI	C11-C9	12.00	1.75	1.53
3	A	401	AOI	C11-C9	12.10	1.75	1.53
3	A	401	AOI	O17-C17	12.38	1.43	1.21
3	C	2401	AOI	O17-C17	12.40	1.43	1.21
3	D	3401	AOI	O17-C17	12.46	1.43	1.21
3	B	1401	AOI	O17-C17	12.50	1.43	1.21

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2401	AOI	C18-C13-C12	-10.51	98.05	111.12
3	A	401	AOI	C18-C13-C12	-10.39	98.20	111.12
3	D	3401	AOI	C18-C13-C12	-10.34	98.26	111.12
3	B	1401	AOI	C18-C13-C12	-10.33	98.28	111.12
3	C	2401	AOI	O17-C17-C16	-8.50	114.84	125.71
3	A	401	AOI	O17-C17-C13	-8.47	113.38	125.93
3	B	1401	AOI	O17-C17-C16	-8.46	114.89	125.71
3	C	2401	AOI	O17-C17-C13	-8.44	113.42	125.93
3	D	3401	AOI	O17-C17-C13	-8.35	113.55	125.93
3	A	401	AOI	O17-C17-C16	-8.34	115.04	125.71
3	B	1401	AOI	O17-C17-C13	-8.32	113.60	125.93
3	D	3401	AOI	O17-C17-C16	-8.29	115.11	125.71
3	A	401	AOI	C15-C16-C17	-6.71	98.67	105.65
3	B	1401	AOI	C15-C16-C17	-6.68	98.70	105.65
3	C	2401	AOI	C15-C16-C17	-6.64	98.75	105.65
3	D	3401	AOI	C15-C16-C17	-6.59	98.80	105.65
3	D	3401	AOI	C19-C10-C1	-6.36	97.50	108.20
3	A	401	AOI	C19-C10-C1	-6.29	97.63	108.20
3	B	1401	AOI	C19-C10-C1	-6.27	97.65	108.20
3	C	2401	AOI	C19-C10-C1	-6.15	97.86	108.20
3	A	401	AOI	C12-C11-C9	-4.51	105.51	113.10
3	B	1401	AOI	C12-C11-C9	-4.50	105.52	113.10
3	B	1401	AOI	C19-C10-C5	-4.48	102.33	110.25
3	C	2401	AOI	C19-C10-C5	-4.47	102.35	110.25
3	D	3401	AOI	C12-C11-C9	-4.46	105.58	113.10
3	D	3401	AOI	C19-C10-C5	-4.38	102.52	110.25
3	C	2401	AOI	C12-C11-C9	-4.33	105.79	113.10
3	A	401	AOI	C19-C10-C5	-4.30	102.66	110.25
3	B	1401	AOI	C7-C8-C14	-3.07	106.94	112.02
3	A	401	AOI	C7-C8-C14	-3.05	106.97	112.02
3	D	3401	AOI	C7-C8-C14	-2.99	107.06	112.02
2	B	1300	NAI	C2B-C1B-N9A	-2.93	109.81	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2401	AOI	C7-C8-C14	-2.88	107.25	112.02
3	A	401	AOI	C10-C9-C8	-2.85	109.22	112.40
2	A	300	NAI	C2B-C1B-N9A	-2.85	109.94	114.29
3	C	2401	AOI	C11-C9-C8	-2.82	107.65	111.74
2	D	3300	NAI	PN-O3-PA	-2.81	124.83	132.73
3	C	2401	AOI	C10-C9-C8	-2.77	109.31	112.40
3	A	401	AOI	C11-C9-C8	-2.74	107.77	111.74
2	C	2300	NAI	PN-O3-PA	-2.72	125.08	132.73
3	B	1401	AOI	C11-C9-C8	-2.72	107.79	111.74
3	D	3401	AOI	C10-C9-C8	-2.72	109.36	112.40
3	D	3401	AOI	C15-C14-C13	-2.71	101.42	104.06
3	B	1401	AOI	C10-C9-C8	-2.68	109.42	112.40
3	C	2401	AOI	C15-C14-C13	-2.67	101.46	104.06
3	D	3401	AOI	C11-C9-C8	-2.65	107.90	111.74
3	B	1401	AOI	C16-C17-C13	-2.60	106.07	108.64
3	D	3401	AOI	C16-C17-C13	-2.57	106.09	108.64
3	A	401	AOI	C15-C14-C13	-2.55	101.58	104.06
3	B	1401	AOI	C15-C14-C13	-2.53	101.59	104.06
2	A	300	NAI	PN-O3-PA	-2.53	125.62	132.73
2	B	1300	NAI	O5B-C5B-C4B	-2.52	99.82	109.12
3	C	2401	AOI	C16-C17-C13	-2.50	106.17	108.64
3	A	401	AOI	C16-C17-C13	-2.49	106.18	108.64
2	C	2300	NAI	C2B-C1B-N9A	-2.46	110.53	114.29
2	D	3300	NAI	O5B-C5B-C4B	-2.41	100.24	109.12
2	C	2300	NAI	O5B-C5B-C4B	-2.29	100.67	109.12
2	A	300	NAI	O5B-C5B-C4B	-2.22	100.94	109.12
2	B	1300	NAI	PN-O3-PA	-2.03	127.03	132.73
2	A	300	NAI	O1N-PN-O3	2.12	114.71	105.09
3	A	401	AOI	C18-C13-C14	2.13	116.41	112.94
2	B	1300	NAI	O1N-PN-O3	2.15	114.84	105.09
3	D	3401	AOI	C9-C10-C5	2.15	111.86	108.67
3	B	1401	AOI	C18-C13-C14	2.19	116.49	112.94
3	C	2401	AOI	C18-C13-C14	2.19	116.51	112.94
3	D	3401	AOI	C18-C13-C14	2.22	116.54	112.94
3	A	401	AOI	C9-C10-C5	2.24	111.99	108.67
2	B	1300	NAI	C4A-C5A-N7A	2.27	111.57	109.48
2	D	3300	NAI	C4A-C5A-N7A	2.27	111.57	109.48
3	B	1401	AOI	C9-C10-C5	2.29	112.06	108.67
3	D	3401	AOI	C18-C13-C17	2.33	109.89	105.19
2	A	300	NAI	C4A-C5A-N7A	2.41	111.69	109.48
3	C	2401	AOI	C9-C10-C5	2.43	112.27	108.67
3	A	401	AOI	C18-C13-C17	2.44	110.11	105.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2300	NAI	C4A-C5A-N7A	2.44	111.72	109.48
3	B	1401	AOI	C18-C13-C17	2.47	110.18	105.19
3	C	2401	AOI	C18-C13-C17	2.51	110.26	105.19
3	B	1401	AOI	C15-C14-C8	3.15	123.99	119.03
3	C	2401	AOI	C15-C14-C8	3.19	124.07	119.03
3	A	401	AOI	C15-C14-C8	3.20	124.08	119.03
3	D	3401	AOI	C12-C13-C14	3.20	113.78	108.99
3	C	2401	AOI	C12-C13-C14	3.23	113.81	108.99
3	D	3401	AOI	C15-C14-C8	3.23	124.13	119.03
3	A	401	AOI	C12-C13-C14	3.33	113.96	108.99
3	B	1401	AOI	C12-C13-C14	3.33	113.97	108.99
3	B	1401	AOI	C6-C5-C10	3.38	118.50	112.26
3	A	401	AOI	C6-C5-C10	3.39	118.52	112.26
3	C	2401	AOI	C6-C5-C10	3.42	118.56	112.26
3	D	3401	AOI	C6-C5-C10	3.49	118.70	112.26
3	D	3401	AOI	O3-C3-C2	4.08	121.61	110.05
3	B	1401	AOI	O3-C3-C2	4.15	121.79	110.05
3	C	2401	AOI	O3-C3-C2	4.17	121.85	110.05
3	A	401	AOI	O3-C3-C2	4.22	121.98	110.05
3	C	2401	AOI	C14-C8-C9	4.24	114.63	109.06
3	A	401	AOI	C14-C8-C9	4.33	114.75	109.06
3	D	3401	AOI	C14-C8-C9	4.36	114.79	109.06
3	B	1401	AOI	C14-C8-C9	4.38	114.81	109.06
3	D	3401	AOI	C7-C6-C5	4.68	121.43	111.92
3	C	2401	AOI	C7-C6-C5	4.71	121.48	111.92
3	A	401	AOI	C7-C6-C5	4.75	121.56	111.92
3	B	1401	AOI	C5-C4-C3	4.75	119.99	112.91
3	D	3401	AOI	C5-C4-C3	4.80	120.05	112.91
3	C	2401	AOI	C5-C4-C3	4.81	120.07	112.91
3	B	1401	AOI	C7-C6-C5	4.84	121.75	111.92
3	A	401	AOI	C5-C4-C3	4.95	120.28	112.91
3	D	3401	AOI	C2-C1-C10	5.88	123.34	112.84
3	B	1401	AOI	C2-C1-C10	5.98	123.52	112.84
3	C	2401	AOI	C2-C1-C10	5.99	123.54	112.84
3	A	401	AOI	C2-C1-C10	6.00	123.55	112.84
3	A	401	AOI	C1-C10-C9	6.82	122.44	111.45
3	C	2401	AOI	C1-C10-C9	6.85	122.50	111.45
3	D	3401	AOI	C1-C10-C9	6.86	122.52	111.45
3	B	1401	AOI	C1-C10-C9	6.87	122.53	111.45
3	A	401	AOI	C4-C3-C2	10.98	124.52	110.52
3	D	3401	AOI	C4-C3-C2	11.20	124.80	110.52
3	B	1401	AOI	C4-C3-C2	11.24	124.84	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2401	AOI	C4-C3-C2	11.29	124.92	110.52
3	D	3401	AOI	C4-C5-C10	12.36	126.28	112.66
3	C	2401	AOI	C4-C5-C10	12.42	126.34	112.66
3	A	401	AOI	C4-C5-C10	12.54	126.47	112.66
3	B	1401	AOI	C4-C5-C10	12.55	126.48	112.66

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	401	AOI	C3
3	A	401	AOI	C5
3	B	1401	AOI	C3
3	B	1401	AOI	C5
3	C	2401	AOI	C3
3	C	2401	AOI	C5
3	D	3401	AOI	C3
3	D	3401	AOI	C5

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NAI	1	0
3	A	401	AOI	4	0
2	B	1300	NAI	2	0
3	B	1401	AOI	4	0
2	C	2300	NAI	1	0
3	C	2401	AOI	6	0
2	D	3300	NAI	2	0
3	D	3401	AOI	8	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	244/260 (93%)	-0.41	10 (4%) 41 42	24, 35, 60, 80	0
1	B	244/260 (93%)	-0.56	3 (1%) 81 81	20, 30, 53, 68	0
1	C	244/260 (93%)	-0.51	4 (1%) 74 74	22, 34, 55, 68	0
1	D	244/260 (93%)	-0.36	9 (3%) 45 46	24, 36, 59, 72	0
All	All	976/1040 (93%)	-0.46	26 (2%) 58 57	20, 34, 59, 80	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	7.6
1	C	2	SER	7.3
1	D	2	SER	5.9
1	A	2	SER	5.6
1	A	132	ARG	3.6
1	D	192	ASP	3.1
1	D	52	ALA	2.9
1	A	49	ALA	2.8
1	A	193	TRP	2.8
1	A	192	ASP	2.8
1	D	103	THR	2.7
1	D	45	LYS	2.7
1	B	52	ALA	2.7
1	D	193	TRP	2.7
1	C	132	ARG	2.5
1	C	192	ASP	2.5
1	A	189	PRO	2.4
1	A	99	ASP	2.3
1	A	129	GLU	2.2
1	A	77	THR	2.2
1	C	42	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	131	GLY	2.1
1	A	42	GLU	2.0
1	B	99	ASP	2.0
1	D	99	ASP	2.0
1	D	77	THR	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	AOI	C	2401	21/21	0.49	0.66	15.73	51,52,54,54	21
3	AOI	D	3401	21/21	0.48	0.76	11.96	51,53,54,54	21
3	AOI	B	1401	21/21	0.60	0.67	11.81	52,53,54,58	21
3	AOI	A	401	21/21	0.60	0.71	10.94	49,52,54,54	21
2	NAI	D	3300	44/44	0.94	0.11	-0.11	37,46,50,51	0
2	NAI	A	300	44/44	0.95	0.12	-0.16	38,45,48,52	0
2	NAI	C	2300	44/44	0.97	0.09	-0.52	34,39,44,46	0
2	NAI	B	1300	44/44	0.97	0.09	-0.84	25,30,35,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.