W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2023 – 05:15 PM EDT

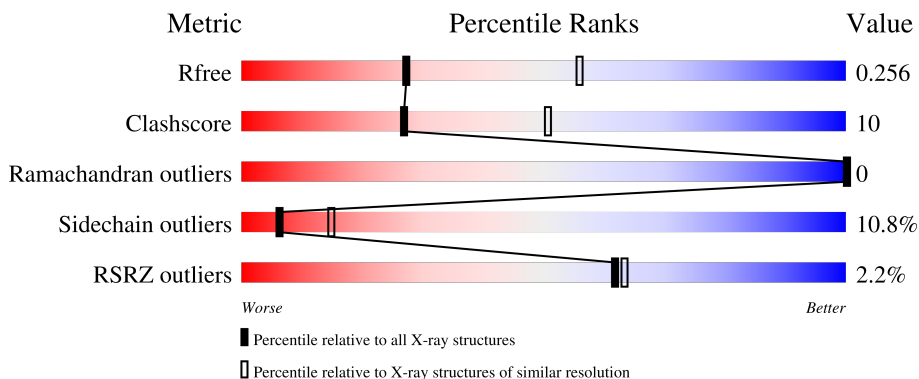|		
PDB ID	:	3VYL
Title	:	Structure of L-ribulose 3-epimerase
Authors	:	Uechi, K.; Sakuraba, H.; Takata, G.
Deposited on	:	2012-09-27
Resolution	:	2.70 Å(reported)

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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 2.70 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.
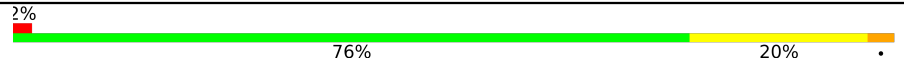
Metric	Percentile Ranks	Value
Rfree		0.256
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		10.8%
RSRZ outliers		2.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	297	77% 18% 5%
1	B	297	82% 15% •
1	C	297	80% 16% •
1	D	297	80% 16% •
1	E	297	76% 20% •

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Mol	Chain	Length	Quality of chain
1	F	297	2% 76% 20%
1	G	297	8% 72% 24%
1	H	297	6% 74% 22%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 18302 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 L-ribulose 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	B	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	C	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	D	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	E	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	F	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	G	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	H	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total　Mn 1　　1	0	0
2	H	1	Total　Mn 1　　1	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
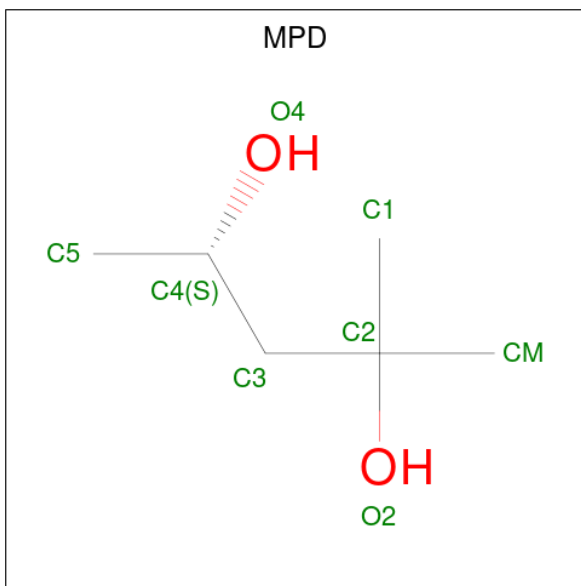
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total　C　O 8　　6　2	0	0
3	B	1	Total　C　O 8　　6　2	0	0
3	D	1	Total　C　O 8　　6　2	0	0
3	E	1	Total　C　O 8　　6　2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	58	Total　O 58　　58	0	0
4	B	60	Total　O 60　　60	0	0
4	C	64	Total　O 64　　64	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	72	Total 72	O 72	0	0
4	E	29	Total 29	O 29	0	0
4	F	11	Total 11	O 11	0	0
4	G	11	Total 11	O 11	0	0
4	H	21	Total 21	O 21	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 vi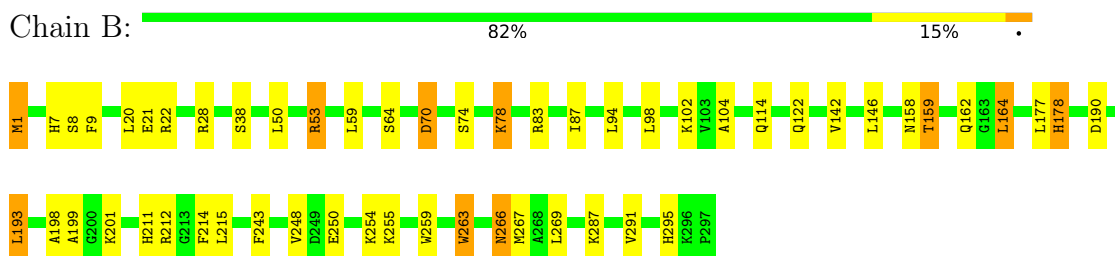ew annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.
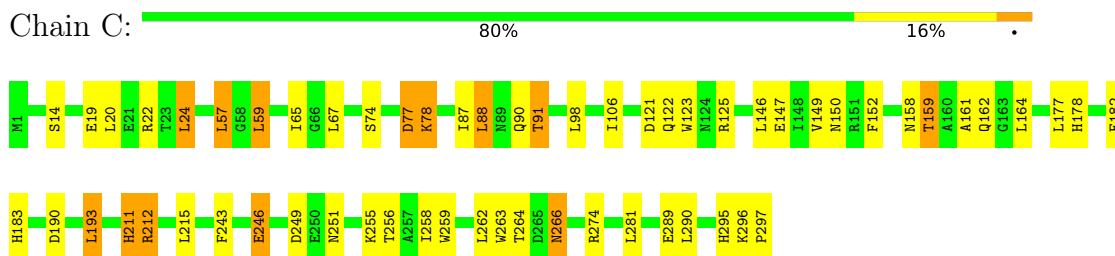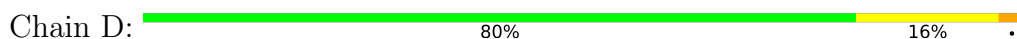
• Molecule 1: L-ribulose 3-epimerase

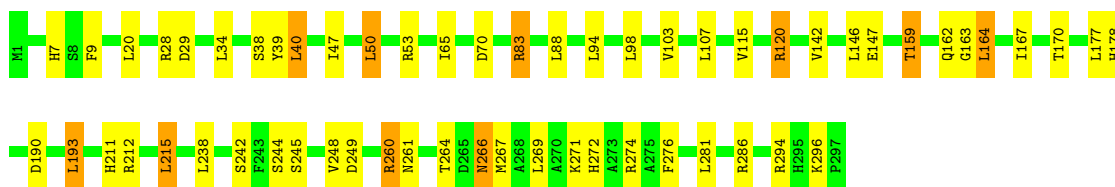Chain A:

• Molecule 1: L-ribulose 3-epimerase

Chain B:

• Molecule 1: L-ribulose 3-epimerase

Chain C:

• Molecule 1: L-ribulose 3-epimerase

Chain D:

M1 H7 S8 F9 L20 R28 D29 L34 S38 Y39 L40 I47 L50 R53 I65 D70 R83 L88 L94 L98 V103 L107 V115 R120 V142 L146 E147 T159 Q162 G163 L164 I167 T170 L177 H178

D190 L193 H211 R212 L215 L238 S242 F243 S244 S245 V248 D249 R260 N261 T264 D265 N266 M267 A268 L269 A270 K271 H272 A273 R274 A275 F276 L281 R286 R294 H295 K296 P297

• Molecule 1: L-ribulose 3-epimerase

Chain E:　76%　20%

M1 A2 R3 H7 V10 S14 E19 D33 S38 P42 A43 D44 R49 L50 L57 G58 L59 S64 L67 S74 D77 V80 R83 L88 L94 K102 V103 I106 L107 S108 A109 G110 H111 E116 D121 Q122 W123 N124 R125

A137 V142 E147 I148 V149 E153 S154 N155 N158 T159 A160 A161 Q162 G163 L164 I167 T170 L177 H178 H183 D190 L193 G203 L215 F240 S245 E246 D249 E250 S253 K254 K255 W259 R260 N261 L262 W263 T264 D265 N266 M267

L279 R285 P297

• Molecule 1: L-ribulose 3-epimerase

Chain F:　76%　20%

M1 A2 R3 I4 G5 I6 H7 S8 F9 V10 W11 E21 L24 R28 L34 Y39 K52 R53 D56 L57 G58 L59 I65 G66 A69 D70 S74 S75 A76 D77 K78 A79 R83 L94 T95 R96 D97 L98 K102 V103 A104 G105 I106 L107 S108 H111

Q114 P118 T119 R120 D121 R125 S126 L146 E147 N155 T159 A160 A161 L164 L177 H178 H179 D180 T181 F182 H183 M184 D190 V191 G192 L193 Y204 G208 E209 S210 H211 R212 L215 I220 D221 F222 D237 L238 S253 K254 K255 W259 L262

W263 N266 K296 P297

• Molecule 1: L-ribulose 3-epimerase

Chain G:　72%　24%

M1 A2 R3 S18 E21 T27 R28 D29 A30 G31 F32 D33 Y39 L40 D41 P42 A43 D44 V45 D46 I47 G48 R49 L50 A51 K52 R53 I54 A55 D56 L57 G58 L59 G60 S64 L67 D72 I73 S74 S75 A76 D77 K78 A79 V80 G84 T95 R96 D97 R101

A104 G105 I106 L107 H111 G112 L113 Q114 V115 E116 A117 P118 D121 Q122 W123 E147 I148 V149 N150 R151 F152 N155 N158 T159 Q162 G163 L164 I167 I175 F176 L177 H178 H183 D190 L193 E209 S210 H211 R212 L215 D236 D237 F240

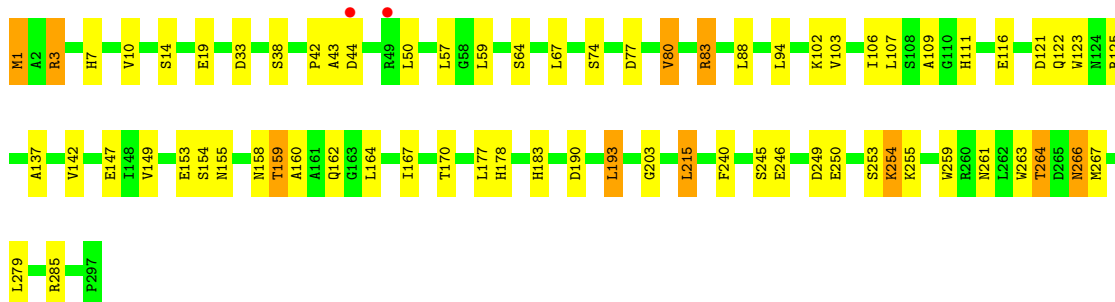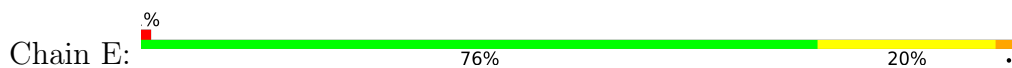F243 S244 S245 E246 I247 V248 D249 E250 K254 K255 I258 W259 R260 N261 L262 W263 T264 D265 N266 M267 A268 R274 L290 V291 S292 A293 R294 H295 K296 P297

• Molecule 1: L-ribulose 3-epimerase

Chain H:

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	202.51Å 206.23Å 121.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.48 – 2.70 34.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.48-2.70) 99.6 (34.48-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.16 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.264 0.202 , 0.256	Depositor DCC
R_{free} test set	3536 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18302	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MN, MPD

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	0.67	2/2278 (0.1%)	0.66	0/3082
1	B	0.68	2/2278 (0.1%)	0.66	0/3082
1	C	0.66	1/2278 (0.0%)	0.67	0/3082
1	D	0.72	0/2278	0.65	0/3082
1	E	0.69	1/2278 (0.0%)	0.64	0/3082
1	F	0.65	3/2278 (0.1%)	0.65	0/3082
1	G	0.68	2/2278 (0.1%)	0.67	0/3082
1	H	0.67	2/2278 (0.1%)	0.64	1/3082 (0.0%)
All	All	0.68	13/18224 (0.1%)	0.66	1/24656 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	259	TRP	CD2-CE2	5.42	1.47	1.41
1	F	259	TRP	CD2-CE2	5.40	1.47	1.41
1	A	263	TRP	CD2-CE2	5.37	1.47	1.41
1	H	123	TRP	CD2-CE2	5.32	1.47	1.41
1	A	153	GLU	CD-OE1	-5.31	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	11	TRP	N-CA-C	5.38	125.53	111.00

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	2242	0	2229	64	0
1	B	2242	0	2229	32	0
1	C	2242	0	2229	44	0
1	D	2242	0	2229	34	0
1	E	2242	0	2229	48	0
1	F	2242	0	2229	50	0
1	G	2242	0	2229	63	0
1	H	2242	0	2229	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
3	D	8	0	14	1	0
3	E	8	0	14	1	0
4	A	58	0	0	0	0
4	B	60	0	0	1	0
4	C	64	0	0	1	0
4	D	72	0	0	0	0
4	E	29	0	0	1	0
4	F	11	0	0	0	0
4	G	11	0	0	0	0
4	H	21	0	0	0	0
All	All	18302	0	17888	367	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 10.

The worst 5 of 367 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:C:78:LYS:H	1:C:78:LYS:CD	1.50	1.18
1:G:3:ARG:HH21	1:G:60:GLY:CA	1.56	1.17
1:C:78:LYS:HD2	1:C:78:LYS:N	1.51	1.15
1:D:39:TYR:O	1:D:40:LEU:HD13	1.48	1.10
1:F:53:ARG:HG3	1:F:53:ARG:HH11	1.00	1.09

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/297 (99%)	292 (99%)	3 (1%)	0	100	100
1	B	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
1	C	295/297 (99%)	289 (98%)	6 (2%)	0	100	100
1	D	295/297 (99%)	293 (99%)	2 (1%)	0	100	100
1	E	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	F	295/297 (99%)	290 (98%)	5 (2%)	0	100	100
1	G	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	H	295/297 (99%)	287 (97%)	8 (3%)	0	100	100
All	All	2360/2376 (99%)	2318 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	225/225 (100%)	198 (88%)	27 (12%)	5	11
1	B	225/225 (100%)	200 (89%)	25 (11%)	6	14
1	C	225/225 (100%)	202 (90%)	23 (10%)	7	17
1	D	225/225 (100%)	199 (88%)	26 (12%)	5	12
1	E	225/225 (100%)	208 (92%)	17 (8%)	13	30
1	F	225/225 (100%)	205 (91%)	20 (9%)	9	22
1	G	225/225 (100%)	197 (88%)	28 (12%)	4	11
1	H	225/225 (100%)	197 (88%)	28 (12%)	4	11
All	All	1800/1800 (100%)	1606 (89%)	194 (11%)	6	15

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	264	THR
1	G	46	ASP
1	F	24	LEU
1	F	146	LEU
1	G	114	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	272	HIS
1	H	7	HIS
1	H	211	HIS
1	C	158	ASN
1	C	150	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	MPD	A	1002	-	7,7,7	0.20	0	9,10,10	0.31	0
3	MPD	D	1002	-	7,7,7	0.27	0	9,10,10	0.54	0
3	MPD	E	1002	-	7,7,7	0.26	0	9,10,10	0.35	0
3	MPD	B	1002	-	7,7,7	0.38	0	9,10,10	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
3	MPD	A	1002	-	-	4/5/5/5	-
3	MPD	D	1002	-	-	5/5/5/5	-
3	MPD	E	1002	-	-	0/5/5/5	-
3	MPD	B	1002	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1002	MPD	C2-C3-C4-C5
3	B	1002	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	D	1002	MPD	O2-C2-C3-C4
3	A	1002	MPD	C2-C3-C4-C5
3	A	1002	MPD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1002	MPD	1	0
3	E	1002	MPD	1	0
3	B	1002	MPD	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	297/297 (100%)	-0.32	0	100	100	19, 36, 60, 79	0
1	B	297/297 (100%)	-0.29	0	100	100	18, 36, 60, 87	0
1	C	297/297 (100%)	-0.40	0	100	100	20, 33, 52, 65	0
1	D	297/297 (100%)	-0.50	0	100	100	18, 31, 58, 78	0
1	E	297/297 (100%)	-0.24	2 (0%)	87	89	26, 44, 72, 92	0
1	F	297/297 (100%)	-0.05	7 (2%)	59	60	26, 49, 72, 96	0
1	G	297/297 (100%)	0.55	24 (8%)	12	10	38, 67, 100, 130	0
1	H	297/297 (100%)	0.30	19 (6%)	19	18	36, 59, 99, 123	0
All	All	2376/2376 (100%)	-0.12	52 (2%)	62	63	18, 43, 84, 130	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	39	TYR	6.1
1	G	40	LEU	5.7
1	G	1	MET	5.6
1	H	39	TYR	5.5
1	H	42	PRO	4.6

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th 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	B-factors($Å^2$)	Q<0.9
3	MPD	B	1002	8/8	0.79	0.25	46,50,53,56	0
3	MPD	D	1002	8/8	0.81	0.25	62,66,76,80	0
3	MPD	A	1002	8/8	0.86	0.23	59,61,67,70	0
3	MPD	E	1002	8/8	0.88	0.21	57,60,64,68	0
2	MN	E	1001	1/1	0.97	0.17	33,33,33,33	0
2	MN	G	1001	1/1	0.98	0.14	50,50,50,50	0
2	MN	H	1001	1/1	0.98	0.10	43,43,43,43	0
2	MN	C	1001	1/1	0.99	0.16	26,26,26,26	0
2	MN	D	1001	1/1	0.99	0.16	22,22,22,22	0
2	MN	A	1001	1/1	0.99	0.15	21,21,21,21	0
2	MN	F	1001	1/1	0.99	0.18	41,41,41,41	0
2	MN	B	1001	1/1	0.99	0.14	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.