



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:04 PM GMT

PDB ID : 3VZ0  
Title : Structural insights into cofactor and substrate selection by Gox0499  
Authors : Yuan, Y.A.; Yuan, Z.; Yin, B.; Wei, D.  
Deposited on : 2012-10-09  
Resolution : 2.30 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

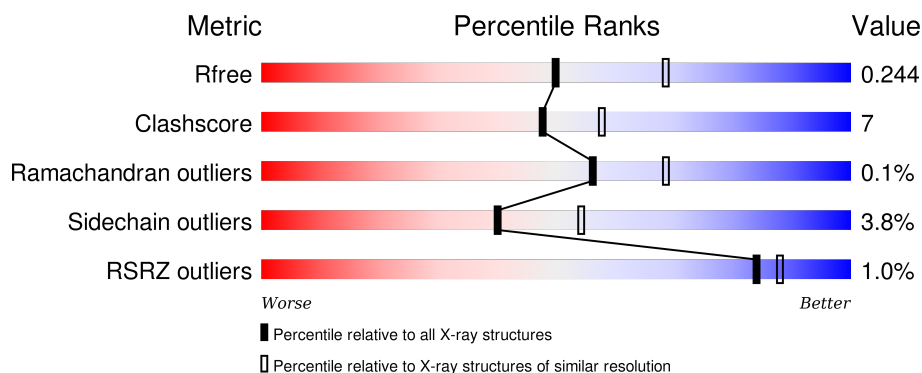
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	459	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	459	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	459	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	459	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2PE	A	501	-	-	-	X
2	2PE	C	501	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14671 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.

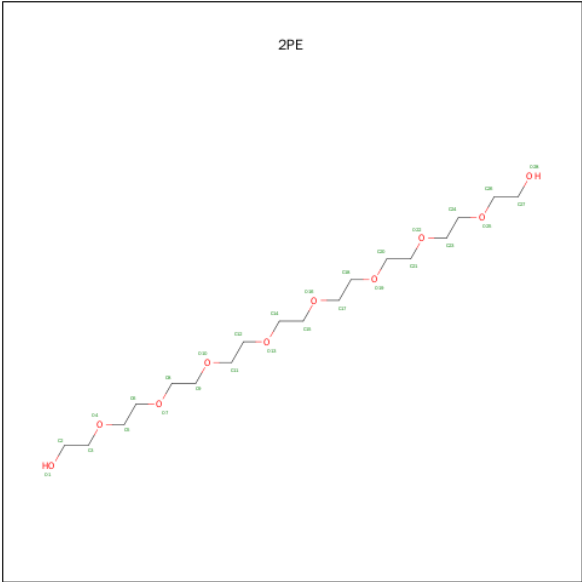
- Molecule 1 is a protein called Putative NAD-dependent aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	Se	0	0	0
			3498	2217	612	655	3	11			
1	B	456	Total	C	N	O	S	Se	0	0	0
			3498	2217	612	655	3	11			
1	C	456	Total	C	N	O	S	Se	0	0	0
			3498	2217	612	655	3	11			
1	D	456	Total	C	N	O	S	Se	0	0	0
			3498	2217	612	655	3	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q5FTL8
A	-1	SER	-	EXPRESSION TAG	UNP Q5FTL8
A	0	HIS	-	EXPRESSION TAG	UNP Q5FTL8
B	-2	GLY	-	EXPRESSION TAG	UNP Q5FTL8
B	-1	SER	-	EXPRESSION TAG	UNP Q5FTL8
B	0	HIS	-	EXPRESSION TAG	UNP Q5FTL8
C	-2	GLY	-	EXPRESSION TAG	UNP Q5FTL8
C	-1	SER	-	EXPRESSION TAG	UNP Q5FTL8
C	0	HIS	-	EXPRESSION TAG	UNP Q5FTL8
D	-2	GLY	-	EXPRESSION TAG	UNP Q5FTL8
D	-1	SER	-	EXPRESSION TAG	UNP Q5FTL8
D	0	HIS	-	EXPRESSION TAG	UNP Q5FTL8

- Molecule 2 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	18	10		
2	B	1	Total	C	O	0	0
			28	18	10		
2	C	1	Total	C	O	0	0
			28	18	10		
2	D	1	Total	C	O	0	0
			28	18	10		

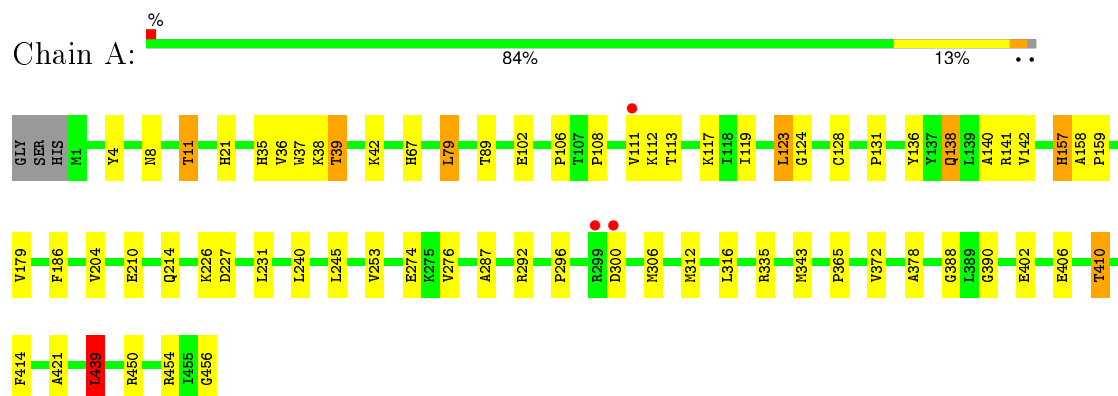
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	131	Total	O	0	0
			131	131		
3	C	112	Total	O	0	0
			112	112		
3	D	142	Total	O	0	0
			142	142		

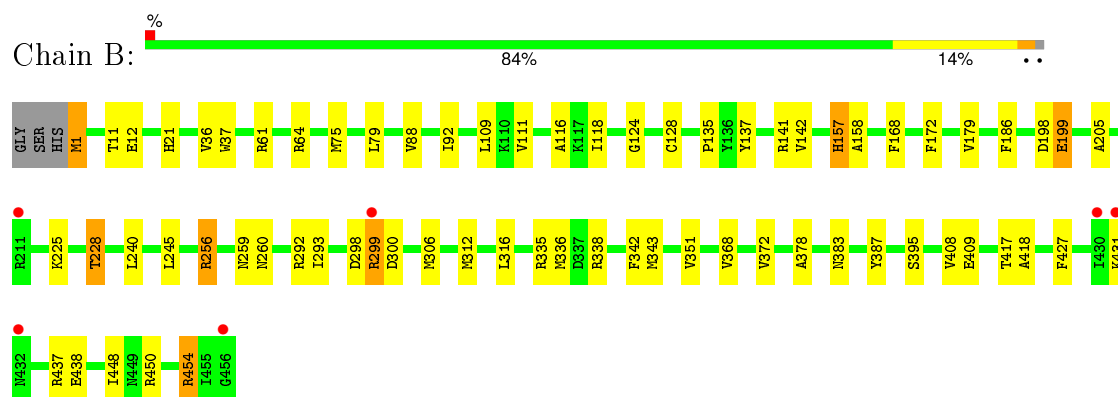
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

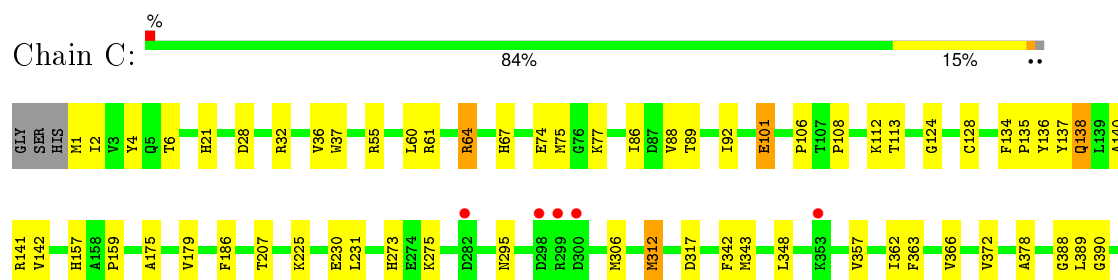
- Molecule 1: Putative NAD-dependent aldehyde dehydrogenase



- Molecule 1: Putative NAD-dependent aldehyde dehydrogenase

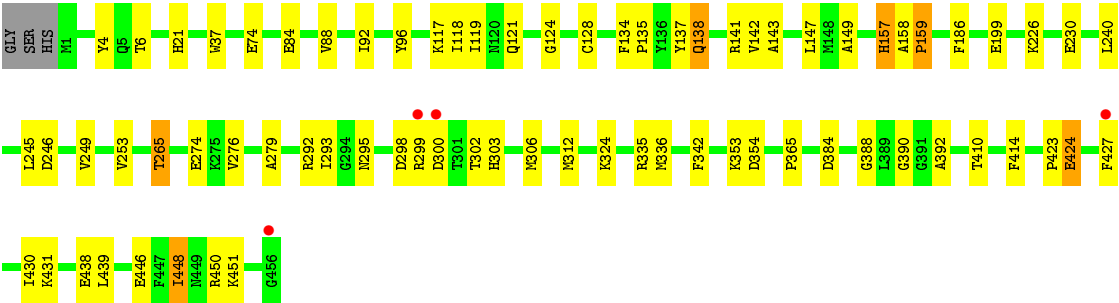
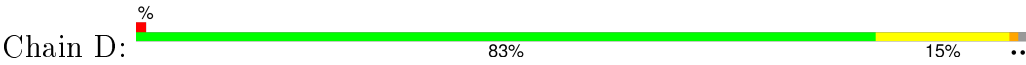


- Molecule 1: Putative NAD-dependent aldehyde dehydrogenase





● Molecule 1: Putative NAD-dependent aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.52Å 254.60Å 76.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.30 48.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.49-2.30) 99.8 (48.49-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.45 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.244 0.187 , 0.244	Depositor DCC
$R_{free}$ test set	4084 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 81596 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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: 2PE

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	0.65	2/3556 (0.1%)	0.67	1/4803 (0.0%)
1	B	0.58	0/3556	0.65	0/4803
1	C	0.54	0/3556	0.64	0/4803
1	D	0.60	0/3556	0.66	0/4803
All	All	0.59	2/14224 (0.0%)	0.66	1/19212 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	GLY	C-O	12.81	1.44	1.23
1	A	456	GLY	CA-C	9.42	1.67	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	GLY	CA-C-O	-9.42	103.64	120.60

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	3498	0	3502	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3498	0	3502	61	0
1	C	3498	0	3502	43	0
1	D	3498	0	3502	58	0
2	A	28	0	38	3	0
2	B	28	0	38	1	0
2	C	28	0	38	4	0
2	D	28	0	38	3	0
3	A	182	0	0	1	0
3	B	131	0	0	0	0
3	C	112	0	0	1	0
3	D	142	0	0	2	0
All	All	14671	0	14160	209	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 (209) 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:128:CYS:SG	1:C:142:VAL:HG11	1.73	1.28
1:D:128:CYS:SG	1:D:142:VAL:HG11	1.81	1.21
1:A:128:CYS:SG	1:A:142:VAL:HG11	1.86	1.15
1:B:293:ILE:HG21	1:B:336:MSE:HE1	1.40	0.99
1:C:21:HIS:HD2	1:C:186:PHE:H	1.12	0.96
1:A:141:ARG:HG3	1:A:439:LEU:HD13	1.47	0.96
1:D:117:LYS:HE3	1:D:119:ILE:HD11	1.49	0.95
1:D:128:CYS:SG	1:D:142:VAL:CG1	2.59	0.91
1:B:21:HIS:HD2	1:B:186:PHE:H	1.12	0.90
1:A:11:THR:HG21	3:A:629:HOH:O	1.71	0.89
1:D:21:HIS:HD2	1:D:186:PHE:H	1.18	0.89
1:A:128:CYS:SG	1:A:142:VAL:CG1	2.62	0.87
1:C:128:CYS:SG	1:C:142:VAL:CG1	2.62	0.86
1:A:21:HIS:HD2	1:A:186:PHE:H	1.22	0.84
1:B:312:MSE:HE1	1:B:335:ARG:HG3	1.59	0.84
1:D:390:GLY:O	1:D:410:THR:HG21	1.78	0.83
1:D:149:ALA:HB1	1:D:448:ILE:HD11	1.59	0.82
1:A:108:PRO:HB2	1:C:108:PRO:HB2	1.62	0.82
1:B:306:MSE:CG	1:B:343:MSE:HE3	2.10	0.80
1:B:135:PRO:O	1:B:157:HIS:HE1	1.64	0.80
1:C:21:HIS:CD2	1:C:186:PHE:H	2.00	0.78
1:B:336:MSE:HE2	1:B:343:MSE:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:VAL:HG11	1:B:454:ARG:HH12	1.50	0.77
1:C:312:MSE:CE	1:C:343:MSE:HB2	2.14	0.77
1:B:260:ASN:HB3	1:B:306:MSE:HE1	1.67	0.77
1:D:245:LEU:HD13	1:D:276:VAL:HB	1.67	0.75
1:A:312:MSE:HE1	1:A:335:ARG:HG3	1.69	0.75
1:B:306:MSE:HG3	1:B:343:MSE:CE	2.17	0.74
1:B:306:MSE:SE	1:B:343:MSE:HE3	2.37	0.74
1:D:312:MSE:HE1	1:D:335:ARG:CG	2.19	0.73
1:B:61:ARG:O	1:B:64:ARG:HG3	1.89	0.72
1:D:312:MSE:HE1	1:D:335:ARG:HG2	1.72	0.71
1:B:383:ASN:HD21	1:B:409:GLU:H	1.39	0.71
1:C:312:MSE:HE2	1:C:343:MSE:HB2	1.72	0.70
1:B:79:LEU:HD23	1:B:299:ARG:HG3	1.73	0.70
1:A:390:GLY:O	1:A:410:THR:HG21	1.92	0.69
1:B:21:HIS:CD2	1:B:186:PHE:H	2.03	0.69
1:D:312:MSE:CE	1:D:342:PHE:O	2.41	0.69
1:D:312:MSE:HE3	1:D:342:PHE:O	1.94	0.69
1:B:312:MSE:HA	1:B:343:MSE:HE2	1.76	0.67
1:B:417:THR:HG22	1:B:418:ALA:O	1.94	0.67
1:C:138:GLN:HE22	1:C:141:ARG:HH21	1.40	0.67
1:D:427:PHE:CD2	2:D:501:2PE:H272	2.30	0.67
1:B:256:ARG:HD2	1:B:256:ARG:O	1.95	0.67
1:B:141:ARG:HD3	1:B:438:GLU:OE2	1.94	0.66
1:D:312:MSE:CE	1:D:335:ARG:HG3	2.26	0.66
1:B:383:ASN:ND2	1:B:409:GLU:H	1.94	0.65
1:C:273:HIS:HD2	1:C:275:LYS:H	1.43	0.65
1:C:295:ASN:HB3	3:C:618:HOH:O	1.98	0.64
1:A:102:GLU:HG3	1:C:112:LYS:HE2	1.78	0.64
1:B:199:GLU:H	1:B:199:GLU:CD	2.00	0.64
1:D:353:LYS:HE3	1:D:384:ASP:OD2	1.99	0.63
1:A:388:GLY:C	1:A:410:THR:HG22	2.18	0.63
1:D:427:PHE:HD2	2:D:501:2PE:H272	1.63	0.62
1:D:292:ARG:NE	1:D:300:ASP:O	2.32	0.62
1:B:111:VAL:HG11	1:B:454:ARG:NH1	2.13	0.62
1:B:306:MSE:SE	1:B:343:MSE:CE	2.96	0.62
1:D:141:ARG:HG2	1:D:439:LEU:HD21	1.83	0.61
1:B:75:MSE:HE1	1:B:259:ASN:HD21	1.65	0.61
1:D:121:GLN:HE22	1:D:451:LYS:NZ	1.99	0.61
1:D:312:MSE:HE3	1:D:342:PHE:C	2.21	0.61
1:C:421:ALA:HA	2:C:501:2PE:H271	1.82	0.60
1:C:61:ARG:O	1:C:64:ARG:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:MSE:HE1	1:A:335:ARG:CG	2.32	0.60
1:A:21:HIS:CD2	1:A:186:PHE:H	2.12	0.59
1:D:21:HIS:CD2	1:D:186:PHE:H	2.09	0.59
1:A:35:HIS:CE1	1:A:39:THR:HG21	2.38	0.59
1:C:390:GLY:O	1:C:410:THR:HG21	2.02	0.58
1:C:1:MSE:HG2	1:C:2:ILE:H	1.67	0.58
1:D:149:ALA:CB	1:D:448:ILE:HD11	2.32	0.58
1:B:312:MSE:HE1	1:B:335:ARG:CG	2.31	0.57
1:D:138:GLN:HA	1:D:138:GLN:HE21	1.69	0.57
1:A:35:HIS:O	1:A:39:THR:HB	2.03	0.57
1:A:117:LYS:HE3	1:A:119:ILE:HD11	1.86	0.57
1:C:427:PHE:CD1	2:C:501:2PE:H272	2.39	0.57
1:A:111:VAL:HG12	1:A:113:THR:H	1.70	0.56
1:D:312:MSE:HE1	1:D:335:ARG:HG3	1.86	0.56
1:A:141:ARG:HG3	1:A:439:LEU:CD1	2.29	0.56
1:D:312:MSE:CE	1:D:335:ARG:CG	2.84	0.56
1:A:8:ASN:HB3	1:A:11:THR:HG22	1.87	0.56
1:A:421:ALA:HB2	2:A:501:2PE:H231	1.86	0.56
1:A:123:LEU:HD21	1:A:226:LYS:HE3	1.89	0.55
1:B:306:MSE:CG	1:B:343:MSE:CE	2.78	0.55
1:B:128:CYS:SG	1:B:142:VAL:HG11	2.47	0.55
1:B:293:ILE:HG21	1:B:336:MSE:CE	2.26	0.55
1:D:135:PRO:O	1:D:157:HIS:HE1	1.91	0.54
1:A:157:HIS:CD2	1:A:158:ALA:H	2.26	0.54
1:D:149:ALA:HB1	1:D:448:ILE:CD1	2.35	0.54
1:A:421:ALA:HA	2:A:501:2PE:H271	1.88	0.54
1:C:36:VAL:HG21	1:C:179:VAL:O	2.08	0.54
1:B:198:ASP:O	1:B:225:LYS:NZ	2.42	0.53
1:B:205:ALA:HA	1:B:228:THR:HG22	1.89	0.53
1:A:38:LYS:HA	1:A:42:LYS:HD3	1.90	0.53
1:D:388:GLY:C	1:D:410:THR:HG22	2.28	0.53
1:A:421:ALA:CA	2:A:501:2PE:H271	2.38	0.53
1:D:293:ILE:HD13	1:D:336:MSE:HE1	1.89	0.53
1:D:295:ASN:HB2	3:D:715:HOH:O	2.08	0.53
1:A:36:VAL:HG21	1:A:179:VAL:O	2.08	0.53
1:B:306:MSE:HG3	1:B:343:MSE:HE3	1.76	0.52
1:B:260:ASN:CB	1:B:306:MSE:HE1	2.39	0.52
1:D:199:GLU:HG2	3:D:694:HOH:O	2.09	0.52
1:D:121:GLN:NE2	1:D:451:LYS:HE3	2.25	0.52
1:A:316:LEU:HD23	1:A:343:MSE:HE3	1.92	0.52
1:B:336:MSE:HE2	1:B:343:MSE:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:CD2	1:D:279:ALA:HB1	2.40	0.51
1:B:88:VAL:O	1:B:92:ILE:HG12	2.10	0.51
1:C:388:GLY:HA2	1:C:410:THR:HG22	1.92	0.51
1:C:312:MSE:HE1	1:C:342:PHE:C	2.31	0.51
1:C:92:ILE:HD12	1:C:439:LEU:HD22	1.92	0.51
1:B:312:MSE:HG3	1:B:343:MSE:HE2	1.93	0.51
1:A:157:HIS:HD2	1:A:158:ALA:H	1.59	0.50
1:A:402:GLU:O	1:A:406:GLU:HG3	2.11	0.50
1:C:135:PRO:O	1:C:157:HIS:HE1	1.94	0.50
1:D:312:MSE:HE1	1:D:342:PHE:O	2.12	0.50
1:C:67:HIS:HD2	1:C:136:TYR:OH	1.94	0.50
1:A:138:GLN:HE22	1:A:141:ARG:NH2	2.10	0.50
1:B:109:LEU:HD21	1:B:118:ILE:HD12	1.94	0.50
1:B:312:MSE:HA	1:B:343:MSE:CE	2.42	0.49
1:A:4:TYR:CD1	1:A:159:PRO:HA	2.47	0.49
1:A:388:GLY:CA	1:A:410:THR:HG22	2.43	0.49
1:C:134:PHE:O	1:C:138:GLN:HG2	2.13	0.49
1:A:372:VAL:HG21	1:A:378:ALA:HB2	1.94	0.49
1:C:421:ALA:CA	2:C:501:2PE:H271	2.42	0.49
1:C:426:PRO:HG3	1:D:118:ILE:HD11	1.95	0.48
1:C:60:LEU:HD22	1:C:86:ILE:HG23	1.95	0.48
1:D:306:MSE:SE	1:D:365:PRO:HD3	2.64	0.48
1:C:4:TYR:CD1	1:C:159:PRO:HA	2.49	0.48
1:A:89:THR:HG23	1:A:140:ALA:HB2	1.95	0.47
1:A:388:GLY:HA2	1:A:410:THR:HG22	1.96	0.47
1:A:312:MSE:HE2	1:A:316:LEU:HD11	1.97	0.47
1:A:112:LYS:HB2	1:C:101:GLU:HG2	1.96	0.47
1:D:245:LEU:CD2	1:D:279:ALA:CB	2.93	0.47
1:B:1:MSE:HE2	1:B:1:MSE:O	2.15	0.47
1:D:37:TRP:CE2	1:D:124:GLY:HA2	2.49	0.47
1:B:36:VAL:HG21	1:B:179:VAL:O	2.15	0.46
1:A:414:PHE:CD2	1:B:454:ARG:HG3	2.50	0.46
1:A:312:MSE:HE1	1:A:335:ARG:CB	2.46	0.46
1:C:88:VAL:O	1:C:92:ILE:HG12	2.14	0.46
1:A:210:GLU:O	1:A:214:GLN:HG3	2.14	0.46
1:A:450:ARG:O	1:B:437:ARG:NH1	2.48	0.46
1:B:312:MSE:CG	1:B:343:MSE:HE2	2.45	0.46
1:A:106:PRO:O	1:A:108:PRO:HD3	2.15	0.46
1:B:312:MSE:HE2	1:B:316:LEU:HD11	1.98	0.46
1:D:4:TYR:CD1	1:D:159:PRO:HA	2.50	0.46
1:B:298:ASP:HB3	1:B:300:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:MSE:SE	1:C:77:LYS:HB2	2.66	0.45
1:D:121:GLN:HE21	1:D:451:LYS:HE3	1.81	0.45
1:D:430:ILE:HG13	1:D:431:LYS:HG3	1.97	0.45
1:B:336:MSE:CE	1:B:343:MSE:O	2.59	0.45
1:A:67:HIS:HD2	1:A:136:TYR:OH	2.00	0.45
1:D:157:HIS:HD2	1:D:158:ALA:H	1.65	0.45
1:B:240:LEU:HD12	1:B:395:SER:HB2	1.99	0.45
1:C:55:ARG:HD2	1:C:175:ALA:O	2.16	0.45
1:A:292:ARG:NE	1:A:300:ASP:O	2.47	0.45
1:B:135:PRO:O	1:B:157:HIS:CE1	2.55	0.44
1:B:312:MSE:CE	1:B:342:PHE:O	2.66	0.44
1:C:37:TRP:CE2	1:C:124:GLY:HA2	2.53	0.44
1:B:168:PHE:CE2	1:B:172:PHE:HE2	2.36	0.44
1:D:88:VAL:O	1:D:92:ILE:HG12	2.18	0.44
1:B:37:TRP:CE2	1:B:124:GLY:HA2	2.53	0.44
1:B:372:VAL:HG21	1:B:378:ALA:HB2	1.99	0.43
1:A:312:MSE:HE3	1:A:343:MSE:HB2	1.99	0.43
1:A:204:VAL:O	1:A:227:ASP:HA	2.18	0.43
1:C:312:MSE:HE3	1:C:312:MSE:HB2	1.78	0.43
1:A:131:PRO:HD2	1:A:138:GLN:HG3	2.01	0.43
1:D:265:THR:O	1:D:265:THR:HG23	2.18	0.43
1:C:89:THR:HG23	1:C:140:ALA:HB2	2.00	0.43
1:D:6:THR:HG23	1:D:74:GLU:HG2	2.01	0.43
1:D:134:PHE:O	1:D:138:GLN:HG2	2.20	0.42
1:D:134:PHE:CE1	2:D:501:2PE:H202	2.55	0.42
1:D:96:TYR:OH	1:D:439:LEU:HA	2.20	0.42
1:D:128:CYS:HG	1:D:142:VAL:CG1	2.31	0.42
1:A:138:GLN:HE22	1:A:141:ARG:CZ	2.31	0.42
1:B:111:VAL:HG21	1:B:116:ALA:HB3	2.02	0.42
1:B:448:ILE:HD11	1:B:450:ARG:HD3	2.01	0.42
1:C:362:ILE:HG21	1:C:366:VAL:HB	2.01	0.42
1:D:424:GLU:CD	1:D:424:GLU:H	2.22	0.42
1:C:6:THR:HG23	1:C:74:GLU:HG2	2.01	0.42
1:C:372:VAL:HG21	1:C:378:ALA:HB2	2.02	0.42
1:C:306:MSE:HG3	1:C:312:MSE:HB2	2.00	0.42
1:C:427:PHE:CE1	2:C:501:2PE:H272	2.55	0.42
1:A:245:LEU:HD11	1:A:276:VAL:HB	2.01	0.42
1:B:11:THR:O	1:B:12:GLU:HB2	2.19	0.42
1:C:106:PRO:O	1:C:108:PRO:HD3	2.20	0.41
1:C:435:PHE:HB2	1:D:226:LYS:HE2	2.01	0.41
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:VAL:O	1:D:253:VAL:HG23	2.20	0.41
1:A:306:MSE:SE	1:A:365:PRO:HD3	2.70	0.41
1:B:79:LEU:CD2	1:B:299:ARG:HG3	2.48	0.41
1:D:92:ILE:HD13	1:D:423:PRO:HG3	2.03	0.41
1:B:351:VAL:HG21	1:B:368:VAL:HG13	2.02	0.41
1:B:383:ASN:HD21	1:B:408:VAL:HA	1.86	0.41
1:C:28:ASP:HB3	1:C:32:ARG:NH2	2.36	0.41
1:B:292:ARG:NH1	1:B:300:ASP:O	2.50	0.41
1:A:253:VAL:HG21	1:A:287:ALA:CB	2.50	0.41
1:B:427:PHE:CE2	2:B:501:2PE:H272	2.55	0.41
1:B:306:MSE:SE	1:B:343:MSE:HE1	2.70	0.41
1:D:245:LEU:HD21	1:D:279:ALA:CB	2.51	0.41
1:B:387:TYR:O	1:B:431:LYS:HD2	2.20	0.41
1:D:302:THR:OG1	1:D:303:HIS:HD2	2.03	0.41
1:C:207:THR:HA	1:C:230:GLU:O	2.20	0.41
1:D:128:CYS:HG	1:D:142:VAL:HG11	1.77	0.41
1:D:392:ALA:HA	1:D:414:PHE:O	2.20	0.40
1:A:37:TRP:CE2	1:A:124:GLY:HA2	2.56	0.40
1:B:157:HIS:HD2	1:B:158:ALA:H	1.69	0.40
1:D:121:GLN:NE2	1:D:451:LYS:CE	2.84	0.40
1:A:138:GLN:HE21	1:A:138:GLN:HA	1.87	0.40
1:A:79:LEU:HB2	1:A:296:PRO:O	2.22	0.40
1:D:143:ALA:O	1:D:147:LEU:HB2	2.21	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	454/459 (99%)	438 (96%)	14 (3%)	2 (0%)	39 48
1	B	454/459 (99%)	439 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	454/459 (99%)	438 (96%)	16 (4%)	0	100	100
1	D	454/459 (99%)	439 (97%)	15 (3%)	0	100	100
All	All	1816/1836 (99%)	1754 (97%)	60 (3%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	GLU
1	A	439	LEU

### 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	359/350 (103%)	348 (97%)	11 (3%)	47	64
1	B	359/350 (103%)	349 (97%)	10 (3%)	51	68
1	C	359/350 (103%)	344 (96%)	15 (4%)	36	49
1	D	359/350 (103%)	340 (95%)	19 (5%)	28	37
All	All	1436/1400 (103%)	1381 (96%)	55 (4%)	40	54

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	39	THR
1	A	79	LEU
1	A	123	LEU
1	A	138	GLN
1	A	157	HIS
1	A	231	LEU
1	A	240	LEU
1	A	410	THR
1	A	439	LEU

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Mol	Chain	Res	Type
1	A	454	ARG
1	B	1	MSE
1	B	137	TYR
1	B	157	HIS
1	B	199	GLU
1	B	228	THR
1	B	245	LEU
1	B	256	ARG
1	B	299	ARG
1	B	338	ARG
1	B	454	ARG
1	C	64	ARG
1	C	101	GLU
1	C	113	THR
1	C	137	TYR
1	C	138	GLN
1	C	225	LYS
1	C	231	LEU
1	C	312	MSE
1	C	317	ASP
1	C	348	LEU
1	C	357	VAL
1	C	363	PHE
1	C	389	LEU
1	C	448	ILE
1	C	454	ARG
1	D	84	GLU
1	D	137	TYR
1	D	138	GLN
1	D	157	HIS
1	D	159	PRO
1	D	230	GLU
1	D	240	LEU
1	D	246	ASP
1	D	265	THR
1	D	274	GLU
1	D	298	ASP
1	D	299	ARG
1	D	324	LYS
1	D	354	ASP
1	D	424	GLU
1	D	438	GLU

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Mol	Chain	Res	Type
1	D	446	GLU
1	D	448	ILE
1	D	450	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	65	GLN
1	A	67	HIS
1	A	138	GLN
1	A	157	HIS
1	A	163	GLN
1	B	21	HIS
1	B	157	HIS
1	B	259	ASN
1	B	260	ASN
1	B	383	ASN
1	C	21	HIS
1	C	65	GLN
1	C	67	HIS
1	C	138	GLN
1	C	157	HIS
1	C	163	GLN
1	C	273	HIS
1	D	21	HIS
1	D	65	GLN
1	D	67	HIS
1	D	121	GLN
1	D	138	GLN
1	D	157	HIS
1	D	163	GLN
1	D	303	HIS

### 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 ⓘ

4 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	2PE	A	501	-	27,27,27	0.81	1 (3%)	26,26,26	0.89	2 (7%)
2	2PE	B	501	-	27,27,27	0.78	1 (3%)	26,26,26	0.78	1 (3%)
2	2PE	C	501	-	27,27,27	0.77	1 (3%)	26,26,26	0.81	2 (7%)
2	2PE	D	501	-	27,27,27	0.76	1 (3%)	26,26,26	0.90	2 (7%)

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	2PE	A	501	-	-	0/25/25/25	0/0/0/0
2	2PE	B	501	-	-	0/25/25/25	0/0/0/0
2	2PE	C	501	-	-	0/25/25/25	0/0/0/0
2	2PE	D	501	-	-	0/25/25/25	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	2PE	C12-C11	-2.97	1.33	1.48
2	C	501	2PE	C12-C11	-2.95	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	2PE	C12-C11	-2.95	1.33	1.48
2	A	501	2PE	C12-C11	-2.86	1.34	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	2PE	O13-C12-C11	2.20	120.16	110.36
2	C	501	2PE	O10-C11-C12	2.21	120.17	110.36
2	A	501	2PE	C11-O10-C9	2.22	122.83	113.31
2	B	501	2PE	O10-C11-C12	2.39	120.99	110.36
2	D	501	2PE	O13-C12-C11	2.78	122.70	110.36
2	D	501	2PE	O10-C11-C12	2.95	123.49	110.36
2	A	501	2PE	O13-C12-C11	2.96	123.52	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	2PE	3	0
2	B	501	2PE	1	0
2	C	501	2PE	4	0
2	D	501	2PE	3	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	445/459 (96%)	-0.35	3 (0%) 89 92	15, 25, 45, 61	0
1	B	445/459 (96%)	-0.27	6 (1%) 79 84	17, 30, 48, 62	0
1	C	445/459 (96%)	-0.24	5 (1%) 82 86	20, 34, 52, 59	0
1	D	445/459 (96%)	-0.35	4 (0%) 85 89	15, 26, 42, 53	0
All	All	1780/1836 (96%)	-0.30	18 (1%) 84 88	15, 28, 49, 62	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430	ILE	4.0
1	B	299	ARG	3.3
1	B	431	LYS	2.9
1	C	299	ARG	2.8
1	C	298	ASP	2.7
1	D	300	ASP	2.6
1	D	299	ARG	2.6
1	D	427	PHE	2.5
1	B	432	ASN	2.4
1	A	111	VAL	2.4
1	B	456	GLY	2.4
1	D	456	GLY	2.3
1	C	300	ASP	2.3
1	C	282	ASP	2.2
1	A	299	ARG	2.2
1	B	211	ARG	2.2
1	C	353	LYS	2.2
1	A	300	ASP	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	2PE	A	501	28/28	0.85	0.19	4.02	48,53,57,58	0
2	2PE	C	501	28/28	0.85	0.22	2.58	54,64,70,70	0
2	2PE	B	501	28/28	0.85	0.17	1.59	59,63,66,66	0
2	2PE	D	501	28/28	0.91	0.17	1.01	49,56,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.