



# Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 03:44 AM GMT

PDB ID : 3KBO  
Title : 2.14 Angstrom Crystal Structure of Putative Oxidoreductase (ycdW) from *Salmonella typhimurium* in Complex with NADP  
Authors : Minasov, G.; Wawrzak, Z.; Skarina, T.; Onopriyenko, O.; Papazisi, L.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2009-10-20  
Resolution : 2.14 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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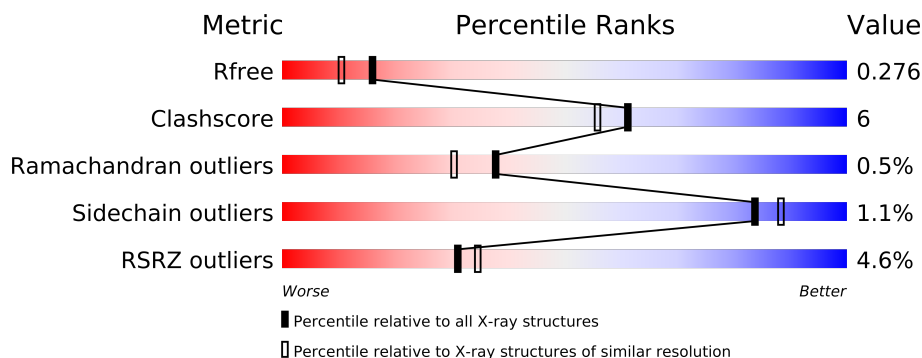
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.14 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))
$R_{free}$	66092	1116 (2.16-2.12)
Clashscore	79885	1302 (2.16-2.12)
Ramachandran outliers	78287	1281 (2.16-2.12)
Sidechain outliers	78261	1281 (2.16-2.12)
RSRZ outliers	66119	1116 (2.16-2.12)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	C	315	
1	D	315	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NDB	A	314	-	X
4	CL	D	315	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10785 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

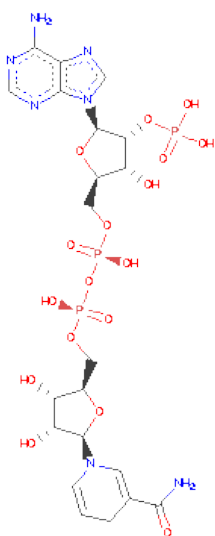
- Molecule 1 is a protein called Glyoxylate/hydroxypyruvatereductase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	Se	0	4	0
			2510	1606	442	453	1	8			
1	B	312	Total	C	N	O	S	Se	0	2	0
			2490	1595	439	447	1	8			
1	C	312	Total	C	N	O	S	Se	0	1	0
			2484	1592	438	445	1	8			
1	D	312	Total	C	N	O	S	Se	0	2	0
			2490	1595	439	447	1	8			

There are 12 discrepancies between the modelled and reference sequences:

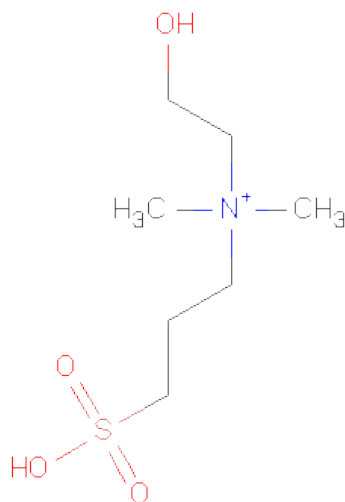
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
A	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
A	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30
B	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
B	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
B	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30
C	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
C	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
C	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30
D	-2	SER	-	EXPRESSION TAG	UNP Q8ZQ30
D	-1	ASN	-	EXPRESSION TAG	UNP Q8ZQ30
D	0	ALA	-	EXPRESSION TAG	UNP Q8ZQ30

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is N-(2-HYDROXYETHYL)-N,N-DIMETHYL-3-SULFOPROPAN-1-AMINIUM M (three-letter code: NDB) (formula:  $C_7H_{18}NO_4S$ ).

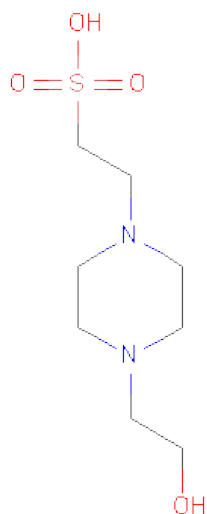


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		
4	D	2	Total	Cl	0	0
			2	2		
4	C	2	Total	Cl	0	0
			2	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

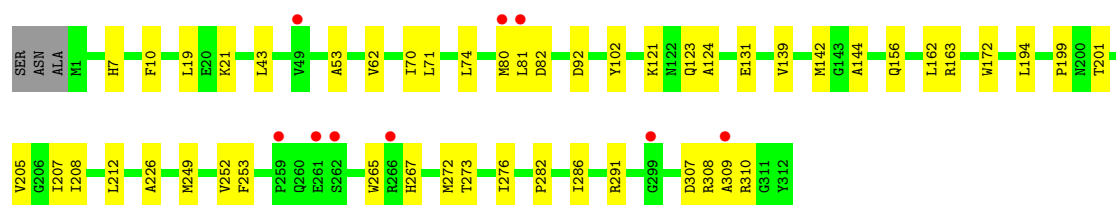
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total 152	O 152	0	6
6	B	125	Total 127	O 127	0	2
6	C	179	Total 184	O 184	0	5
6	D	104	Total 105	O 105	0	1

### 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.

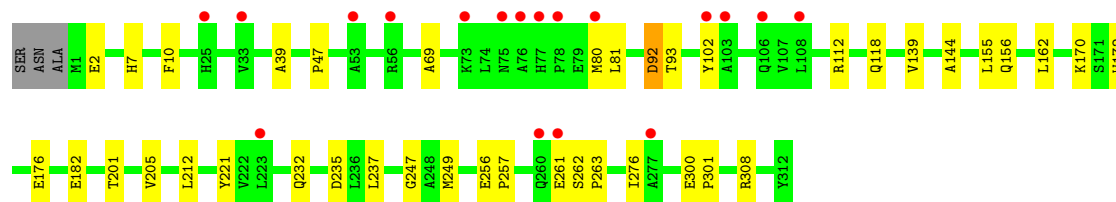
- Molecule 1: Glyoxylate/hydroxypyruvatereductase A

Chain A: 



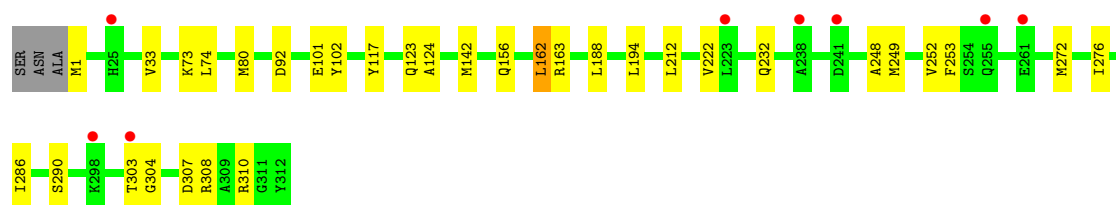
- Molecule 1: Glyoxylate/hydroxypyruvatereductase A

Chain B: 



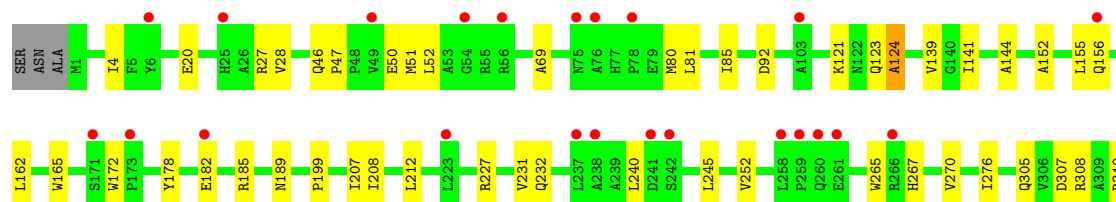
- Molecule 1: Glyoxylate/hydroxypyruvatereductase A

Chain C: 



- Molecule 1: Glyoxylate/hydroxypyruvatereductase A

Chain D: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.62Å 45.59Å 112.33Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	29.93 – 2.14 29.83 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.93-2.14) 98.0 (29.83-2.14)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.48 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.211 , 0.269 0.220 , 0.276	Depositor DCC
$R_{free}$ test set	3806 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	7 of 75670 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.53 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2269e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, NDB, EPE, CL

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	0.66	0/2568	0.71	0/3485
1	B	0.59	0/2548	0.68	0/3457
1	C	0.70	0/2542	0.72	0/3449
1	D	0.54	0/2548	0.67	0/3457
All	All	0.63	0/10206	0.69	0/13848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2510	0	2490	34	0
1	B	2490	0	2478	29	0
1	C	2484	0	2474	22	0
1	D	2490	0	2478	41	0
2	A	48	0	25	2	0
2	B	48	0	26	1	0
2	C	48	0	26	0	0
2	D	48	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	13	0	18	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	15	0	17	0	0
5	D	15	0	17	0	0
6	A	152	0	0	2	0
6	B	127	0	0	3	0
6	C	184	0	0	1	0
6	D	105	0	0	3	0
All	All	10785	0	10075	118	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:232[B]:GLN:N	1:D:232[B]:GLN:HE21	1.64	0.96
1:A:121:LYS:NZ	1:D:267:HIS:O	2.23	0.70
1:A:121:LYS:NZ	1:D:270:VAL:O	2.22	0.69
1:C:156:GLN:HB2	1:C:162:LEU:HD13	1.79	0.65
1:A:307:ASP:HB3	1:A:310:ARG:HG2	1.79	0.64
1:A:139:VAL:HB	1:A:162:LEU:HD22	1.81	0.63
1:D:232[B]:GLN:H	1:D:232[B]:GLN:HE21	1.44	0.63
1:A:131:GLU:HA	6:A:403:HOH:O	1.98	0.63
1:D:123:GLN:O	1:D:124:ALA:HB3	1.99	0.63
1:D:47:PRO:HG2	1:D:80:MSE:HE1	1.81	0.62
1:B:276:ILE:HD13	1:C:117:TYR:CE2	2.35	0.62
1:B:201:THR:O	1:B:205:VAL:HG23	1.99	0.62
1:D:52:LEU:HD12	1:D:80:MSE:HE2	1.81	0.62
1:D:208:ILE:HB	1:D:231:VAL:HG22	1.82	0.61
1:C:303:THR:HB	1:C:304:GLY:HA2	1.87	0.57
1:C:307:ASP:HB3	1:C:310:ARG:HG2	1.86	0.57
1:A:273:THR:HB	1:A:276:ILE:HD11	1.87	0.57
1:A:139:VAL:HB	1:A:162:LEU:CD2	2.35	0.56
1:D:144:ALA:HB1	1:D:172:TRP:CH2	2.41	0.56
1:A:212:LEU:HD23	1:A:212:LEU:C	2.27	0.55
1:B:182:GLU:CD	1:B:182:GLU:H	2.10	0.55
1:C:252:VAL:C	1:C:253:PHE:CD2	2.80	0.55
1:B:300:GLU:HB3	1:B:301:PRO:CD	2.37	0.54
1:A:142:MSE:HG3	1:A:194:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:310:ARG:HD2	1:D:312:TYR:CZ	2.42	0.54
1:A:308:ARG:HB3	6:A:426:HOH:O	2.08	0.53
1:C:276:ILE:C	1:C:276:ILE:HD12	2.28	0.53
1:A:253:PHE:CZ	1:A:272:MSE:HE3	2.43	0.53
1:A:144:ALA:HB1	1:A:172:TRP:CH2	2.44	0.53
1:A:70:ILE:HG22	1:A:71:LEU:N	2.22	0.53
1:C:74:LEU:HD21	1:C:308:ARG:NH2	2.23	0.52
1:D:141:ILE:HD12	1:D:152:ALA:HB2	1.91	0.52
1:A:53:ALA:HA	1:A:80:MSE:HA	1.92	0.52
1:D:69:ALA:HB3	6:D:373:HOH:O	2.08	0.52
1:B:139:VAL:HB	1:B:162:LEU:HD23	1.91	0.51
1:A:282:PRO:O	1:A:286:ILE:HG12	2.09	0.51
1:D:20:GLU:HG2	1:D:28:VAL:HG23	1.92	0.51
1:A:201:THR:O	1:A:205:VAL:HG23	2.11	0.51
1:D:139:VAL:HG11	1:D:155:LEU:HD13	1.93	0.51
1:A:124:ALA:HA	1:D:265:TRP:CE3	2.46	0.51
1:A:265:TRP:CE3	1:D:124:ALA:HA	2.46	0.51
1:B:262:SER:HA	6:B:379[A]:HOH:O	2.11	0.51
1:B:47:PRO:HG2	1:B:80:MSE:HE1	1.93	0.50
1:D:232[B]:GLN:HE21	1:D:232[B]:GLN:CA	2.24	0.50
1:B:300:GLU:HB3	1:B:301:PRO:HD2	1.93	0.50
1:D:240:LEU:HD23	1:D:245:LEU:HB2	1.93	0.50
1:A:207:ILE:HG23	1:A:208:ILE:HG13	1.93	0.49
1:D:305:GLN:HB2	6:D:320:HOH:O	2.13	0.49
1:D:165:TRP:HA	1:D:178:TYR:O	2.13	0.49
1:D:139:VAL:HB	1:D:162:LEU:HD23	1.95	0.48
1:B:276:ILE:HD13	1:C:117:TYR:CZ	2.49	0.48
1:D:123:GLN:O	1:D:124:ALA:CB	2.61	0.48
1:D:46:GLN:N	1:D:47:PRO:CD	2.77	0.48
1:D:85:ILE:O	1:D:308:ARG:NH1	2.48	0.47
1:D:81:LEU:HD11	1:D:85:ILE:HG21	1.96	0.47
1:C:73:LYS:HG2	1:C:80:MSE:CE	2.43	0.47
1:D:199:PRO:HD3	2:D:313:NDP:H52A	1.97	0.47
1:B:102:TYR:OH	1:B:249:MSE:HE2	2.15	0.47
1:B:176:GLU:HG2	6:B:384:HOH:O	2.13	0.47
1:D:182:GLU:CD	1:D:182:GLU:H	2.17	0.47
1:A:62:VAL:CG2	1:A:70:ILE:HD12	2.45	0.47
1:C:253:PHE:CD2	1:C:253:PHE:N	2.82	0.47
1:D:212:LEU:C	1:D:212:LEU:HD23	2.36	0.46
1:B:170:LYS:NZ	2:B:313:NDP:O3X	2.29	0.46
1:D:276:ILE:C	1:D:276:ILE:HD12	2.35	0.46
1:C:102:TYR:OH	1:C:249:MSE:HE2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2:GLU:HB3	1:B:39:ALA:HA	1.98	0.46
1:D:47:PRO:HG2	1:D:80:MSE:CE	2.45	0.46
1:B:276:ILE:CD1	1:C:117:TYR:CE2	2.99	0.45
1:A:252:VAL:C	1:A:253:PHE:CD2	2.89	0.45
1:A:253:PHE:CE1	1:A:272:MSE:HE3	2.51	0.45
1:B:144:ALA:HB1	1:B:172:TRP:CH2	2.51	0.45
1:A:19:LEU:HD22	1:A:43:LEU:HD22	1.98	0.45
1:A:7:HIS:CD2	1:A:10:PHE:CD2	3.04	0.45
1:C:142:MSE:HG3	1:C:194:LEU:HD11	1.97	0.45
1:D:232[B]:GLN:N	1:D:232[B]:GLN:NE2	2.48	0.45
1:C:212:LEU:HD23	1:C:212:LEU:C	2.36	0.45
1:A:81:LEU:O	1:A:82:ASP:C	2.55	0.45
1:A:123:GLN:O	1:A:124:ALA:C	2.55	0.45
1:B:7:HIS:CD2	1:B:10:PHE:CD2	3.05	0.45
1:B:69:ALA:HB3	6:B:453:HOH:O	2.16	0.44
1:B:221:TYR:HA	1:B:247:GLY:O	2.17	0.44
1:B:237:LEU:HD11	1:B:263:PRO:HG2	1.98	0.44
1:D:156:GLN:HB2	1:D:162:LEU:CD1	2.47	0.44
1:D:227:ARG:CA	1:D:252:VAL:HG21	2.48	0.43
1:B:92:ASP:O	1:B:93:THR:OG1	2.33	0.43
1:B:102:TYR:CZ	1:B:249:MSE:HE2	2.54	0.43
1:C:33:VAL:O	1:C:33:VAL:HG23	2.17	0.43
1:C:1:MSE:N	6:C:424:HOH:O	2.52	0.43
1:C:286:ILE:O	1:C:290:SER:CB	2.67	0.43
1:A:226:ALA:HA	2:A:313:NDP:H1D	2.00	0.42
1:B:81:LEU:HD23	1:B:308:ARG:NH2	2.34	0.42
1:A:267:HIS:O	1:D:121:LYS:NZ	2.53	0.42
1:B:261:GLU:O	1:B:262:SER:C	2.58	0.42
1:D:207:ILE:O	1:D:212:LEU:HD13	2.19	0.42
1:C:123:GLN:O	1:C:124:ALA:HB3	2.20	0.42
1:B:212:LEU:HD23	1:B:212:LEU:C	2.39	0.42
1:D:307:ASP:HB3	1:D:310:ARG:HG2	2.01	0.42
1:D:310:ARG:HD2	1:D:312:TYR:CE2	2.55	0.42
1:C:188:LEU:HD11	1:C:212:LEU:HG	2.02	0.42
1:A:307:ASP:OD2	1:A:309:ALA:HB3	2.20	0.41
1:B:139:VAL:HG11	1:B:155:LEU:HD13	2.02	0.41
3:A:314:NDB:HAG	3:A:314:NDB:HAH	2.00	0.41
1:D:46:GLN:N	1:D:47:PRO:HD3	2.34	0.41
1:C:222:VAL:O	1:C:248:ALA:HA	2.20	0.41
1:A:71:LEU:HA	1:A:74:LEU:HG	2.01	0.41
1:A:199:PRO:HD3	2:A:313:NDP:H52A	2.01	0.41
1:B:256:GLU:HA	1:B:257:PRO:C	2.40	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:156:GLN:N	1:D:162:LEU:HD11	2.35	0.41
1:D:185:ARG:HB3	6:D:376:HOH:O	2.20	0.41
1:B:156:GLN:N	1:B:162:LEU:HD11	2.36	0.41
1:B:112:ARG:HD3	1:C:101:GLU:OE1	2.20	0.41
1:B:232[B]:GLN:HB3	1:B:235:ASP:HB2	2.02	0.41
1:C:276:ILE:C	1:C:276:ILE:CD1	2.88	0.41
1:D:4:ILE:HD12	1:D:51:MSE:HE3	2.02	0.41
1:A:102:TYR:OH	1:A:249:MSE:HE2	2.22	0.40
1:A:19:LEU:HD22	1:A:43:LEU:CD2	2.51	0.40
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.90	0.40

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	314/315 (100%)	302 (96%)	11 (4%)	1 (0%)	50	46
1	B	312/315 (99%)	296 (95%)	15 (5%)	1 (0%)	50	46
1	C	311/315 (99%)	301 (97%)	9 (3%)	1 (0%)	50	46
1	D	312/315 (99%)	291 (93%)	18 (6%)	3 (1%)	22	12
All	All	1249/1260 (99%)	1190 (95%)	53 (4%)	6 (0%)	38	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	92	ASP
1	D	124	ALA
1	D	189	ASN
1	A	92	ASP
1	B	92	ASP
1	D	92	ASP

### 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	261/251 (104%)	257 (98%)	4 (2%)	76	82
1	B	259/251 (103%)	258 (100%)	1 (0%)	95	98
1	C	258/251 (103%)	254 (98%)	4 (2%)	75	80
1	D	259/251 (103%)	257 (99%)	2 (1%)	89	94
All	All	1037/1004 (103%)	1026 (99%)	11 (1%)	84	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	156	GLN
1	A	163	ARG
1	A	291	ARG
1	B	118	GLN
1	C	162	LEU
1	C	163	ARG
1	C	232	GLN
1	C	272	MSE
1	D	27	ARG
1	D	50	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	17	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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$
2	NDP	A	313	-	52,52,52	1.84	9 (17%)	80,80,80	1.75	12 (15%)
3	NDB	A	314	-	12,12,12	1.70	2 (16%)	17,17,17	2.02	5 (29%)
2	NDP	B	313	-	52,52,52	1.82	10 (19%)	80,80,80	1.98	15 (18%)
5	EPE	B	314	-	15,15,15	0.79	1 (6%)	20,20,20	1.70	4 (20%)
2	NDP	C	313	-	52,52,52	1.89	10 (19%)	80,80,80	1.77	11 (13%)
2	NDP	D	313	-	52,52,52	1.78	10 (19%)	80,80,80	1.84	12 (15%)
5	EPE	D	314	-	15,15,15	0.64	1 (6%)	20,20,20	1.79	2 (10%)

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	NDP	A	313	-	-	0/35/77/77	0/3/5/5
3	NDB	A	314	-	-	0/12/12/12	0/0/0/0
2	NDP	B	313	-	-	0/35/77/77	0/3/5/5
5	EPE	B	314	-	-	0/9/19/19	0/1/1/1
2	NDP	C	313	-	-	0/35/77/77	0/3/5/5
2	NDP	D	313	-	-	0/35/77/77	0/3/5/5
5	EPE	D	314	-	-	0/9/19/19	0/1/1/1

All (43) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	313	NDP	C4N-C3N	-6.70	1.37	1.50
2	B	313	NDP	O7N-C7N	6.62	1.41	1.24
2	D	313	NDP	O7N-C7N	6.28	1.40	1.24
2	A	313	NDP	C4N-C3N	-6.15	1.38	1.50
2	A	313	NDP	O7N-C7N	5.98	1.40	1.24
2	D	313	NDP	C4N-C3N	-5.93	1.38	1.50
2	C	313	NDP	O7N-C7N	5.77	1.39	1.24
2	B	313	NDP	C4N-C3N	-5.60	1.39	1.50
2	B	313	NDP	C2A-N3A	3.88	1.39	1.32
3	A	314	NDB	CAK-SAM	3.85	1.83	1.77
2	A	313	NDP	C4N-C5N	-3.75	1.40	1.49
2	D	313	NDP	C4N-C5N	-3.72	1.40	1.49
2	B	313	NDP	C4N-C5N	-3.65	1.41	1.49
2	C	313	NDP	C4N-C5N	-3.61	1.41	1.49
2	D	313	NDP	C2A-N3A	3.60	1.39	1.32
2	A	313	NDP	C2A-N3A	3.55	1.39	1.32
2	C	313	NDP	C2A-N3A	3.39	1.38	1.32
2	C	313	NDP	C2A-N1A	3.37	1.40	1.33
2	D	313	NDP	C2A-N1A	3.32	1.40	1.33
2	B	313	NDP	C2A-N1A	3.17	1.40	1.33
2	C	313	NDP	C2N-C3N	2.84	1.40	1.34
2	A	313	NDP	O2D-C2D	-2.69	1.36	1.43
2	A	313	NDP	C2A-N1A	2.67	1.39	1.33
5	B	314	EPE	C10-S	2.63	1.81	1.77
2	D	313	NDP	C7N-C3N	2.61	1.53	1.47
2	D	313	NDP	C2N-C3N	2.55	1.39	1.34
2	C	313	NDP	PN-O2N	-2.53	1.43	1.55
2	B	313	NDP	C7N-C3N	2.42	1.52	1.47
2	B	313	NDP	O4D-C4D	-2.40	1.39	1.45
3	A	314	NDB	CAI-NAL	-2.35	1.46	1.52
2	B	313	NDP	C2N-C3N	2.29	1.39	1.34
2	C	313	NDP	O4D-C4D	-2.28	1.39	1.45
2	C	313	NDP	O2D-C2D	-2.28	1.37	1.43
2	D	313	NDP	O4D-C4D	-2.27	1.39	1.45
2	A	313	NDP	C6N-C5N	2.20	1.37	1.33
2	D	313	NDP	C6N-C5N	2.18	1.37	1.33
2	A	313	NDP	PN-O2N	-2.17	1.45	1.55
2	B	313	NDP	C6N-C5N	2.16	1.37	1.33
5	D	314	EPE	C10-S	2.13	1.80	1.77
2	D	313	NDP	PN-O2N	-2.09	1.45	1.55
2	A	313	NDP	O4D-C1D	2.07	1.47	1.42
2	C	313	NDP	C7N-C3N	2.04	1.51	1.47
2	B	313	NDP	PN-O2N	-2.01	1.46	1.55

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	313	NDP	N3A-C2A-N1A	-12.00	118.67	128.71
2	D	313	NDP	N3A-C2A-N1A	-11.06	119.46	128.71
2	A	313	NDP	N3A-C2A-N1A	-10.87	119.62	128.71
2	C	313	NDP	N3A-C2A-N1A	-9.07	121.13	128.71
5	D	314	EPE	O2S-S-C10	6.93	112.75	106.81
2	C	313	NDP	O4B-C1B-N9A	6.43	114.42	108.44
2	B	313	NDP	O4B-C1B-N9A	5.10	113.19	108.44
5	B	314	EPE	O2S-S-C10	4.81	110.93	106.81
3	A	314	NDB	OAD-SAM-CAK	4.61	111.77	105.93
2	D	313	NDP	O4B-C1B-N9A	4.58	112.70	108.44
3	A	314	NDB	CAG-CAI-NAL	-3.60	112.18	116.22
3	A	314	NDB	OAC-SAM-CAK	3.60	109.89	106.81
2	A	313	NDP	N3A-C4A-N9A	3.26	131.31	125.43
2	D	313	NDP	O3X-P2B-O2B	3.25	116.45	107.09
2	B	313	NDP	N3A-C4A-N9A	3.16	131.14	125.43
2	D	313	NDP	N3A-C4A-N9A	3.13	131.08	125.43
2	B	313	NDP	C1B-N9A-C4A	-3.10	121.28	126.64
2	B	313	NDP	C5N-C4N-C3N	3.09	120.96	112.60
2	C	313	NDP	N3A-C4A-N9A	3.03	130.90	125.43
2	B	313	NDP	C4N-C3N-C2N	-2.94	118.10	121.68
2	B	313	NDP	O3X-P2B-O2B	2.88	115.40	107.09
5	B	314	EPE	O1S-S-C10	2.85	109.25	106.81
2	C	313	NDP	C1B-N9A-C4A	-2.82	121.77	126.64
2	C	313	NDP	C8A-N9A-C4A	2.79	109.03	106.90
2	B	313	NDP	C4A-C5A-N7A	-2.73	107.18	109.52
2	A	313	NDP	N7A-C8A-N9A	-2.69	106.74	114.36
2	D	313	NDP	C4N-C3N-C2N	-2.69	118.41	121.68
2	D	313	NDP	O2N-PN-O1N	2.67	127.12	112.21
5	B	314	EPE	O3S-S-C10	2.67	109.31	105.93
2	A	313	NDP	C3N-C2N-N1N	-2.67	119.26	123.05
2	A	313	NDP	C1B-N9A-C4A	-2.62	122.11	126.64
2	C	313	NDP	C5N-C4N-C3N	2.62	119.69	112.60
2	D	313	NDP	C5N-C4N-C3N	2.61	119.66	112.60
2	D	313	NDP	O4B-C1B-C2B	-2.58	104.53	106.95
2	C	313	NDP	N7A-C8A-N9A	-2.58	107.07	114.36
2	A	313	NDP	C4A-C5A-N7A	-2.56	107.33	109.52
3	A	314	NDB	OAF-SAM-CAK	2.47	108.92	106.81
2	A	313	NDP	C8A-N9A-C4A	2.44	108.76	106.90
2	A	313	NDP	O2N-PN-O1N	2.41	125.69	112.21
2	D	313	NDP	O3X-P2B-O1X	-2.37	102.69	110.44
2	B	313	NDP	C2A-N3A-C4A	2.37	120.75	114.01
2	A	313	NDP	C5N-C4N-C3N	2.36	119.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	313	NDP	O2N-PN-O1N	2.33	125.24	112.21
2	B	313	NDP	N7A-C8A-N9A	-2.28	107.90	114.36
2	C	313	NDP	C3D-C2D-C1D	2.21	105.75	101.35
2	C	313	NDP	C3N-C2N-N1N	-2.21	119.92	123.05
5	D	314	EPE	C2-C3-N4	2.18	114.90	110.61
2	C	313	NDP	O3X-P2B-O2X	2.16	116.01	107.61
2	D	313	NDP	N7A-C8A-N9A	-2.14	108.31	114.36
2	A	313	NDP	O3X-P2B-O2X	2.13	115.90	107.61
5	B	314	EPE	C6-N1-C2	2.12	114.14	108.86
2	D	313	NDP	C1B-N9A-C4A	-2.12	122.97	126.64
2	B	313	NDP	C5A-C4A-N3A	-2.11	121.10	125.70
2	B	313	NDP	C2D-C1D-N1N	2.10	118.58	113.21
2	B	313	NDP	C8A-N9A-C1B	2.10	130.52	126.38
2	C	313	NDP	C2B-C1B-N9A	-2.08	105.85	113.74
2	B	313	NDP	O5B-PA-O1A	2.07	117.47	109.37
3	A	314	NDB	CAH-CAJ-NAL	-2.06	110.35	115.39
2	A	313	NDP	C4N-C5N-C6N	-2.05	118.85	122.61
2	A	313	NDP	C8A-N7A-C5A	2.04	109.90	103.58
2	D	313	NDP	C5N-C6N-N1N	-2.01	118.93	123.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	312/315 (99%)	0.32	9 (2%) 49 52	9, 29, 49, 58	0
1	B	312/315 (99%)	0.45	18 (5%) 22 25	17, 34, 53, 68	0
1	C	312/315 (99%)	0.22	8 (2%) 53 56	14, 28, 41, 51	0
1	D	312/315 (99%)	0.62	23 (7%) 14 16	16, 39, 54, 67	0
All	All	1248/1260 (99%)	0.40	58 (4%) 31 34	9, 31, 52, 68	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	261	GLU	4.1
1	A	299	GLY	3.9
1	A	261	GLU	3.7
1	B	33	VAL	3.7
1	B	25	HIS	3.7
1	B	260	GLN	3.4
1	B	76	ALA	3.3
1	D	238	ALA	3.2
1	B	75	ASN	3.2
1	B	73	LYS	3.2
1	D	75	ASN	3.2
1	D	76	ALA	3.2
1	D	56	ARG	3.1
1	D	54	GLY	2.9
1	D	261	GLU	2.9
1	C	25	HIS	2.8
1	C	303	THR	2.8
1	B	261	GLU	2.8
1	D	266	ARG	2.8
1	A	49	VAL	2.7
1	A	81	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	241	ASP	2.6
1	D	223	LEU	2.6
1	D	156	GLN	2.6
1	B	103	ALA	2.5
1	D	25	HIS	2.5
1	D	173	PRO	2.5
1	A	262	SER	2.5
1	D	259	PRO	2.4
1	B	53	ALA	2.4
1	B	277	ALA	2.4
1	B	78	PRO	2.4
1	C	238	ALA	2.4
1	D	78	PRO	2.3
1	D	182	GLU	2.3
1	D	237	LEU	2.3
1	D	6	TYR	2.3
1	B	106	GLN	2.3
1	D	242	SER	2.3
1	D	49	VAL	2.2
1	D	171	SER	2.2
1	A	309	ALA	2.2
1	C	298	LYS	2.2
1	D	260	GLN	2.2
1	A	259	PRO	2.2
1	B	102	TYR	2.1
1	B	77	HIS	2.1
1	B	223	LEU	2.1
1	A	80	MSE	2.1
1	C	241	ASP	2.1
1	C	255	GLN	2.1
1	D	258	LEU	2.1
1	B	108	LEU	2.1
1	D	103	ALA	2.1
1	C	223	LEU	2.0
1	B	80	MSE	2.0
1	A	266	ARG	2.0
1	B	56	ARG	2.0

## 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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	D	315	1/1	0.23	4.21	55,55,55,55	0
3	NDB	A	314	13/13	0.20	2.27	31,33,40,45	0
4	CL	B	315	1/1	0.17	1.13	54,54,54,54	0
4	CL	A	315	1/1	0.15	1.08	52,52,52,52	0
5	EPE	B	314	15/15	0.20	0.88	41,56,64,64	0
5	EPE	D	314	15/15	0.18	0.65	48,57,61,62	0
2	NDP	D	313	48/48	0.11	-0.84	20,28,35,37	0
4	CL	D	316	1/1	0.09	-0.99	62,62,62,62	0
2	NDP	B	313	48/48	0.09	-1.19	15,25,29,34	0
4	CL	C	314	1/1	0.07	-1.50	44,44,44,44	0
2	NDP	C	313	48/48	0.08	-1.72	13,19,24,27	0
2	NDP	A	313	48/48	0.09	-1.73	11,19,25,27	0
4	CL	B	316	1/1	0.06	-4.92	61,61,61,61	0
4	CL	A	316	1/1	0.04	-5.65	62,62,62,62	0
4	CL	C	315	1/1	0.06	-6.93	63,63,63,63	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.