



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:56 PM GMT

PDB ID : 4IZ6  
Title : Structure of EntE and EntB, an NRPS adenylation-PCP fusion protein with pseudo translational symmetry  
Authors : Gulick, A.M.; Sundlov, J.A.  
Deposited on : 2013-01-29  
Resolution : 2.40 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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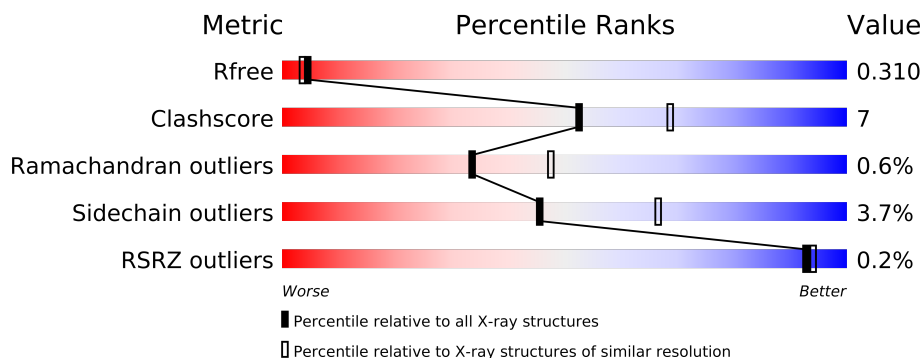
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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. 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	635	
1	B	635	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9564 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 Enterobactin synthase component E, Isochorismatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	1	0
			4644	2949	802	875	18			
1	B	612	Total	C	N	O	S	0	0	0
			4609	2936	790	865	18			

There are 48 discrepancies between the modelled and reference sequences:

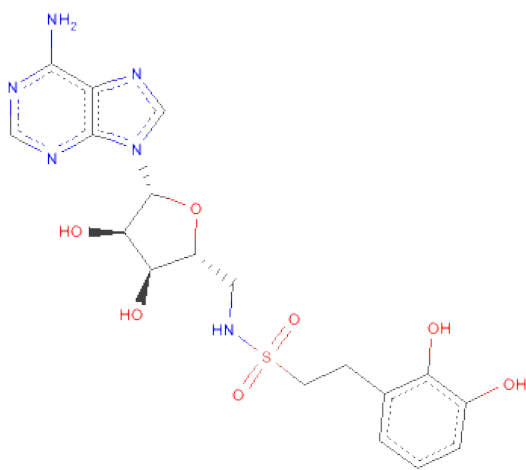
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P10378
A	-18	GLY	-	EXPRESSION TAG	UNP P10378
A	-17	SER	-	EXPRESSION TAG	UNP P10378
A	-16	SER	-	EXPRESSION TAG	UNP P10378
A	-15	HIS	-	EXPRESSION TAG	UNP P10378
A	-14	HIS	-	EXPRESSION TAG	UNP P10378
A	-13	HIS	-	EXPRESSION TAG	UNP P10378
A	-12	HIS	-	EXPRESSION TAG	UNP P10378
A	-11	HIS	-	EXPRESSION TAG	UNP P10378
A	-10	SER	-	EXPRESSION TAG	UNP P10378
A	-9	SER	-	EXPRESSION TAG	UNP P10378
A	-8	GLY	-	EXPRESSION TAG	UNP P10378
A	-7	GLU	-	EXPRESSION TAG	UNP P10378
A	-6	ASN	-	EXPRESSION TAG	UNP P10378
A	-5	LEU	-	EXPRESSION TAG	UNP P10378
A	-4	TYR	-	EXPRESSION TAG	UNP P10378
A	-3	PHE	-	EXPRESSION TAG	UNP P10378
A	-2	GLN	-	EXPRESSION TAG	UNP P10378
A	-1	GLY	-	EXPRESSION TAG	UNP P10378
A	0	HIS	-	EXPRESSION TAG	UNP P10378
A	537	GLY	-	LINKER	UNP P10378
A	538	ARG	-	LINKER	UNP P10378
A	539	ALA	-	LINKER	UNP P10378
A	540	SER	-	LINKER	UNP P10378
B	-19	MET	-	EXPRESSION TAG	UNP P10378

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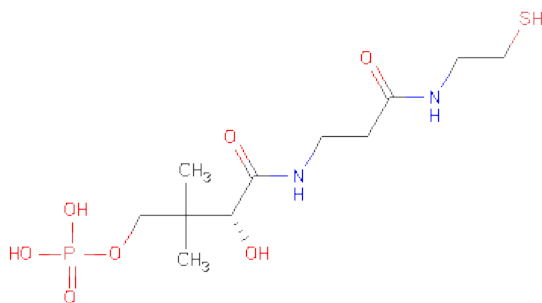
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP P10378
B	-17	SER	-	EXPRESSION TAG	UNP P10378
B	-16	SER	-	EXPRESSION TAG	UNP P10378
B	-15	HIS	-	EXPRESSION TAG	UNP P10378
B	-14	HIS	-	EXPRESSION TAG	UNP P10378
B	-13	HIS	-	EXPRESSION TAG	UNP P10378
B	-12	HIS	-	EXPRESSION TAG	UNP P10378
B	-11	HIS	-	EXPRESSION TAG	UNP P10378
B	-10	SER	-	EXPRESSION TAG	UNP P10378
B	-9	SER	-	EXPRESSION TAG	UNP P10378
B	-8	GLY	-	EXPRESSION TAG	UNP P10378
B	-7	GLU	-	EXPRESSION TAG	UNP P10378
B	-6	ASN	-	EXPRESSION TAG	UNP P10378
B	-5	LEU	-	EXPRESSION TAG	UNP P10378
B	-4	TYR	-	EXPRESSION TAG	UNP P10378
B	-3	PHE	-	EXPRESSION TAG	UNP P10378
B	-2	GLN	-	EXPRESSION TAG	UNP P10378
B	-1	GLY	-	EXPRESSION TAG	UNP P10378
B	0	HIS	-	EXPRESSION TAG	UNP P10378
B	537	GLY	-	LINKER	UNP P10378
B	538	ARG	-	LINKER	UNP P10378
B	539	ALA	-	LINKER	UNP P10378
B	540	SER	-	LINKER	UNP P10378

- Molecule 2 is 5'-DEOXY-5'-({[2-(2,3-DIHYDROXYPHENYL)ETHYL]SULFONYL}AMINO)ADENOSINE (three-letter code: 1HZ) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>6</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	18	6	7	1		
2	B	1	Total	C	N	O	S	0	0
			32	18	6	7	1		

- Molecule 3 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

- Molecule 4 is water.

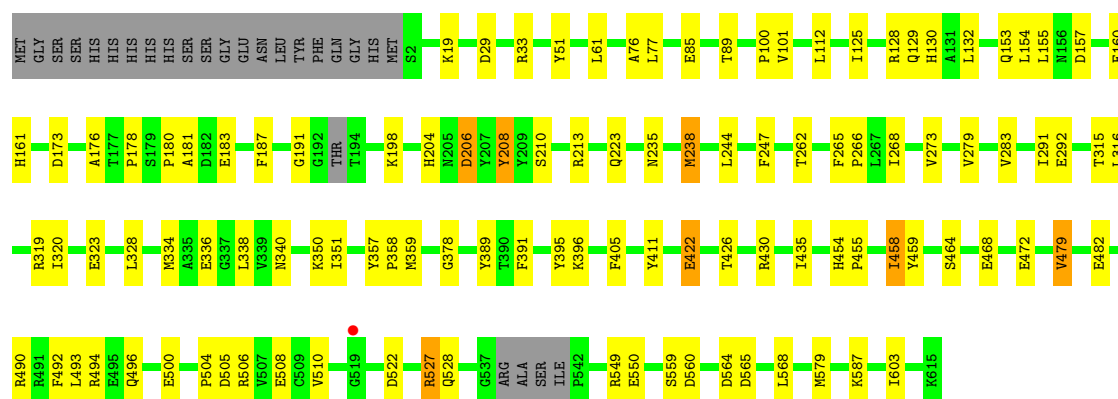
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	0
			99	99		
4	B	106	Total	O	0	0
			106	106		

### 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.

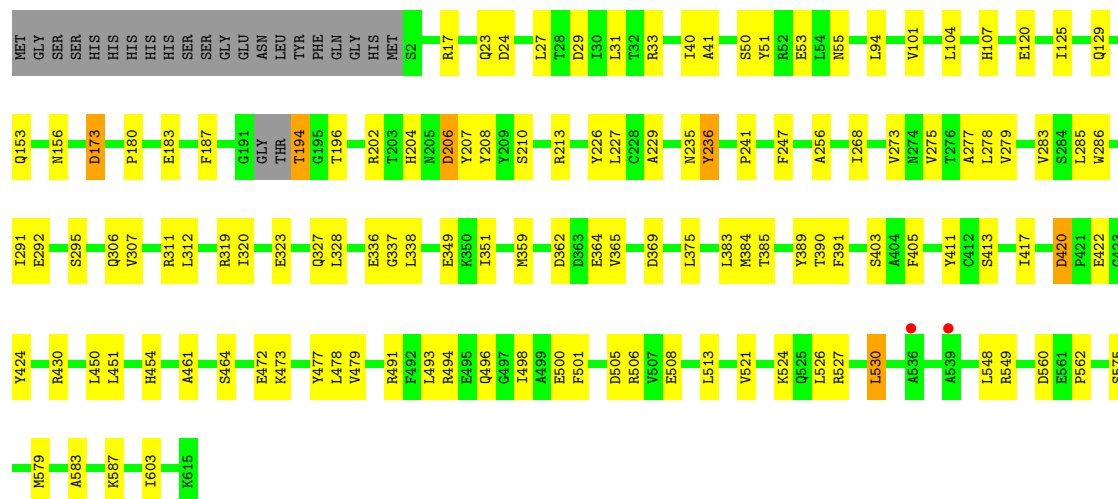
- Molecule 1: Enterobactin synthase component E, Isochorismatase

Chain A:



- Molecule 1: Enterobactin synthase component E, Isochorismatase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.99Å 119.11Å 99.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 2.40 76.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.50-2.40) 97.7 (76.48-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_837)	Depositor
R, $R_{free}$	0.250 , 0.313 0.248 , 0.310	Depositor DCC
$R_{free}$ test set	2655 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 21.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 51230 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 59.58 % 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 1.7283e-05. 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: 1HZ, PNS

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	0.43	0/4748	0.61	0/6470
1	B	0.44	0/4711	0.60	0/6431
All	All	0.43	0/9459	0.60	0/12901

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	4644	0	4499	64	0
1	B	4609	0	4431	72	0
2	A	32	0	20	1	0
2	B	32	0	20	1	0
3	A	21	0	20	1	0
3	B	21	0	20	1	0
4	A	99	0	0	3	0
4	B	106	0	0	4	0
All	All	9564	0	9010	131	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 7.

All (131) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:210:SER:HA	1:B:359:MET:HE1	1.61	0.83
1:A:292:GLU:O	1:B:587:LYS:NZ	2.18	0.75
1:A:206:ASP:HB2	1:A:389:TYR:HA	1.69	0.75
1:B:180:PRO:HB2	1:B:183:GLU:HG3	1.71	0.72
3:A:702:PNS:H371	1:B:279:VAL:HG11	1.74	0.69
1:A:129:GLN:OE1	4:A:892:HOH:O	2.08	0.69
1:A:29:ASP:OD2	1:A:33:ARG:NH2	2.27	0.68
1:A:180:PRO:HB2	1:A:183:GLU:HG3	1.76	0.68
1:B:206:ASP:HB2	1:B:389:TYR:HA	1.76	0.67
1:B:129:GLN:HG3	1:B:156:ASN:ND2	2.11	0.66
1:B:194:THR:HG23	1:B:196:THR:H	1.60	0.66
1:A:587:LYS:NZ	1:B:292:GLU:O	2.30	0.65
1:B:210:SER:HA	1:B:359:MET:CE	2.28	0.63
1:A:549:ARG:NH2	1:A:564:ASP:OD2	2.30	0.61
1:B:27:LEU:HB2	1:B:94:LEU:HD13	1.84	0.60
1:B:268:ILE:HG23	1:B:273:VAL:HB	1.84	0.59
1:A:279:VAL:HG11	3:B:702:PNS:H371	1.85	0.58
1:B:125:ILE:HG12	1:B:153:GLN:HB2	1.85	0.58
1:A:336:GLU:HG2	1:A:411:TYR:CZ	2.39	0.58
1:B:336:GLU:HG2	1:B:411:TYR:CZ	2.39	0.57
1:A:268:ILE:HG23	1:A:273:VAL:HB	1.87	0.57
1:B:501:PHE:O	4:B:828:HOH:O	2.17	0.57
1:B:50:SER:HB2	1:B:53:GLU:H	1.70	0.57
1:B:505:ASP:O	1:B:506:ARG:NH1	2.36	0.57
1:A:210:SER:O	1:A:359:MET:HE1	2.05	0.56
1:B:227:LEU:HB2	1:B:273:VAL:HG21	1.87	0.56
1:B:575:SER:O	1:B:579:MET:HG3	2.06	0.55
1:A:315:THR:O	1:A:319:ARG:HG3	2.07	0.55
1:A:61:LEU:HD23	1:A:89:THR:HA	1.88	0.55
1:B:27:LEU:HG	1:B:204:HIS:ND1	2.21	0.55
1:B:29:ASP:OD2	1:B:33:ARG:NH2	2.39	0.55
1:B:549:ARG:NH2	1:B:562:PRO:O	2.22	0.54
1:B:364:GLU:O	1:B:385:THR:HA	2.08	0.54
1:B:454:HIS:O	4:B:826:HOH:O	2.18	0.54
1:A:459:TYR:HB2	1:A:479:VAL:HG13	1.89	0.54
1:B:213:ARG:HB3	1:B:359:MET:CE	2.38	0.53
1:A:494:ARG:HH12	1:A:500:GLU:HG2	1.74	0.53
1:B:337:GLY:HA3	1:B:390:THR:HA	1.91	0.52
1:A:336:GLU:N	1:A:336:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:PHE:HB2	1:A:266:PRO:HD3	1.91	0.51
1:A:125:ILE:HG12	1:A:153:GLN:HB2	1.91	0.51
1:A:458:ILE:HG12	1:A:479:VAL:O	2.11	0.51
1:B:51:TYR:OH	1:B:247:PHE:HA	2.11	0.51
1:B:320:ILE:HD13	1:B:328:LEU:HD13	1.94	0.50
1:A:430:ARG:NH1	1:A:472:GLU:OE2	2.32	0.50
1:A:603:ILE:HD12	1:A:603:ILE:H	1.77	0.50
1:A:454:HIS:CG	1:A:455:PRO:HD2	2.46	0.50
1:B:405:PHE:CE2	1:B:411:TYR:HB2	2.47	0.49
1:B:526:LEU:O	1:B:530:LEU:HB2	2.12	0.49
1:A:154:LEU:HD12	1:A:161:HIS:HB2	1.95	0.49
1:B:235:ASN:HB3	2:B:701:1HZ:O14	2.13	0.49
1:A:426:THR:OG1	4:A:872:HOH:O	2.19	0.49
1:A:176:ALA:HB1	1:A:178:PRO:HD3	1.94	0.48
1:B:17:ARG:NH1	1:B:24:ASP:OD1	2.47	0.48
1:A:334:MET:HG3	1:A:336:GLU:HB2	1.96	0.48
1:A:568:LEU:HD21	1:A:603:ILE:HD11	1.94	0.48
1:A:378:GLY:O	1:B:349:GLU:HB2	2.12	0.48
1:A:395:TYR:CZ	1:A:396:LYS:HE3	2.49	0.48
1:B:213:ARG:HB3	1:B:359:MET:HE3	1.96	0.47
1:B:319:ARG:O	1:B:323:GLU:HB2	2.14	0.47
1:B:311:ARG:HA	4:B:820:HOH:O	2.14	0.47
1:B:549:ARG:HG2	1:B:603:ILE:HD13	1.97	0.47
1:B:101:VAL:HG22	1:B:187:PHE:HB2	1.96	0.47
1:B:29:ASP:O	1:B:33:ARG:HD2	2.15	0.47
1:A:77:LEU:HD21	1:A:112:LEU:HD22	1.97	0.46
1:B:31:LEU:HD21	1:B:55:ASN:HA	1.96	0.46
1:B:461:ALA:HB2	1:B:521:VAL:HG11	1.97	0.46
1:A:191:GLY:HA3	4:A:828:HOH:O	2.16	0.46
1:A:128:ARG:NE	1:A:157:ASP:OD1	2.41	0.46
1:A:493:LEU:HA	1:A:493:LEU:HD23	1.68	0.45
1:B:548:LEU:HD23	1:B:603:ILE:HG23	1.98	0.45
1:A:181:ALA:HA	1:A:204:HIS:HB2	1.97	0.45
1:A:130:HIS:HE1	1:A:132:LEU:HG	1.82	0.45
1:B:307:VAL:HG11	1:B:312:LEU:HD22	1.98	0.45
1:A:505:ASP:O	1:A:506:ARG:NH1	2.49	0.45
1:A:235:ASN:HB3	2:A:701:1HZ:O14	2.15	0.45
1:A:435:ILE:HD12	1:A:464:SER:HB3	1.99	0.45
1:B:241:PRO:HD3	1:B:306:GLN:HE22	1.81	0.45
1:B:479:VAL:HG23	1:B:513:LEU:HD12	1.98	0.44
1:B:365:VAL:HA	1:B:384:MET:O	2.17	0.44
1:A:213:ARG:HB3	1:A:359:MET:CE	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:336:GLU:N	1:B:336:GLU:OE1	2.51	0.44
1:B:420:ASP:HB3	1:B:422:GLU:H	1.83	0.44
1:A:238:MET:O	1:A:244:LEU:HG	2.17	0.44
1:A:283:VAL:HG11	1:A:320:ILE:HD11	2.00	0.44
1:A:357:TYR:HB2	1:A:358:PRO:HD2	2.00	0.43
1:A:492:PHE:O	1:A:496:GLN:HG2	2.18	0.43
1:B:369:ASP:HB3	1:B:375:LEU:HD21	2.00	0.43
1:A:198:LYS:HA	1:A:198:LYS:HD3	1.81	0.43
1:B:451:LEU:HD13	1:B:478:LEU:HD21	2.00	0.43
1:B:477:TYR:CD1	1:B:508:GLU:HB3	2.54	0.43
1:A:405:PHE:CE2	1:A:411:TYR:HB2	2.53	0.43
1:B:411:TYR:HE1	4:B:849:HOH:O	2.02	0.43
1:B:494:ARG:NH2	1:B:500:GLU:OE2	2.47	0.43
1:A:160:GLU:OE1	1:A:160:GLU:N	2.41	0.43
1:A:33:ARG:NH2	1:A:208:TYR:OH	2.51	0.42
1:B:328:LEU:HD23	1:B:351:ILE:HG22	2.01	0.42
1:A:319:ARG:NH2	1:A:323:GLU:OE1	2.49	0.42
1:B:424:TYR:N	1:B:424:TYR:CD2	2.87	0.42
1:B:278:LEU:HD11	1:B:286:TRP:CZ3	2.55	0.42
1:B:226:TYR:HA	1:B:275:VAL:O	2.19	0.42
1:B:41:ALA:HB2	1:B:51:TYR:CD1	2.55	0.42
1:B:383:LEU:HD22	1:B:413:SER:OG	2.20	0.42
1:A:490:ARG:HD3	1:A:504:PRO:O	2.20	0.42
1:A:316:LEU:HA	1:A:316:LEU:HD12	1.89	0.42
1:A:579:MET:HB2	1:B:285:LEU:HD21	2.01	0.42
1:B:493:LEU:HA	1:B:496:GLN:HG2	2.02	0.42
1:B:229:ALA:HB2	1:B:256:ALA:HB3	2.02	0.42
1:B:213:ARG:HB3	1:B:359:MET:HE2	2.02	0.41
1:A:101:VAL:HG22	1:A:187:PHE:HB2	2.01	0.41
1:B:383:LEU:HD12	1:B:417:ILE:HD13	2.01	0.41
1:B:430:ARG:NH1	1:B:472:GLU:OE2	2.54	0.41
1:A:130:HIS:CE1	1:A:132:LEU:HG	2.55	0.41
1:B:104:LEU:HD12	1:B:107:HIS:NE2	2.36	0.41
1:A:494:ARG:HH12	1:A:500:GLU:CG	2.33	0.41
1:A:262:THR:HG21	1:B:583:ALA:HA	2.03	0.41
1:B:40:ILE:N	1:B:40:ILE:HD12	2.35	0.41
1:B:450:LEU:HD13	1:B:498:ILE:HG21	2.02	0.41
1:A:85:GLU:HG2	1:A:155:LEU:HD13	2.03	0.41
1:B:202:ARG:CZ	1:B:207:TYR:HD1	2.34	0.41
1:A:76:ALA:O	1:A:100:PRO:HA	2.21	0.41
1:A:51:TYR:OH	1:A:247:PHE:HA	2.20	0.41
1:A:19:LYS:HE2	1:A:19:LYS:HB3	1.96	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:LYS:HE3	1:A:422:GLU:OE2	2.20	0.40
1:B:236:TYR:CE2	1:B:277:ALA:HB1	2.56	0.40
1:A:565:ASP:OD1	1:A:565:ASP:N	2.53	0.40
1:A:328:LEU:HD23	1:A:351:ILE:HG22	2.04	0.40
1:A:506:ARG:HD3	1:A:506:ARG:HA	1.74	0.40
1:B:464:SER:HA	1:B:473:LYS:O	2.21	0.40
1:B:283:VAL:HG11	1:B:320:ILE:HD11	2.04	0.40
1:A:527:ARG:HH21	1:A:528:GLN:HB3	1.87	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	604/635 (95%)	584 (97%)	17 (3%)	3 (0%)	38	53
1	B	608/635 (96%)	581 (96%)	23 (4%)	4 (1%)	30	43
All	All	1212/1270 (95%)	1165 (96%)	40 (3%)	7 (1%)	33	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	GLU
1	A	338	LEU
1	B	173	ASP
1	B	524	LYS
1	B	527	ARG
1	A	559	SER
1	B	338	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	475/525 (90%)	457 (96%)	18 (4%)	44	65
1	B	462/525 (88%)	445 (96%)	17 (4%)	45	66
All	All	937/1050 (89%)	902 (96%)	35 (4%)	45	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	A	206	ASP
1	A	208	TYR
1	A	223	GLN
1	A	238	MET
1	A	291	ILE
1	A	340	ASN
1	A	391	PHE
1	A	458	ILE
1	A	468	GLU
1	A	479	VAL
1	A	482	GLU
1	A	508	GLU
1	A	510	VAL
1	A	522	ASP
1	A	527	ARG
1	A	550	GLU
1	A	560	ASP
1	B	23	GLN
1	B	120	GLU
1	B	173	ASP
1	B	194	THR
1	B	206	ASP
1	B	208	TYR
1	B	236	TYR
1	B	291	ILE
1	B	295	SER
1	B	327	GLN
1	B	362	ASP
1	B	391	PHE
1	B	403	SER
1	B	420	ASP
1	B	491	ARG

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Mol	Chain	Res	Type
1	B	530	LEU
1	B	560	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

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	1HZ	A	701	3	35,35,35	1.04	2 (5%)	52,52,52	1.93	9 (17%)
3	PNS	A	702	1,2	20,20,21	0.48	0	25,26,29	1.74	5 (20%)
2	1HZ	B	701	3	35,35,35	0.99	2 (5%)	52,52,52	1.95	10 (19%)
3	PNS	B	702	1,2	20,20,21	0.50	0	25,26,29	1.67	7 (28%)

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	1HZ	A	701	3	-	0/16/32/32	0/2/4/4
3	PNS	A	702	1,2	-	0/26/26/27	0/0/0/0
2	1HZ	B	701	3	-	0/16/32/32	0/2/4/4
3	PNS	B	702	1,2	-	0/26/26/27	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	1HZ	C22-S	-3.74	1.68	1.78
2	B	701	1HZ	C22-S	-3.39	1.69	1.78
2	B	701	1HZ	C4-N9	-2.98	1.33	1.37
2	A	701	1HZ	C4-N9	-2.49	1.34	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	1HZ	N3-C2-N1	-9.60	120.68	128.71
2	A	701	1HZ	N3-C2-N1	-8.38	121.70	128.71
3	A	702	PNS	C43-C42-N41	-4.95	101.36	112.45
2	B	701	1HZ	N3-C4-N9	4.15	132.93	125.43
2	A	701	1HZ	O2P-S-O1P	-3.98	111.98	119.30
2	A	701	1HZ	N3-C4-N9	3.96	132.58	125.43
2	B	701	1HZ	O2P-S-O1P	-3.63	112.64	119.30
3	B	702	PNS	C43-C42-N41	-3.53	104.55	112.45
3	A	702	PNS	C38-C37-N36	-3.53	104.27	111.87
2	A	701	1HZ	C5'-C4'-C3'	-3.24	110.78	116.76
2	B	701	1HZ	C8-N9-C4	3.23	109.36	106.90
2	A	701	1HZ	C4-C5-N7	-3.04	106.92	109.52
2	A	701	1HZ	C8-N9-C4	2.95	109.15	106.90
3	B	702	PNS	O25-P24-O27	-2.81	104.52	113.42
2	A	701	1HZ	O4'-C4'-C5'	2.78	112.43	108.56
3	B	702	PNS	C38-C37-N36	-2.70	106.06	111.87
3	A	702	PNS	C37-C38-C39	-2.63	107.77	112.25
2	A	701	1HZ	C5-C4-N3	-2.54	120.17	125.70
3	B	702	PNS	C42-N41-C39	2.44	127.80	122.84
3	B	702	PNS	C29-C32-C34	2.39	115.05	112.73
3	A	702	PNS	C29-C32-C34	2.38	115.04	112.73
2	B	701	1HZ	C5-C4-N3	-2.38	120.51	125.70
2	B	701	1HZ	C5'-C4'-C3'	-2.29	112.55	116.76
2	B	701	1HZ	C22-S-N5'	2.26	112.25	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	1HZ	C2-N3-C4	2.16	120.16	114.01
3	B	702	PNS	C37-C38-C39	-2.12	108.64	112.25
3	A	702	PNS	C30-C29-C32	2.10	112.46	108.82
3	B	702	PNS	O27-C28-C29	-2.09	105.11	108.99
2	A	701	1HZ	N7-C8-N9	-2.08	108.46	114.36
2	B	701	1HZ	C22-C21-C19	2.01	115.84	111.97
2	B	701	1HZ	C3'-C2'-C1'	2.00	104.04	100.91

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	609/635 (95%)	-0.28	1 (0%) 93 94	13, 24, 48, 67	0
1	B	612/635 (96%)	-0.32	2 (0%) 91 92	11, 23, 43, 68	0
All	All	1221/1270 (96%)	-0.30	3 (0%) 93 94	11, 24, 45, 68	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	519	GLY	3.8
1	B	539	ALA	3.5
1	B	536	ALA	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( $\text{\AA}^2$ )	Q<0.9
3	PNS	A	702	21/22	0.12	-0.09	12,17,22,22	0
2	1HZ	A	701	32/32	0.14	-0.27	15,22,29,31	0
2	1HZ	B	701	32/32	0.14	-0.51	12,21,29,31	0
3	PNS	B	702	21/22	0.10	-0.88	14,16,22,24	0

## 6.5 Other polymers

There are no such residues in this entry.