



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 12:29 AM EDT

PDB ID : 1PV8  
Title : Crystal structure of a low activity F12L mutant of human porphobilinogen synthase  
Authors : Breinig, S.; Kervinen, J.; Stith, L.; Wasson, A.S.; Fairman, R.; Wlodawer, A.; Zdanov, A.; Jaffe, E.K.  
Deposited on : 2003-06-26  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

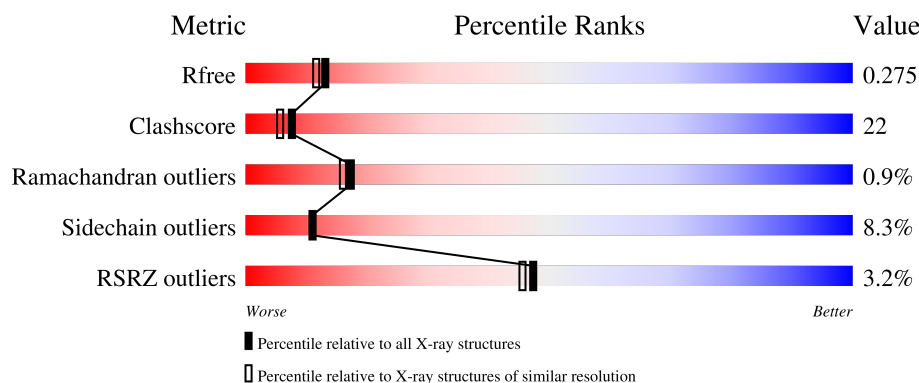
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	330	
1	B	330	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PB1	A	350	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4497 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 Delta-aminolevulinic acid dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2108	1353	362	379	14			
1	B	280	Total	C	N	O	S	0	0	0
			2130	1371	365	381	13			

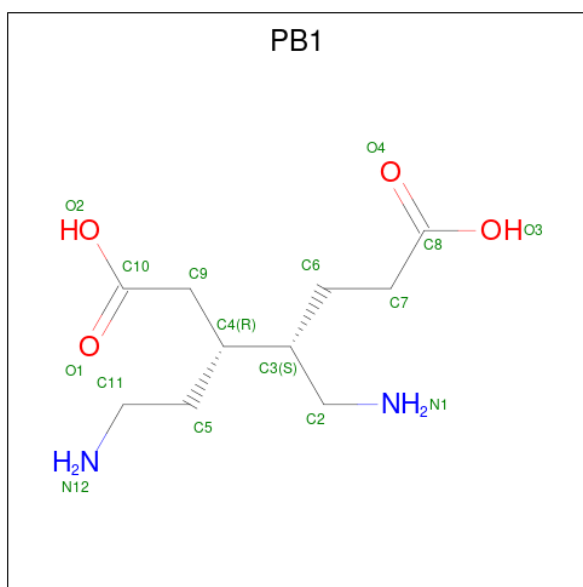
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LEU	PHE	engineered mutation	UNP P13716
B	12	LEU	PHE	engineered mutation	UNP P13716

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 3-(2-AMINOETHYL)-4-(AMINOMETHYL)HEPTANEDIOIC ACID (three-letter code: PB1) (formula: C<sub>10</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	10	2	4		

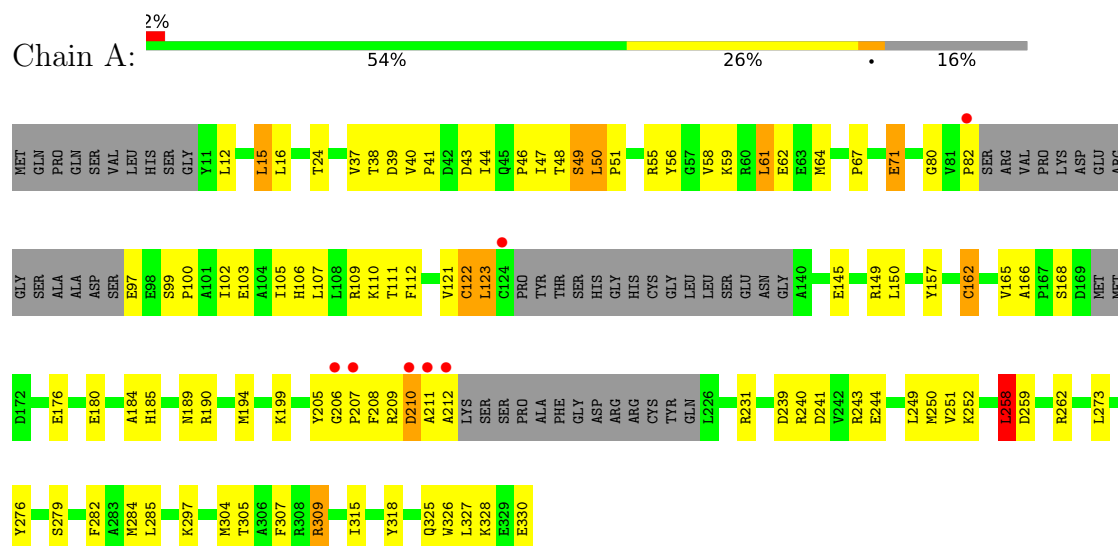
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	118	Total	O	0	0
			118	118		

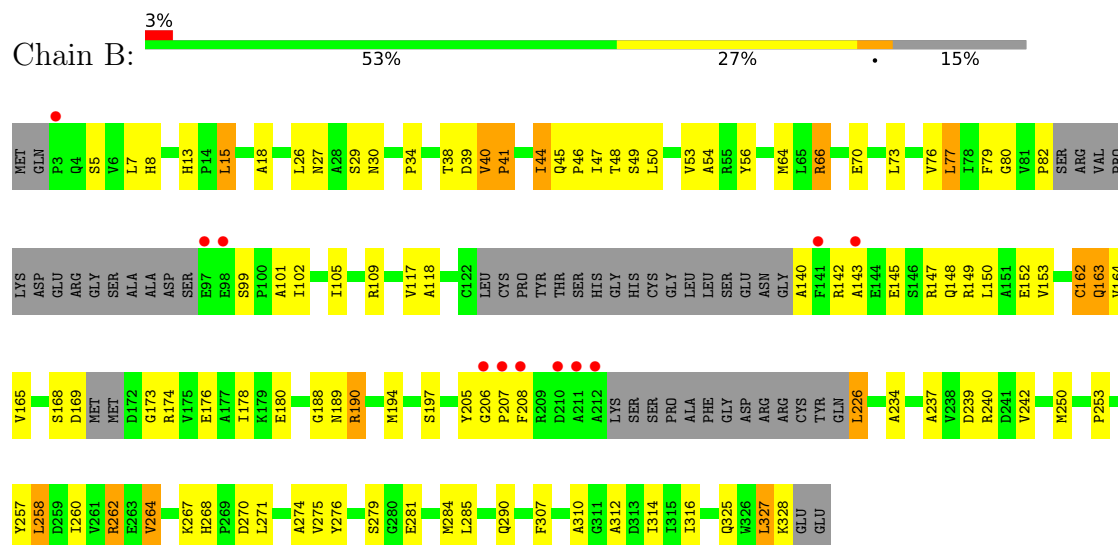
### 3 Residue-property plots

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 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: Delta-aminolevulinic acid dehydratase



#### • Molecule 1: Delta-aminolevulinic acid dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.57Å 89.57Å 153.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 2.20 34.60 – 2.21	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.00-2.20) 95.6 (34.60-2.21)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.284 0.189 , 0.275	Depositor DCC
$R_{free}$ test set	3346 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.229 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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, 0.333 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: ZN, PB1

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	0.74	0/2152	0.94	4/2923 (0.1%)
1	B	0.75	0/2177	0.91	1/2960 (0.0%)
All	All	0.74	0/4329	0.92	5/5883 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	258	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	226	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	330	GLU	N-CA-C	-5.30	96.70	111.00
1	A	15	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	309	ARG	NE-CZ-NH1	-5.18	117.71	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	TYR	Sidechain



## 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	2108	0	2106	97	0
1	B	2130	0	2130	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	15	21	0
4	A	123	0	0	10	0
4	B	118	0	0	3	0
All	All	4497	0	4251	187	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 22.

All (187) 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:B:194:MET:CE	1:B:194:MET:SD	2.04	1.46
3:A:350:PB1:N1	3:A:350:PB1:H112	1.57	1.19
1:B:49:SER:HB2	1:B:207:PRO:HB3	1.17	1.09
1:A:49:SER:HB3	1:A:207:PRO:HB3	1.37	1.06
1:B:117:VAL:H	1:B:163:GLN:NE2	1.61	0.98
1:B:260:ILE:O	1:B:264:VAL:HG12	1.65	0.97
1:B:27:ASN:HD22	1:B:29:SER:H	1.14	0.94
1:A:106:HIS:O	1:A:110:LYS:HE2	1.67	0.93
1:A:107:LEU:O	1:A:111:THR:HG22	1.68	0.92
1:B:49:SER:CB	1:B:207:PRO:HB3	2.02	0.89
1:B:49:SER:HB2	1:B:207:PRO:CB	2.03	0.89
1:B:47:ILE:HG13	1:B:54:ALA:HA	1.58	0.85
4:A:535:HOH:O	1:B:207:PRO:HD3	1.75	0.85
1:B:239:ASP:OD2	1:B:267:LYS:HE2	1.80	0.81
3:A:350:PB1:N12	3:A:350:PB1:H91	1.94	0.81
1:A:24:THR:CG2	1:A:305:THR:HG23	2.12	0.80
3:A:350:PB1:H112	3:A:350:PB1:HN11	1.44	0.78
1:A:99:SER:O	1:A:103:GLU:HG3	1.85	0.76
1:A:207:PRO:HB2	1:A:279:SER:HB2	1.68	0.75
1:A:240:ARG:HH11	1:A:240:ARG:HB3	1.50	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLY:O	1:B:82:PRO:HD3	1.87	0.74
1:A:59:LYS:N	1:A:59:LYS:HD3	1.99	0.74
1:A:49:SER:O	1:A:51:PRO:HD3	1.88	0.74
1:A:105:ILE:O	1:A:109:ARG:HG2	1.88	0.74
1:B:145:GLU:O	1:B:149:ARG:HG3	1.87	0.74
1:B:27:ASN:ND2	1:B:29:SER:H	1.84	0.74
3:A:350:PB1:H91	3:A:350:PB1:HN11	1.52	0.73
1:A:37:VAL:HG12	1:A:100:PRO:HB2	1.70	0.73
1:B:117:VAL:H	1:B:163:GLN:HE21	1.37	0.72
1:A:207:PRO:O	1:A:210:ASP:HB2	1.90	0.72
1:B:39:ASP:O	1:B:41:PRO:HD3	1.89	0.71
1:A:39:ASP:O	1:A:41:PRO:HD3	1.91	0.70
1:A:24:THR:HG21	1:A:305:THR:HG23	1.74	0.70
1:B:118:ALA:HA	1:B:164:VAL:HB	1.73	0.69
3:A:350:PB1:HN11	3:A:350:PB1:C9	2.04	0.69
1:A:49:SER:CB	1:A:207:PRO:HB3	2.20	0.69
1:A:176:GLU:O	1:A:180:GLU:HG2	1.93	0.69
1:A:282:PHE:CD2	1:A:318:TYR:HB2	2.28	0.68
1:A:162:CYS:SG	1:A:165:VAL:CG1	2.84	0.66
3:A:350:PB1:N1	3:A:350:PB1:C11	2.49	0.66
1:B:188:GLY:C	1:B:189:ASN:HD22	1.98	0.66
1:A:259:ASP:HB2	1:B:262:ARG:HG3	1.79	0.65
1:B:44:ILE:HG12	1:B:44:ILE:O	1.96	0.64
1:A:284:MET:HE2	1:B:284:MET:SD	2.37	0.64
1:B:50:LEU:HD21	1:B:279:SER:HB2	1.79	0.63
1:A:37:VAL:CG1	1:A:100:PRO:HB2	2.29	0.63
1:B:77:LEU:HD13	1:B:79:PHE:CE2	2.36	0.61
1:A:109:ARG:HA	4:A:549:HOH:O	1.99	0.61
1:A:162:CYS:SG	1:A:165:VAL:HG13	2.41	0.61
1:A:41:PRO:HB3	1:A:59:LYS:HE2	1.82	0.61
1:B:99:SER:HB3	1:B:102:ILE:HD13	1.83	0.61
1:B:46:PRO:HA	1:B:54:ALA:HB2	1.84	0.60
1:B:117:VAL:H	1:B:163:GLN:HE22	1.47	0.60
1:B:150:LEU:O	1:B:150:LEU:HD23	2.02	0.59
1:A:47:ILE:HG22	1:A:50:LEU:H	1.67	0.59
1:A:208:PHE:HB2	3:A:350:PB1:C8	2.32	0.59
1:A:122:CYS:O	1:A:122:CYS:SG	2.60	0.59
1:A:309:ARG:NH2	4:A:511:HOH:O	2.26	0.59
1:B:190:ARG:HH11	1:B:190:ARG:HG2	1.67	0.59
1:A:48:THR:HA	4:A:583:HOH:O	2.02	0.58
1:B:150:LEU:HD22	1:B:178:ILE:HD11	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:CYS:SG	1:A:165:VAL:HG12	2.44	0.58
1:B:281:GLU:O	1:B:285:LEU:HD23	2.03	0.58
1:A:210:ASP:O	1:A:212:ALA:N	2.28	0.58
1:B:73:LEU:HD21	1:B:76:VAL:HG13	1.85	0.58
1:A:40:VAL:HG11	1:A:43:ASP:OD1	2.04	0.58
1:A:50:LEU:HD13	1:A:207:PRO:CB	2.35	0.57
1:B:189:ASN:HD22	1:B:189:ASN:N	2.00	0.57
1:A:24:THR:HG23	1:A:305:THR:HG23	1.88	0.56
1:B:250:MET:HA	1:B:274:ALA:O	2.05	0.56
1:A:58:VAL:HG23	4:A:541:HOH:O	2.04	0.56
1:B:275:VAL:HG21	1:B:312:ALA:HB2	1.88	0.56
1:A:240:ARG:HB3	1:A:240:ARG:NH1	2.20	0.56
1:A:157:TYR:O	1:A:162:CYS:HB3	2.06	0.55
1:B:149:ARG:O	1:B:153:VAL:HG23	2.06	0.55
1:B:258:LEU:HD11	1:B:307:PHE:CD1	2.42	0.55
1:A:304:MET:SD	1:A:315:ILE:HG21	2.46	0.55
1:A:67:PRO:O	1:A:71:GLU:HG2	2.07	0.55
1:B:189:ASN:N	1:B:189:ASN:ND2	2.55	0.55
1:A:71:GLU:HA	1:A:328:LYS:NZ	2.20	0.55
1:B:50:LEU:HD21	1:B:279:SER:CB	2.37	0.55
1:A:239:ASP:O	1:A:243:ARG:HG3	2.07	0.54
1:A:284:MET:CE	1:B:284:MET:SD	2.94	0.54
1:B:13:HIS:CE1	1:B:15:LEU:HB2	2.42	0.54
1:A:297:LYS:HA	1:A:326:TRP:CH2	2.42	0.54
1:A:97:GLU:HG2	1:A:97:GLU:O	2.09	0.53
1:A:208:PHE:CE2	3:A:350:PB1:H92	2.44	0.53
1:B:27:ASN:HD22	1:B:29:SER:N	1.95	0.53
1:A:50:LEU:HD13	1:A:207:PRO:HB2	1.91	0.53
1:B:148:GLN:O	1:B:152:GLU:HG2	2.09	0.52
1:B:275:VAL:CG2	1:B:312:ALA:HB2	2.39	0.52
1:B:270:ASP:HB2	4:B:506:HOH:O	2.09	0.52
1:B:77:LEU:HD13	1:B:79:PHE:HE2	1.73	0.52
1:B:50:LEU:HB2	1:B:53:VAL:HB	1.91	0.52
1:B:262:ARG:HG2	1:B:310:ALA:O	2.09	0.51
1:A:80:GLY:C	1:A:82:PRO:HD3	2.29	0.51
1:A:208:PHE:CG	3:A:350:PB1:C8	2.93	0.51
1:A:208:PHE:CB	3:A:350:PB1:C8	2.88	0.51
1:A:145:GLU:CB	1:A:149:ARG:NH2	2.74	0.50
1:A:121:VAL:HG22	1:A:157:TYR:CD2	2.47	0.50
1:B:207:PRO:HB2	1:B:279:SER:HB2	1.94	0.50
1:A:184:ALA:HB3	1:A:185:HIS:HD1	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:TYR:CZ	1:B:64:MET:HG3	2.47	0.50
1:A:328:LYS:HE2	4:A:597:HOH:O	2.11	0.49
1:A:44:ILE:O	1:A:46:PRO:HD3	2.12	0.49
1:A:58:VAL:HA	1:A:61:LEU:HD22	1.94	0.49
1:B:239:ASP:CG	1:B:267:LYS:HE2	2.33	0.49
1:B:271:LEU:HD22	1:B:271:LEU:H	1.78	0.49
1:A:168:SER:HB2	3:A:350:PB1:H111	1.94	0.49
3:A:350:PB1:N1	3:A:350:PB1:C9	2.75	0.49
1:A:284:MET:HE3	1:B:284:MET:HG3	1.95	0.49
1:A:38:THR:CG2	1:A:55:ARG:HB3	2.43	0.48
1:B:44:ILE:O	1:B:44:ILE:CG1	2.61	0.48
1:B:176:GLU:O	1:B:180:GLU:HG3	2.13	0.48
1:B:284:MET:HG3	1:B:285:LEU:HD22	1.96	0.48
1:B:162:CYS:SG	1:B:165:VAL:HG12	2.53	0.48
1:B:143:ALA:O	1:B:147:ARG:HD3	2.14	0.48
1:B:66:ARG:HD2	1:B:70:GLU:OE2	2.13	0.48
1:A:150:LEU:O	1:A:150:LEU:HD13	2.13	0.48
3:A:350:PB1:H92	3:A:350:PB1:H61	1.54	0.48
1:B:27:ASN:N	1:B:30:ASN:OD1	2.40	0.48
1:A:325:GLN:HE21	1:A:325:GLN:HA	1.78	0.48
1:A:252:LYS:CE	3:A:350:PB1:C5	2.93	0.47
1:A:189:ASN:HB3	4:A:691:HOH:O	2.13	0.47
3:A:350:PB1:N12	3:A:350:PB1:C9	2.73	0.47
1:B:169:ASP:C	1:B:174:ARG:HH11	2.18	0.47
1:A:184:ALA:HB3	1:A:185:HIS:ND1	2.30	0.47
1:A:282:PHE:HD2	1:A:318:TYR:HB2	1.78	0.47
3:A:350:PB1:HN11	3:A:350:PB1:C11	2.21	0.46
1:A:150:LEU:HD13	1:A:150:LEU:C	2.35	0.46
1:A:208:PHE:CD2	3:A:350:PB1:H61	2.50	0.46
1:B:150:LEU:CD2	1:B:178:ILE:HD11	2.45	0.46
1:B:242:VAL:HG21	1:B:268:HIS:CE1	2.51	0.46
1:A:71:GLU:O	1:A:328:LYS:HE3	2.16	0.46
1:A:97:GLU:HA	1:A:102:ILE:HG21	1.97	0.46
1:B:169:ASP:H	1:B:174:ARG:HH11	1.63	0.46
1:A:111:THR:HG23	1:A:112:PHE:CD2	2.51	0.46
1:B:140:ALA:C	1:B:142:ARG:N	2.69	0.46
1:B:274:ALA:HA	1:B:314:ILE:O	2.15	0.46
1:B:325:GLN:O	1:B:328:LYS:HG2	2.16	0.46
3:A:350:PB1:H112	3:A:350:PB1:C2	2.42	0.45
1:A:249:LEU:HB2	1:A:273:LEU:CD1	2.46	0.45
1:A:205:TYR:HB2	4:A:589:HOH:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLU:CB	1:A:149:ARG:CZ	2.95	0.45
1:A:252:LYS:HE2	3:A:350:PB1:H21	1.71	0.45
1:A:12:LEU:HD11	1:A:16:LEU:HD13	1.98	0.45
1:A:166:ALA:HA	1:A:194:MET:O	2.17	0.45
4:A:535:HOH:O	1:B:206:GLY:N	2.49	0.45
1:A:252:LYS:HE2	3:A:350:PB1:C5	2.47	0.45
1:B:237:ALA:HA	1:B:240:ARG:NH1	2.32	0.45
1:A:50:LEU:HD13	1:A:207:PRO:HB3	2.00	0.44
1:A:50:LEU:CD1	1:A:207:PRO:HB2	2.47	0.44
1:B:140:ALA:O	1:B:143:ALA:HB3	2.17	0.44
1:A:207:PRO:O	1:A:210:ASP:CB	2.61	0.44
1:A:262:ARG:O	1:A:262:ARG:HD3	2.16	0.44
1:B:117:VAL:N	1:B:163:GLN:NE2	2.46	0.44
1:A:111:THR:HG23	1:A:112:PHE:N	2.33	0.44
1:A:162:CYS:SG	1:A:162:CYS:O	2.75	0.44
1:A:258:LEU:HD11	1:A:307:PHE:HD1	1.83	0.44
1:A:240:ARG:NH2	1:A:241:ASP:OD1	2.51	0.43
1:B:13:HIS:HE1	1:B:15:LEU:HB2	1.82	0.43
1:B:194:MET:CE	1:B:194:MET:CG	2.93	0.43
1:B:208:PHE:HB2	1:B:279:SER:OG	2.18	0.43
1:B:34:PRO:HG3	1:B:316:ILE:CG2	2.48	0.43
1:B:205:TYR:CE1	1:B:253:PRO:HG3	2.53	0.43
1:A:56:TYR:CZ	1:A:64:MET:HG3	2.54	0.42
1:B:18:ALA:HA	4:B:709:HOH:O	2.19	0.42
1:B:109:ARG:HD2	4:B:512:HOH:O	2.19	0.42
1:B:258:LEU:HD11	1:B:307:PHE:HD1	1.83	0.42
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.81	0.42
1:B:5:SER:O	1:B:7:LEU:HD22	2.20	0.42
1:B:38:THR:HG23	1:B:40:VAL:H	1.84	0.42
1:A:176:GLU:HB2	1:A:244:GLU:HG2	2.01	0.42
1:A:185:HIS:ND1	1:A:185:HIS:N	2.68	0.42
1:A:250:MET:HG2	1:A:251:VAL:N	2.35	0.42
1:A:208:PHE:HB2	3:A:350:PB1:O4	2.19	0.42
1:A:297:LYS:HG3	1:A:326:TRP:CE2	2.55	0.42
1:B:226:LEU:HD21	1:B:234:ALA:HA	2.02	0.41
1:A:210:ASP:C	1:A:212:ALA:H	2.17	0.41
1:A:231:ARG:HD2	4:A:513:HOH:O	2.21	0.41
1:A:249:LEU:HB2	1:A:273:LEU:HD12	2.01	0.41
1:A:39:ASP:C	1:A:41:PRO:HD3	2.41	0.40
1:A:297:LYS:HG3	1:A:326:TRP:CD2	2.56	0.40
1:B:190:ARG:HG2	1:B:190:ARG:NH1	2.35	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:O	1:B:105:ILE:HG13	2.21	0.40
1:B:327:LEU:O	1:B:328:LYS:HD3	2.21	0.40
1:A:71:GLU:HA	1:A:328:LYS:HZ1	1.84	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	266/330 (81%)	254 (96%)	10 (4%)	2 (1%)	19	19
1	B	270/330 (82%)	251 (93%)	16 (6%)	3 (1%)	14	12
All	All	536/660 (81%)	505 (94%)	26 (5%)	5 (1%)	17	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ALA
1	B	173	GLY
1	A	206	GLY
1	B	41	PRO
1	B	197	SER

### 5.3.2 Protein sidechains [i](#)

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	216/267 (81%)	199 (92%)	17 (8%)	12	12
1	B	218/267 (82%)	199 (91%)	19 (9%)	10	10
All	All	434/534 (81%)	398 (92%)	36 (8%)	11	11

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	49	SER
1	A	50	LEU
1	A	61	LEU
1	A	62	GLU
1	A	71	GLU
1	A	122	CYS
1	A	123	LEU
1	A	162	CYS
1	A	190	ARG
1	A	199	LYS
1	A	209	ARG
1	A	210	ASP
1	A	258	LEU
1	A	276	TYR
1	A	285	LEU
1	A	327	LEU
1	B	8	HIS
1	B	15	LEU
1	B	26	LEU
1	B	40	VAL
1	B	44	ILE
1	B	45	GLN
1	B	48	THR
1	B	66	ARG
1	B	77	LEU
1	B	162	CYS
1	B	163	GLN
1	B	168	SER
1	B	190	ARG
1	B	258	LEU
1	B	262	ARG
1	B	264	VAL
1	B	276	TYR
1	B	290	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	325	GLN
1	B	27	ASN
1	B	45	GLN
1	B	114	ASN
1	B	163	GLN
1	B	189	ASN
1	B	290	GLN
1	B	325	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	PB1	A	350	1	9,15,15	0.71	0	6,18,18	0.99	1 (16%)

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	PB1	A	350	1	-	5/14/18/18	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	350	PB1	C6-C3-C4	-2.15	106.77	112.55

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	350	PB1	C3-C4-C9-C10
3	A	350	PB1	N1-C2-C3-C6
3	A	350	PB1	N1-C2-C3-C4
3	A	350	PB1	C9-C4-C5-C11
3	A	350	PB1	C5-C4-C9-C10

There are no ring outliers.

1 monomer is involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	350	PB1	21	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	276/330 (83%)	-0.24	7 (2%) 57 55	16, 31, 70, 89	0
1	B	280/330 (84%)	-0.16	11 (3%) 39 37	12, 33, 75, 86	0
All	All	556/660 (84%)	-0.20	18 (3%) 47 45	12, 32, 72, 89	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	ALA	6.9
1	B	212	ALA	6.5
1	A	212	ALA	6.1
1	B	3	PRO	4.5
1	B	210	ASP	4.2
1	A	211	ALA	4.1
1	B	206	GLY	4.1
1	B	207	PRO	3.8
1	A	124	CYS	3.6
1	B	97	GLU	3.5
1	A	207	PRO	3.1
1	B	98	GLU	3.0
1	A	206	GLY	2.9
1	A	82	PRO	2.6
1	A	210	ASP	2.6
1	B	208	PHE	2.5
1	B	143	ALA	2.5
1	B	141	PHE	2.2

### 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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	401	1/1	0.81	0.14	92,92,92,92	1
2	ZN	A	401	1/1	0.90	0.09	92,92,92,92	1
3	PB1	A	350	16/16	0.92	0.20	26,59,92,92	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.