



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3UJF  
Title : Asymmetric complex of human neuron specific enolase-4-PGA/PEP  
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Deposited on : 2011-11-07  
Resolution : 2.10 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

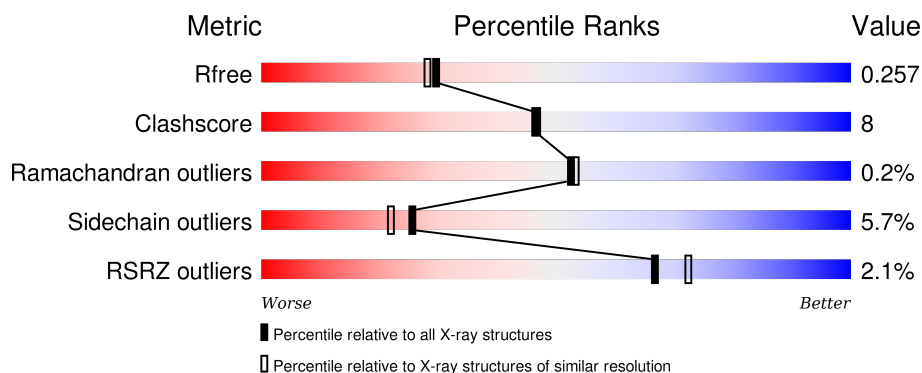
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	443	
1	B	443	

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	MG	A	501	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6835 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 Gamma-enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3314	2084	568	649	13			
1	B	432	Total	C	N	O	S	0	0	0
			3306	2078	567	648	13			

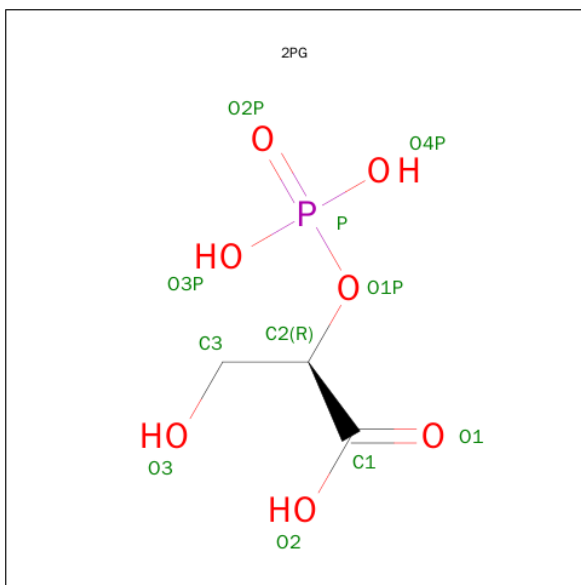
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	HIS	-	EXPRESSION TAG	UNP P09104
A	435	HIS	-	EXPRESSION TAG	UNP P09104
A	436	HIS	-	EXPRESSION TAG	UNP P09104
A	437	HIS	-	EXPRESSION TAG	UNP P09104
A	438	HIS	-	EXPRESSION TAG	UNP P09104
A	439	HIS	-	EXPRESSION TAG	UNP P09104
A	440	HIS	-	EXPRESSION TAG	UNP P09104
A	441	HIS	-	EXPRESSION TAG	UNP P09104
A	442	HIS	-	EXPRESSION TAG	UNP P09104
A	443	HIS	-	EXPRESSION TAG	UNP P09104
B	434	HIS	-	EXPRESSION TAG	UNP P09104
B	435	HIS	-	EXPRESSION TAG	UNP P09104
B	436	HIS	-	EXPRESSION TAG	UNP P09104
B	437	HIS	-	EXPRESSION TAG	UNP P09104
B	438	HIS	-	EXPRESSION TAG	UNP P09104
B	439	HIS	-	EXPRESSION TAG	UNP P09104
B	440	HIS	-	EXPRESSION TAG	UNP P09104
B	441	HIS	-	EXPRESSION TAG	UNP P09104
B	442	HIS	-	EXPRESSION TAG	UNP P09104
B	443	HIS	-	EXPRESSION TAG	UNP P09104

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

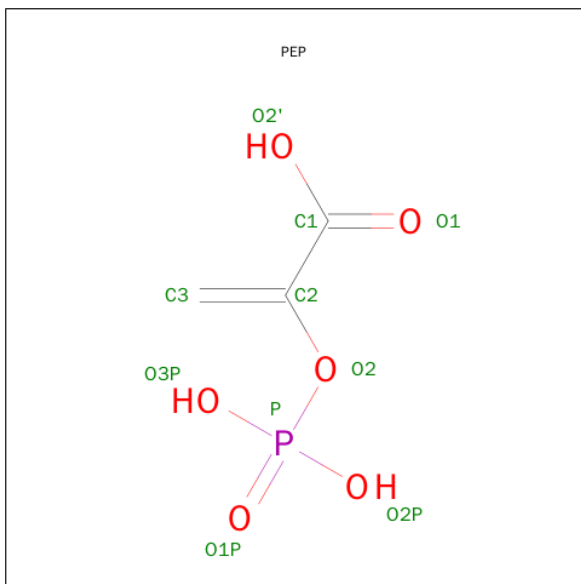
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula:  $C_3H_7O_7P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 11 3 7 1	0	0

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula:  $C_3H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		
5	B	102	Total	O	0	0
			102	102		

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.

[illegible]

Chain B:

2% 80% 15%

S1 W6 D12 G15 L29 F30 V34 Q64 L57 A73 P74 A75 L76 L92 N93 L94 D97 M101 K102 S103 K104 M108 T133 G138 D141 F149 T152 M153 G154 G155 S156 G159 M168 R178 N215 K238 F200 F250 Y251 G254 D257 F260 K261 S262 P263 T264 D265 Y269 D273 Y279 V283 D293 P294 W303 N309 T322 N323 P324 E328 C336 L340 L341 K342 K357 L358 E361 N364 H370 L383 C388 T389 T394 G395 R399 F200

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.61Å 119.34Å 68.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.39 – 2.10 37.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.2 (37.39-2.10) 89.2 (37.39-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.75 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.194 , 0.259 0.194 , 0.257	Depositor DCC
$R_{free}$ test set	2687 reflections (6.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.9	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	0 of 47007 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEP, 2PG

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	1.03	2/3369 (0.1%)	0.87	4/4558 (0.1%)
1	B	1.00	2/3361 (0.1%)	0.89	0/4547
All	All	1.02	4/6730 (0.1%)	0.88	4/9105 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	TYR	CD2-CE2	6.30	1.48	1.39
1	B	34	VAL	CB-CG2	6.16	1.65	1.52
1	A	61	VAL	CB-CG2	5.40	1.64	1.52
1	B	303	TRP	CE3-CZ3	5.09	1.47	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	LEU	CA-CB-CG	6.26	129.71	115.30
1	A	402	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	29	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	402	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3314	0	3289	59	1
1	B	3306	0	3278	49	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	4	2	0
4	B	10	0	2	0	0
5	A	88	0	0	2	0
5	B	102	0	0	1	1
All	All	6835	0	6573	101	1

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 8.

All (101) 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:A:334:LYS:HE3	1:A:334:LYS:HA	1.49	0.93
1:A:271:THR:OG1	1:A:274:GLN:HG3	1.70	0.91
1:A:215:ASN:HD22	1:A:215:ASN:H	1.21	0.86
1:A:101:ASN:H	1:A:101:ASN:HD22	1.24	0.84
1:B:141:ASP:O	1:B:388:CYS:SG	2.37	0.83
1:A:102:LYS:HE2	1:A:346:ILE:O	1.85	0.76
1:B:101:ASN:H	1:B:101:ASN:HD22	1.36	0.73
1:A:400:SER:HB2	1:B:401:GLU:HB3	1.71	0.72
1:B:238:LYS:HE3	5:B:616:HOH:O	1.92	0.70
1:A:205:ASN:OD1	5:A:621:HOH:O	2.10	0.68
1:A:102:LYS:HB2	5:A:620:HOH:O	1.94	0.67
1:A:215:ASN:ND2	1:A:215:ASN:H	1.92	0.66
1:A:401:GLU:HB3	1:B:400:SER:HB2	1.80	0.64
1:A:101:ASN:H	1:A:101:ASN:ND2	1.96	0.62
1:B:294:PRO:HD2	1:B:303:TRP:CH2	2.34	0.62
1:A:73:ALA:O	1:A:77:ILE:HG13	1.98	0.62
1:A:182:ARG:NH1	1:B:54:GLN:O	2.33	0.61
1:A:342:LYS:HZ3	3:A:503:2PG:H2	1.66	0.61
1:B:76:LEU:HD23	1:B:92:LEU:HD23	1.83	0.61
1:B:73:ALA:HB3	1:B:74:PRO:HD3	1.83	0.60
1:B:340:LEU:HD23	1:B:342:LYS:HE3	1.84	0.60
1:A:164:MET:HG2	1:A:245:VAL:HG13	1.85	0.59
1:B:322:THR:HG23	1:B:341:LEU:HD12	1.85	0.58
1:B:357:LYS:O	1:B:361:GLU:HB2	2.04	0.58
1:A:400:SER:CB	1:B:401:GLU:HB3	2.34	0.58
1:A:143:ILE:HD13	1:A:423:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:CD2	1:B:92:LEU:HD23	2.36	0.56
1:A:41:GLY:O	1:A:44:GLU:HG3	2.06	0.55
1:A:143:ILE:HD12	1:A:143:ILE:C	2.27	0.55
1:B:155:GLY:O	1:B:261:LYS:CE	2.55	0.55
1:A:313:GLN:HA	1:A:337:ASN:HD21	1.73	0.54
1:B:328:GLU:HG2	1:B:358:LEU:HD21	1.90	0.54
1:A:68:ILE:HD11	1:A:109:ALA:HA	1.90	0.54
1:B:251:TYR:OH	1:B:254:GLY:HA2	2.09	0.53
1:A:293:ASP:OD2	1:A:317:ASP:HB3	2.10	0.52
1:A:244:ASP:HA	1:A:292:GLU:HB3	1.92	0.51
1:A:245:VAL:HG11	1:A:279:TYR:OH	2.10	0.51
1:B:149:PHE:O	1:B:168:MET:HA	2.11	0.51
1:A:227:LYS:HE3	1:A:286:TYR:CD1	2.46	0.51
1:B:101:ASN:N	1:B:101:ASN:HD22	2.08	0.51
1:B:94:LEU:HD22	1:B:102:LYS:HE3	1.91	0.51
1:B:264:THR:HG22	1:B:265:ASP:N	2.27	0.50
1:A:337:ASN:C	1:A:337:ASN:HD22	2.15	0.50
1:B:293:ASP:HA	1:B:303:TRP:CH2	2.47	0.49
1:A:359:ALA:O	1:A:364:TRP:HB2	2.12	0.49
1:A:101:ASN:HD22	1:A:101:ASN:N	2.02	0.49
1:A:340:LEU:HD23	1:A:342:LYS:HE3	1.95	0.49
1:B:97:ASP:OD1	1:B:104:LYS:HB3	2.12	0.49
1:B:153:ASN:N	1:B:153:ASN:OD1	2.45	0.49
1:B:155:GLY:O	1:B:261:LYS:HD3	2.13	0.49
1:B:257:ASP:OD2	1:B:260:PHE:HA	2.12	0.49
1:A:319:LEU:O	1:A:326:ARG:HD3	2.13	0.49
1:B:155:GLY:O	1:B:261:LYS:NZ	2.46	0.48
1:A:293:ASP:HA	1:A:303:TRP:CH2	2.48	0.48
1:A:183:LEU:HB3	1:A:239:ILE:HD11	1.96	0.48
1:B:416:LEU:HB2	1:B:420:ALA:HB2	1.95	0.48
1:B:156:SER:OG	1:B:249:GLU:HB3	2.13	0.48
1:B:340:LEU:CD2	1:B:342:LYS:HE3	2.44	0.47
1:A:313:GLN:O	1:A:314:ILE:HD13	2.13	0.47
1:B:395:GLY:HA3	1:B:402:ARG:HD2	1.97	0.46
1:A:370:HIS:ND1	1:A:402:ARG:NH1	2.58	0.46
1:A:61:VAL:O	1:A:65:VAL:HG23	2.15	0.46
1:B:429:ASN:HD22	1:B:429:ASN:N	2.13	0.46
1:A:314:ILE:H	1:A:337:ASN:HD21	1.63	0.46
1:B:141:ASP:HB3	1:B:421:ARG:NH1	2.31	0.45
1:B:429:ASN:H	1:B:429:ASN:HD22	1.63	0.45
1:A:183:LEU:O	1:A:187:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:HIS:HE1	1:B:15:GLY:O	1.99	0.45
1:A:314:ILE:H	1:A:337:ASN:ND2	2.14	0.45
1:B:323:ASN:HA	1:B:324:PRO:HD2	1.67	0.45
1:A:4:LYS:HG3	1:A:24:TYR:HB2	1.98	0.45
1:A:334:LYS:HE3	1:A:334:LYS:CA	2.31	0.44
1:A:119:LYS:NZ	1:A:377:ASP:OD2	2.40	0.44
1:B:12:ASP:OD1	1:B:12:ASP:C	2.55	0.44
1:B:6:TRP:HA	1:B:6:TRP:CE3	2.53	0.44
1:B:29:LEU:HD12	1:B:30:PHE:N	2.33	0.43
1:A:257:ASP:HB2	1:A:269:TYR:CD1	2.53	0.43
1:A:44:GLU:CD	1:A:345:GLN:HG2	2.38	0.43
1:A:371:ARG:O	1:A:374:GLU:HG2	2.19	0.43
1:B:178:ARG:NE	1:B:413:GLU:OE1	2.50	0.42
1:B:279:TYR:O	1:B:283:VAL:HG23	2.19	0.42
1:A:401:GLU:HB3	1:B:400:SER:CB	2.48	0.42
1:A:342:LYS:NZ	3:A:503:2PG:H2	2.32	0.42
1:B:57:LEU:N	1:B:57:LEU:HD12	2.34	0.42
1:A:102:LYS:HD3	1:A:110:ILE:HD12	2.01	0.42
1:B:133:ILE:HD13	1:B:383:LEU:HA	2.01	0.42
1:A:141:ASP:O	1:A:388:CYS:SG	2.56	0.42
1:A:164:MET:H	1:A:219:ASN:HD21	1.68	0.42
1:B:394:THR:HG23	1:B:406:TYR:CZ	2.54	0.41
1:B:108:ASN:N	1:B:108:ASN:OD1	2.52	0.41
1:A:426:ASN:HB2	1:A:433:LEU:HD11	2.02	0.41
1:B:6:TRP:HE3	1:B:6:TRP:HA	1.85	0.41
1:A:143:ILE:HD11	1:A:390:GLY:HA2	2.01	0.41
1:A:265:ASP:HA	1:A:266:PRO:HD3	1.89	0.41
1:A:165:GLN:HB3	1:A:166:GLU:HG3	2.03	0.41
1:B:336:CYS:SG	1:B:364:TRP:CH2	3.13	0.41
1:A:292:GLU:OE1	1:A:340:LEU:HD22	2.21	0.41
1:A:284:ARG:HG3	1:A:285:ASP:N	2.37	0.40
1:A:201:LYS:HE3	1:B:261:LYS:HB3	2.04	0.40
1:A:370:HIS:CG	1:A:394:THR:HA	2.57	0.40
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.96	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:SER:OG	5:B:606:HOH:O[3_645]	2.09	0.11

## 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	431/443 (97%)	403 (94%)	28 (6%)	0	100	100
1	B	430/443 (97%)	408 (95%)	20 (5%)	2 (0%)	34	30
All	All	861/886 (97%)	811 (94%)	48 (6%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	TYR
1	B	399	ARG

### 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	350/360 (97%)	329 (94%)	21 (6%)	24	20
1	B	349/360 (97%)	330 (95%)	19 (5%)	27	24
All	All	699/720 (97%)	659 (94%)	40 (6%)	25	22

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	54	GLN
1	A	101	ASN
1	A	150	ASN

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Mol	Chain	Res	Type
1	A	215	ASN
1	A	237	GLU
1	A	264	THR
1	A	312	ILE
1	A	320	THR
1	A	325	LYS
1	A	337	ASN
1	A	344	ASN
1	A	357	LYS
1	A	370	HIS
1	A	372	SER
1	A	388	CYS
1	A	389	THR
1	A	391	GLN
1	A	403	LEU
1	A	418	ASP
1	A	419	GLU
1	B	6	TRP
1	B	29	LEU
1	B	97	ASP
1	B	101	ASN
1	B	141	ASP
1	B	152	ILE
1	B	153	ASN
1	B	178	ARG
1	B	215	ASN
1	B	273	ASP
1	B	309	ASN
1	B	370	HIS
1	B	388	CYS
1	B	389	THR
1	B	403	LEU
1	B	415	GLU
1	B	418	ASP
1	B	419	GLU
1	B	429	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	135	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	150	ASN
1	A	189	HIS
1	A	215	ASN
1	A	219	ASN
1	A	337	ASN
1	A	354	GLN
1	A	426	ASN
1	B	101	ASN
1	B	139	ASN
1	B	150	ASN
1	B	189	HIS
1	B	309	ASN
1	B	345	GLN
1	B	429	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	2PG	A	503	2	6,10,10	0.89	0	5,14,14	1.59	2 (40%)
4	PEP	B	503	2	5,9,9	1.33	1 (20%)	8,13,13	1.99	5 (62%)

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	2PG	A	503	2	-	0/7/11/11	0/0/0/0
4	PEP	B	503	2	-	0/5/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	PEP	O2-C2	2.44	1.46	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	PEP	O2P-P-O2	-2.07	98.49	105.25
4	B	503	PEP	O2-C2-C3	-2.07	120.55	124.73
3	A	503	2PG	P-O1P-C2	-2.04	112.53	121.17
3	A	503	2PG	O3P-P-O2P	2.12	117.39	110.58
4	B	503	PEP	C1-C2-C3	2.28	125.00	120.97
4	B	503	PEP	P-O2-C2	2.74	129.05	122.96
4	B	503	PEP	O2P-P-O1P	2.84	119.72	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	2PG	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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	433/443 (97%)	-0.12	10 (2%) 64 70	19, 33, 50, 60	0
1	B	432/443 (97%)	-0.09	8 (1%) 70 75	18, 33, 49, 64	5 (1%)
All	All	865/886 (97%)	-0.10	18 (2%) 67 72	18, 33, 50, 64	5 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	ASP	4.0
1	A	253	ASP	3.9
1	B	263	PRO	3.2
1	A	418	ASP	3.1
1	B	141	ASP	2.8
1	A	380	ILE	2.6
1	B	159	GLY	2.6
1	A	6	TRP	2.5
1	A	302	ALA	2.5
1	A	54	GLN	2.5
1	B	54	GLN	2.4
1	A	33	ALA	2.4
1	B	403	LEU	2.4
1	A	57	LEU	2.3
1	B	395	GLY	2.2
1	A	265	ASP	2.2
1	A	140	SER	2.2
1	B	138	GLY	2.0

### 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	MG	A	501	1/1	0.97	0.22	3.35	10,10,10,10	0
2	MG	A	502	1/1	0.95	0.14	1.28	13,13,13,13	0
2	MG	B	502	1/1	0.98	0.12	-0.12	9,9,9,9	0
4	PEP	B	503	10/10	0.99	0.12	-0.26	22,24,27,28	0
3	2PG	A	503	11/11	0.98	0.11	-0.32	26,29,36,40	0
2	MG	B	501	1/1	0.98	0.11	-1.26	5,5,5,5	0

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

There are no such residues in this entry.