



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 07:43 PM EST

PDB ID : 3UJR  
Title : Asymmetric complex of human neuron specific enolase-5-PGA/PEP  
Authors : Qin, J.; Chai, G.; Brewer, J.; Lovelace, L.; Lebioda, L.  
Deposited on : 2011-11-08  
Resolution : 1.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

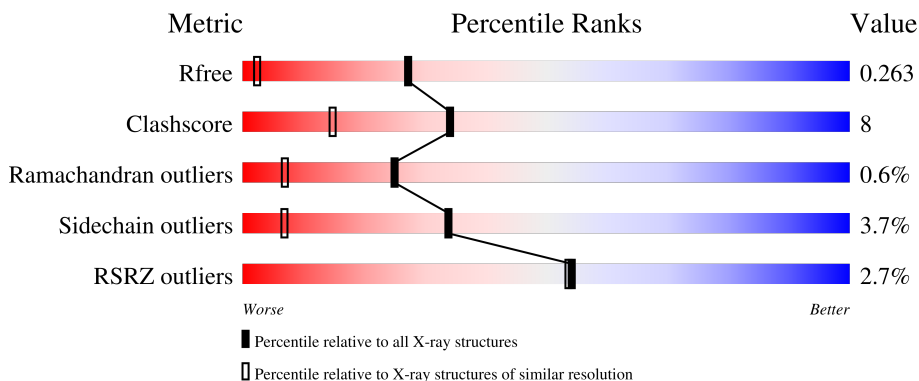
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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))
$R_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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	443	 83% 12% ..
1	B	443	 81% 14% ..

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7247 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
			Total	C	N	O	S			
1	A	433	3314	2084	568	649	13	0	0	0
1	B	432	3306	2078	567	648	13	0	0	0

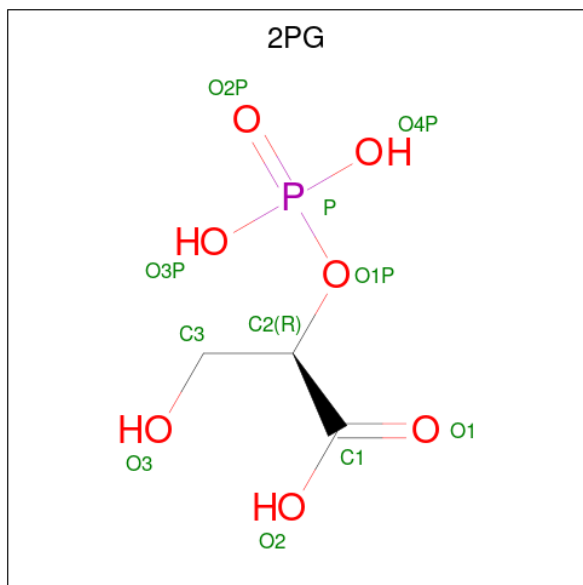
There are 20 discrepancies between the modelled and reference sequences:

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	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

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



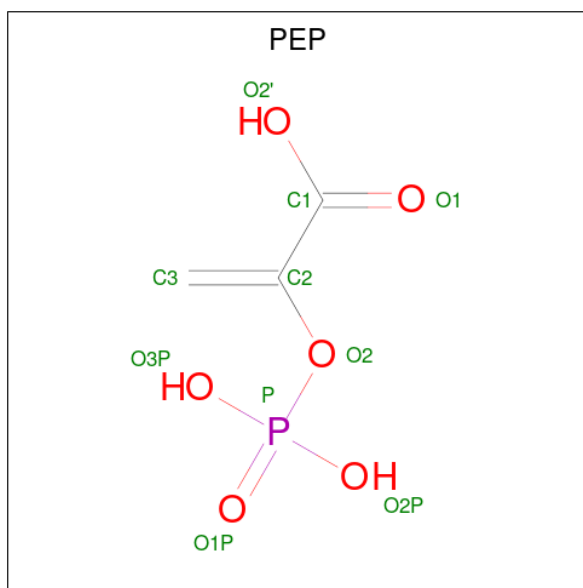
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 11 3 7 1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

- Molecule 5 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C<sub>3</sub>H<sub>5</sub>O<sub>6</sub>P).



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

- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	316	Total 316	O 316	0	0
6	B	278	Total 278	O 278	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.56Å 119.82Å 68.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.67 – 1.40 41.67 – 1.40	Depositor EDS
% Data completeness (in resolution range)	77.8 (41.67-1.40) 61.5 (41.67-1.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 1.40Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.214 , 0.264 0.212 , 0.263	Depositor DCC
$R_{free}$ test set	6887 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	5.0	Xtrriage
Anisotropy	0.097	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.28$ , $\langle L^2 \rangle = 0.12$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7247	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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 [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, TRS

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	1.12	4/3369 (0.1%)	1.08	8/4558 (0.2%)
1	B	1.12	3/3361 (0.1%)	1.07	9/4547 (0.2%)
All	All	1.12	7/6730 (0.1%)	1.08	17/9105 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	CYS	CB-SG	-7.15	1.70	1.82
1	A	413	GLU	CG-CD	-6.99	1.41	1.51
1	A	385	VAL	CB-CG2	-5.98	1.40	1.52
1	A	372	SER	CA-CB	5.51	1.61	1.52
1	B	384	VAL	CB-CG2	5.44	1.64	1.52
1	B	218	GLU	CB-CG	5.28	1.62	1.52
1	B	118	CYS	CB-SG	-5.23	1.73	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	326	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	B	273	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	131	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	326	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	319	LEU	CB-CG-CD1	-6.14	100.56	111.00
1	B	217	LEU	CA-CB-CG	5.95	128.98	115.30
1	B	162	LEU	CB-CG-CD2	-5.50	101.64	111.00
1	A	371	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	217	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	B	50	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	377	ASP	CB-CG-OD2	-5.31	113.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	371	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	183	LEU	CB-CG-CD2	5.17	119.79	111.00
1	B	191	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	A	56	TYR	CD1-CE1-CZ	-5.05	115.25	119.80

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	47	0
1	B	3306	0	3278	67	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	4	2	0
4	A	8	0	12	0	0
5	B	10	0	2	0	0
6	A	316	0	0	3	0
6	B	278	0	0	10	1
All	All	7247	0	6585	111	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 (111) 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:158:ALA:HB3	1:B:261:LYS:NZ	1.23	1.46
1:B:158:ALA:CB	1:B:261:LYS:NZ	2.12	1.11
1:B:257:ASP:OD1	1:B:268:ARG:HG3	1.58	1.01
1:B:158:ALA:O	1:B:160:ASN:N	1.95	0.99
1:B:215:ASN:H	1:B:215:ASN:HD22	1.13	0.94
1:B:158:ALA:HB3	1:B:261:LYS:HZ3	1.21	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ALA:CB	1:B:261:LYS:HZ2	1.82	0.82
1:A:215:ASN:H	1:A:215:ASN:HD22	1.29	0.81
1:B:215:ASN:H	1:B:215:ASN:ND2	1.80	0.79
1:A:421:ARG:CG	1:A:421:ARG:HH11	1.96	0.79
1:A:421:ARG:HH11	1:A:421:ARG:HG2	1.50	0.76
1:A:231:ASP:OD2	1:A:236:THR:OG1	2.04	0.75
1:B:158:ALA:CB	1:B:261:LYS:HZ3	1.87	0.74
1:A:143:ILE:HD11	1:A:390:GLY:HA2	1.68	0.73
1:B:158:ALA:HB3	1:B:261:LYS:HZ2	0.90	0.72
1:B:162:LEU:HB3	6:B:724:HOH:O	1.90	0.71
1:B:155:GLY:O	1:B:261:LYS:CE	2.39	0.69
1:A:14:ARG:HH12	1:A:372:SER:HB3	1.61	0.66
1:A:143:ILE:HD13	1:A:423:ALA:HB2	1.78	0.65
1:B:154:GLY:CA	6:B:724:HOH:O	2.44	0.65
1:A:14:ARG:NH1	1:A:372:SER:HB3	2.12	0.65
1:B:154:GLY:HA2	6:B:724:HOH:O	1.97	0.65
1:B:155:GLY:O	1:B:261:LYS:NZ	2.28	0.65
1:A:421:ARG:HG2	1:A:421:ARG:NH1	2.10	0.64
1:B:429:ASN:HD22	1:B:429:ASN:H	1.42	0.64
1:B:158:ALA:HB1	1:B:160:ASN:OD1	1.99	0.63
1:B:101:ASN:HD22	1:B:101:ASN:H	1.46	0.63
1:A:400:SER:HB2	1:B:401:GLU:HB3	1.80	0.62
1:A:319:LEU:O	1:A:326:ARG:HD3	1.99	0.62
1:B:160:ASN:O	1:B:261:LYS:CE	2.48	0.62
1:B:156:SER:HA	1:B:260:PHE:HE1	1.65	0.61
1:B:429:ASN:HD22	1:B:429:ASN:N	1.96	0.61
1:B:198:LYS:NZ	1:B:221:GLU:OE2	2.31	0.60
1:B:161:LYS:HB2	6:B:741:HOH:O	2.01	0.60
1:A:14:ARG:HH22	1:A:372:SER:HB3	1.66	0.60
1:B:158:ALA:C	1:B:160:ASN:N	2.55	0.60
1:A:14:ARG:NH2	1:A:372:SER:HB3	2.16	0.59
1:A:337:ASN:HD22	1:A:337:ASN:C	2.06	0.58
1:B:155:GLY:O	1:B:261:LYS:CD	2.52	0.58
1:B:160:ASN:O	1:B:261:LYS:HE3	2.03	0.58
1:B:53:LYS:HG3	6:B:719:HOH:O	2.04	0.58
1:B:155:GLY:O	1:B:261:LYS:HD3	2.04	0.57
1:B:94:LEU:CD2	1:B:102:LYS:HE3	2.34	0.57
1:B:259:ASP:O	1:B:261:LYS:N	2.37	0.57
1:B:215:ASN:HD22	1:B:215:ASN:N	1.93	0.56
1:A:78:SER:OG	6:A:640:HOH:O	2.18	0.56
1:A:113:VAL:O	1:A:117:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:SER:HA	1:B:260:PHE:CE1	2.42	0.55
1:A:70:SER:HB2	6:A:895:HOH:O	2.07	0.54
1:A:143:ILE:CD1	1:A:423:ALA:HB2	2.37	0.54
1:A:313:GLN:HA	1:A:337:ASN:HD21	1.73	0.54
1:B:178:ARG:HG2	1:B:410:MET:SD	2.49	0.53
1:A:14:ARG:HH12	1:A:372:SER:CB	2.21	0.53
1:A:29:LEU:C	1:A:29:LEU:HD23	2.29	0.53
1:A:131:ARG:CZ	1:A:142:LEU:HD11	2.39	0.52
1:B:250:PHE:HB3	1:B:260:PHE:CD2	2.43	0.52
1:A:284:ARG:NE	1:A:285:ASP:OD1	2.40	0.52
1:A:416:LEU:O	1:A:419:GLU:HB3	2.10	0.51
1:B:73:ALA:HB3	1:B:74:PRO:HD3	1.92	0.51
1:A:14:ARG:CZ	1:A:372:SER:HB3	2.40	0.51
1:B:149:PHE:O	1:B:168:MET:HA	2.11	0.51
1:B:156:SER:O	1:B:156:SER:OG	2.29	0.50
1:B:161:LYS:HE3	1:B:262:SER:OG	2.11	0.50
1:B:370:HIS:CG	1:B:394:THR:HA	2.46	0.50
1:B:154:GLY:C	1:B:158:ALA:HB2	2.32	0.50
1:B:252:ARG:HH21	1:B:260:PHE:HB2	1.77	0.50
1:B:231:ASP:HB2	6:B:723:HOH:O	2.11	0.50
1:A:342:LYS:HZ3	3:A:503:2PG:H2	1.76	0.50
1:A:29:LEU:HD23	1:A:30:PHE:N	2.27	0.50
1:B:213:ALA:O	1:B:214:PRO:C	2.49	0.50
1:B:213:ALA:C	1:B:214:PRO:O	2.48	0.49
1:B:187:VAL:HG21	1:B:239:ILE:CD1	2.42	0.49
1:A:164:MET:H	1:A:219:ASN:HD21	1.59	0.49
1:A:189:HIS:HD2	6:B:781:HOH:O	1.95	0.49
1:B:265:ASP:O	1:B:268:ARG:HG2	2.13	0.49
1:B:162:LEU:HD11	1:B:219:ASN:HA	1.94	0.48
1:B:160:ASN:HB3	1:B:213:ALA:HB1	1.96	0.48
1:B:162:LEU:HD12	1:B:217:LEU:O	2.14	0.48
1:B:153:ASN:ND2	1:B:211:GLY:H	2.13	0.47
1:A:149:PHE:O	1:A:168:MET:HA	2.15	0.47
1:B:143:ILE:HD11	1:B:423:ALA:HA	1.97	0.46
1:A:314:ILE:H	1:A:337:ASN:HD21	1.62	0.46
1:B:293:ASP:HA	1:B:303:TRP:CH2	2.50	0.46
1:A:143:ILE:HD11	1:A:390:GLY:CA	2.44	0.45
1:A:314:ILE:H	1:A:337:ASN:ND2	2.15	0.45
1:B:65:VAL:HG12	6:B:761:HOH:O	2.17	0.44
1:B:163:ALA:N	6:B:835:HOH:O	2.34	0.44
1:A:189:HIS:HE1	1:B:15:GLY:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:NH2	1:B:260:PHE:HB2	2.33	0.44
1:A:265:ASP:HA	1:A:266:PRO:HD3	1.81	0.43
1:B:53:LYS:CG	6:B:719:HOH:O	2.66	0.43
1:A:342:LYS:HZ1	3:A:503:2PG:C1	2.32	0.43
1:A:83:VAL:HG23	1:A:121:GLY:HA2	2.01	0.43
1:B:429:ASN:N	1:B:429:ASN:ND2	2.66	0.42
1:A:46:LEU:HD22	6:A:679:HOH:O	2.19	0.42
1:A:370:HIS:CG	1:A:394:THR:HA	2.55	0.41
1:B:266:PRO:HA	1:B:269:TYR:CZ	2.55	0.41
1:A:150:ASN:O	1:A:396:ALA:HB2	2.20	0.41
1:B:416:LEU:O	1:B:419:GLU:HB2	2.19	0.41
1:B:131:ARG:NH2	1:B:142:LEU:HD11	2.34	0.41
1:A:166:GLU:HB2	1:A:244:ASP:HB3	2.02	0.41
1:A:390:GLY:HA3	1:A:430:PRO:HG3	2.03	0.41
1:B:265:ASP:HB3	1:B:268:ARG:HD3	2.03	0.41
1:A:215:ASN:HD22	1:A:215:ASN:N	2.06	0.41
1:B:160:ASN:O	1:B:261:LYS:NZ	2.54	0.41
1:B:161:LYS:CE	1:B:262:SER:OG	2.69	0.41
1:B:340:LEU:HD12	1:B:340:LEU:HA	1.94	0.41
1:A:400:SER:CB	1:B:401:GLU:HB3	2.48	0.40
1:A:255:LYS:HB3	1:A:270:ILE:O	2.21	0.40
1:A:131:ARG:O	1:A:134:ALA:HB3	2.21	0.40
1:A:322:THR:HG22	1:A:322:THR:O	2.22	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:B:95:GLU:OE1	6:B:846:HOH:O[2_675]	2.03	0.17

## 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	431/443 (97%)	413 (96%)	17 (4%)	1 (0%)	47	21
1	B	430/443 (97%)	410 (95%)	16 (4%)	4 (1%)	17	3
All	All	861/886 (97%)	823 (96%)	33 (4%)	5 (1%)	25	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	PHE
1	B	159	GLY
1	B	264	THR
1	A	399	ARG
1	B	399	ARG

### 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	350/360 (97%)	334 (95%)	16 (5%)	27	4
1	B	349/360 (97%)	339 (97%)	10 (3%)	42	11
All	All	699/720 (97%)	673 (96%)	26 (4%)	34	7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	92	LEU
1	A	126	GLU
1	A	131	ARG
1	A	140	SER
1	A	201	LYS
1	A	202	ASP
1	A	215	ASN
1	A	284	ARG
1	A	325	LYS
1	A	337	ASN

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Mol	Chain	Res	Type
1	A	344	ASN
1	A	370	HIS
1	A	372	SER
1	A	418	ASP
1	A	421	ARG
1	B	101	ASN
1	B	156	SER
1	B	215	ASN
1	B	216	ILE
1	B	273	ASP
1	B	370	HIS
1	B	391	GLN
1	B	418	ASP
1	B	421	ARG
1	B	429	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	153	ASN
1	A	189	HIS
1	A	215	ASN
1	A	219	ASN
1	A	337	ASN
1	A	354	GLN
1	A	360	GLN
1	B	101	ASN
1	B	150	ASN
1	B	215	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	9,10,10	1.60	3 (33%)	11,14,14	2.45	1 (9%)
4	TRS	A	504	-	7,7,7	0.34	0	9,9,9	1.04	1 (11%)
5	PEP	B	503	2	9,9,9	1.23	1 (11%)	11,13,13	1.47	3 (27%)

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	-	4/11/11/11	-
4	TRS	A	504	-	-	3/9/9/9	-
5	PEP	B	503	2	-	0/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	2PG	O1-C1	2.69	1.30	1.22
3	A	503	2PG	P-O1P	2.29	1.63	1.59
3	A	503	2PG	C2-C1	-2.20	1.50	1.52
5	B	503	PEP	C2-C1	2.15	1.51	1.49

All (5) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	2PG	P-O1P-C2	-7.41	106.04	123.04
5	B	503	PEP	O2P-P-O1P	3.00	122.44	110.68
5	B	503	PEP	O2-C2-C3	-2.37	120.23	124.79
4	A	504	TRS	C2-C-N	2.24	114.66	107.98
5	B	503	PEP	O2P-P-O2	-2.08	98.92	105.25

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	2PG	C1-C2-C3-O3
4	A	504	TRS	C3-C-C2-O2
4	A	504	TRS	C1-C-C2-O2
3	A	503	2PG	O1P-C2-C3-O3
3	A	503	2PG	O1-C1-C2-C3
3	A	503	2PG	O2-C1-C2-C3
4	A	504	TRS	N-C-C2-O2

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	433/443 (97%)	0.27	4 (0%) 84 82	2, 5, 14, 25	0
1	B	432/443 (97%)	0.44	19 (4%) 34 34	2, 6, 18, 29	5 (1%)
All	All	865/886 (97%)	0.36	23 (2%) 54 54	2, 5, 17, 29	5 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	PRO	5.1
1	B	158	ALA	5.1
1	B	260	PHE	5.0
1	B	156	SER	4.3
1	A	418	ASP	4.0
1	B	159	GLY	3.9
1	B	155	GLY	3.7
1	B	142	LEU	3.6
1	B	140	SER	3.4
1	B	266	PRO	3.1
1	A	421	ARG	2.9
1	B	157	HIS	2.8
1	B	162	LEU	2.6
1	A	253	ASP	2.6
1	B	418	ASP	2.6
1	A	420	ALA	2.6
1	B	141	ASP	2.5
1	B	217	LEU	2.4
1	B	262	SER	2.3
1	B	264	THR	2.2
1	B	154	GLY	2.2
1	B	96	LEU	2.1
1	B	215	ASN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
4	TRS	A	504	8/8	0.88	0.13	12,14,16,18	0
3	2PG	A	503	11/11	0.97	0.10	2,2,5,6	0
2	MG	B	501	1/1	0.98	0.07	2,2,2,2	0
5	PEP	B	503	10/10	0.98	0.09	2,4,6,9	0
2	MG	A	502	1/1	0.99	0.07	2,2,2,2	0
2	MG	A	501	1/1	0.99	0.07	2,2,2,2	0
2	MG	B	502	1/1	0.99	0.08	3,3,3,3	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.