Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 08:16 PM EST

PDB ID	:	3UCD
Title	:	Asymmetric complex of human neuron specific enolase-2-PGA/PEP
Authors	:	Qin, J.; Chai, G.; Brewer, J.; Lovelace, L.; Lebioda, L.
Deposited on	:	2011-10-26
Resolution	:	1.41 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

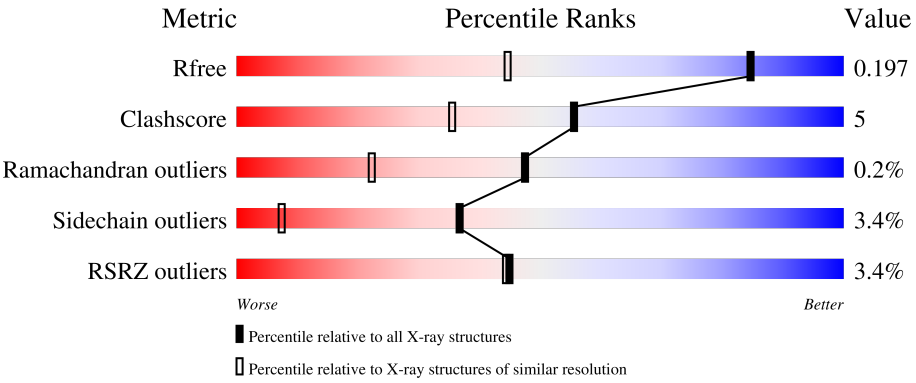
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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 >=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 <=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	439	3% 85% 11%
1	B	439	3% 87% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6975 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 3314	C 2084	N 569	O 648	S 13	0	0	0
1	B	432	Total 3306	C 2078	N 568	O 647	S 13	0	0	0

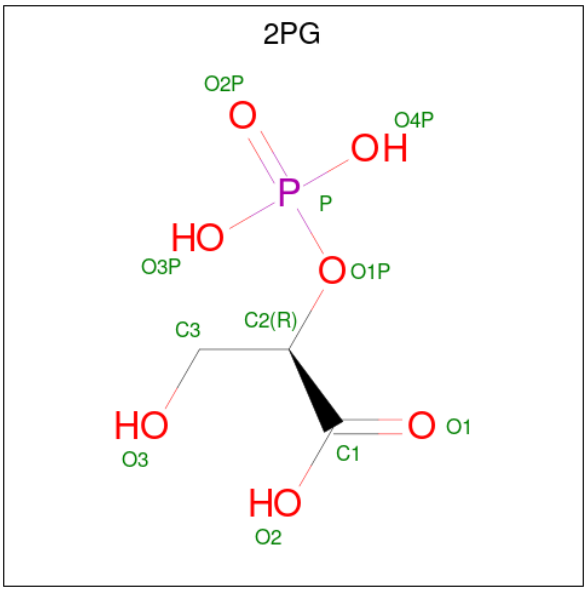
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLN	GLU	conflict	UNP P09104
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
B	3	GLN	GLU	conflict	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

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

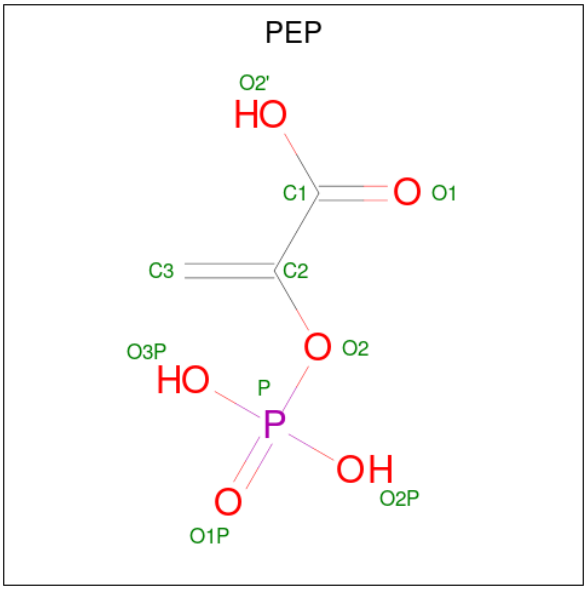
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0

- 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	0	0
			11	3	7	1		

- 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.

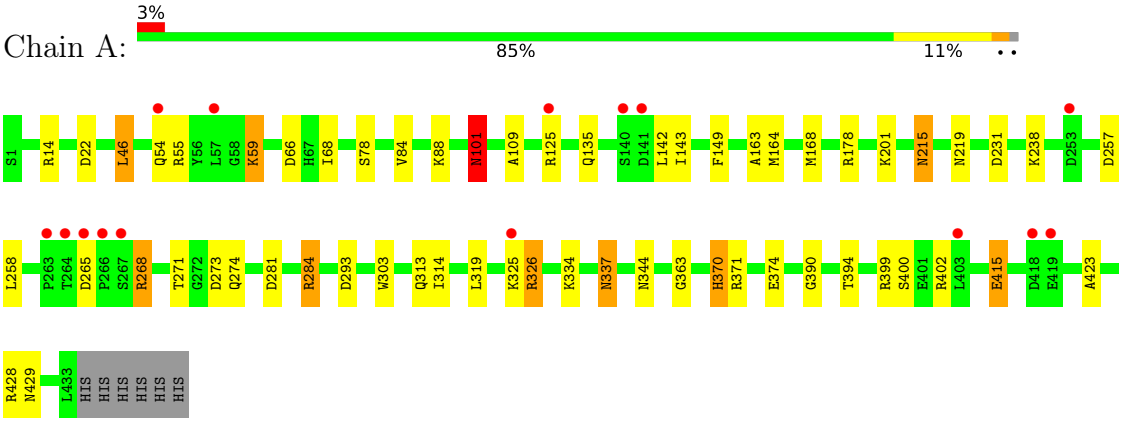
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	170	Total O 170 170	0	0
5	B	160	Total O 160 160	0	0

3 Residue-property plots (i)

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.

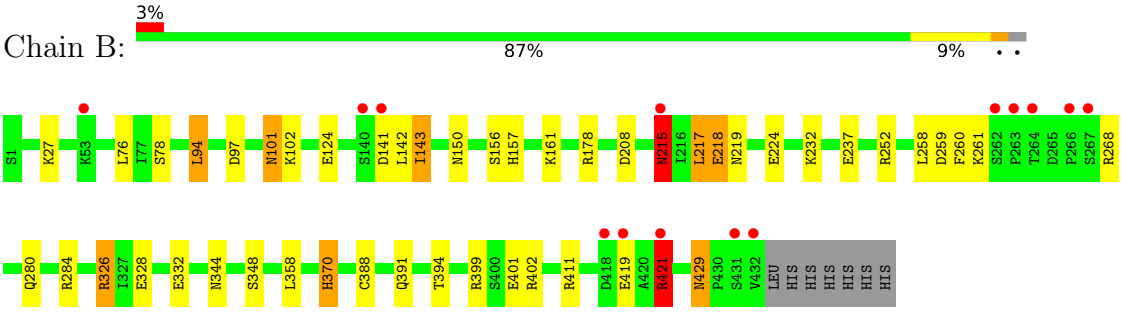
• Molecule 1: Gamma-enolase

Chain A:



• Molecule 1: Gamma-enolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.71Å 118.62Å 67.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.58 – 1.41 41.07 – 1.41	Depositor EDS
% Data completeness (in resolution range)	94.1 (44.58-1.41) 94.0 (41.07-1.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.198 0.160 , 0.197	Depositor DCC
R_{free} test set	7676 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6975	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PEP, MG, 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	1.23	9/3369 (0.3%)	1.19	20/4558 (0.4%)
1	B	1.26	12/3361 (0.4%)	1.08	13/4547 (0.3%)
All	All	1.24	21/6730 (0.3%)	1.14	33/9105 (0.4%)

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	A	0	1
1	B	0	2
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	ASP	CB-CG	9.66	1.72	1.51
1	A	415	GLU	CB-CG	8.57	1.68	1.52
1	A	284	ARG	CB-CG	-7.62	1.31	1.52
1	B	156	SER	CB-OG	6.66	1.50	1.42
1	A	429	ASN	CB-CG	6.63	1.66	1.51
1	B	268	ARG	CB-CG	6.28	1.69	1.52
1	A	326	ARG	CG-CD	6.17	1.67	1.51
1	B	157	HIS	N-CA	6.09	1.58	1.46
1	B	78	SER	CB-OG	-6.06	1.34	1.42
1	B	280	GLN	CG-CD	-5.93	1.37	1.51
1	A	101	ASN	CG-ND2	5.75	1.47	1.32
1	A	326	ARG	CD-NE	-5.67	1.36	1.46
1	B	421	ARG	CG-CD	5.67	1.66	1.51
1	A	135	GLN	CD-NE2	5.59	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ASN	CB-CG	5.55	1.63	1.51
1	B	218	GLU	CG-CD	-5.54	1.43	1.51
1	A	363	GLY	N-CA	5.54	1.54	1.46
1	B	215	ASN	CB-CG	5.33	1.63	1.51
1	B	224	GLU	CG-CD	5.26	1.59	1.51
1	B	348	SER	CA-CB	5.18	1.60	1.52
1	B	161	LYS	CD-CE	5.15	1.64	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	268	ARG	NE-CZ-NH1	19.73	130.16	120.30
1	A	326	ARG	NE-CZ-NH2	-16.34	112.13	120.30
1	A	326	ARG	NE-CZ-NH1	15.79	128.19	120.30
1	A	268	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	A	326	ARG	CD-NE-CZ	10.74	138.64	123.60
1	A	284	ARG	CG-CD-NE	-9.91	91.00	111.80
1	B	421	ARG	NE-CZ-NH2	8.34	124.47	120.30
1	A	268	ARG	CD-NE-CZ	7.68	134.35	123.60
1	A	284	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	326	ARG	CG-CD-NE	-7.23	96.62	111.80
1	B	284	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	161	LYS	CD-CE-NZ	6.75	127.24	111.70
1	A	281	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	217	LEU	CB-CG-CD2	-6.17	100.52	111.00
1	A	428	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	46	LEU	CB-CG-CD2	6.12	121.41	111.00
1	A	326	ARG	CB-CG-CD	-6.07	95.81	111.60
1	B	94	LEU	CB-CG-CD2	6.03	121.24	111.00
1	B	76	LEU	CB-CG-CD2	6.00	121.20	111.00
1	B	178	ARG	CB-CG-CD	5.91	126.96	111.60
1	A	178	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	268	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	22	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	55	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	238	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	B	326	ARG	CG-CD-NE	5.47	123.30	111.80
1	B	252	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	231	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	14	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	411	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	142	LEU	CA-CB-CG	-5.23	103.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	260	PHE	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	ARG	Sidechain
1	B	217	LEU	Mainchain
1	B	402	ARG	Sidechain

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	3291	35	1
1	B	3306	0	3280	35	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	4	0	0
4	B	10	0	2	0	0
5	A	170	0	0	9	0
5	B	160	0	0	5	0
All	All	6975	0	6577	68	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 5.

All (68) 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:143:ILE:CD1	1:B:143:ILE:CG1	1.78	1.58
1:B:143:ILE:CD1	1:B:388:CYS:HB3	1.87	1.04
1:B:143:ILE:HD11	1:B:388:CYS:CB	1.88	1.02
1:A:66:ASP:HB2	5:A:922:HOH:O	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:HB3	5:A:951:HOH:O	1.60	0.99
1:B:143:ILE:HB	5:B:956:HOH:O	0.81	0.98
1:B:143:ILE:HD11	1:B:388:CYS:HB3	1.02	0.98
1:A:319:LEU:O	1:A:326:ARG:HD3	1.77	0.85
1:B:141:ASP:O	1:B:388:CYS:SG	2.35	0.84
1:A:257:ASP:OD1	1:A:268:ARG:HD2	1.80	0.80
1:A:101:ASN:H	1:A:101:ASN:HD22	1.31	0.78
1:B:419:GLU:HG2	1:B:421:ARG:NH1	2.03	0.72
1:B:215:ASN:ND2	5:B:892:HOH:O	2.22	0.71
1:B:419:GLU:O	1:B:421:ARG:CZ	2.39	0.71
1:A:66:ASP:CB	5:A:922:HOH:O	2.28	0.70
1:A:314:ILE:H	1:A:337:ASN:HD21	1.41	0.68
1:A:215:ASN:H	1:A:215:ASN:HD22	1.40	0.68
1:A:78:SER:OG	5:A:820:HOH:O	2.13	0.65
1:B:219:ASN:ND2	5:B:924:HOH:O	2.03	0.63
1:B:215:ASN:H	1:B:215:ASN:HD22	1.48	0.62
1:B:429:ASN:HD22	1:B:429:ASN:H	1.47	0.62
1:B:101:ASN:HD22	1:B:101:ASN:H	1.47	0.61
1:A:314:ILE:H	1:A:337:ASN:ND2	1.98	0.61
1:B:143:ILE:CD1	1:B:388:CYS:CB	2.64	0.61
1:A:265:ASP:O	1:A:268:ARG:HG2	2.02	0.59
1:B:258:LEU:HD22	5:B:924:HOH:O	2.03	0.58
1:A:201:LYS:HE3	1:B:261:LYS:HB3	1.84	0.58
1:B:218:GLU:HG2	5:B:951:HOH:O	2.03	0.57
1:B:429:ASN:HD22	1:B:429:ASN:N	2.03	0.57
1:A:143:ILE:HD13	1:A:423:ALA:HB2	1.86	0.56
1:B:94:LEU:HD22	1:B:102:LYS:HE3	1.88	0.56
1:A:84:VAL:HB	1:A:125:ARG:NH2	2.21	0.55
1:B:143:ILE:CD1	1:B:143:ILE:CG2	2.85	0.55
1:A:164:MET:H	1:A:219:ASN:HD21	1.54	0.54
1:B:215:ASN:HD22	1:B:215:ASN:N	2.04	0.54
1:A:257:ASP:OD1	1:A:268:ARG:CD	2.53	0.54
1:A:215:ASN:H	1:A:215:ASN:ND2	2.06	0.53
1:A:415:GLU:HB2	5:A:958:HOH:O	2.08	0.53
1:B:421:ARG:NH2	1:B:421:ARG:H	2.05	0.53
1:A:337:ASN:HD22	1:A:337:ASN:C	2.12	0.53
1:B:143:ILE:HD13	1:B:388:CYS:SG	2.49	0.53
1:A:143:ILE:CD1	1:A:423:ALA:HB2	2.39	0.52
1:A:319:LEU:O	1:A:326:ARG:CD	2.54	0.52
1:A:101:ASN:H	1:A:101:ASN:ND2	2.03	0.50
1:A:164:MET:HG3	5:A:951:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:H	1:B:421:ARG:HH21	1.60	0.49
1:B:215:ASN:ND2	1:B:215:ASN:H	2.09	0.49
1:A:313:GLN:HA	1:A:337:ASN:HD21	1.78	0.48
1:A:271:THR:OG1	1:A:274:GLN:HG3	2.13	0.48
1:A:143:ILE:HD11	1:A:390:GLY:HA2	1.94	0.48
1:B:232:LYS:HB2	1:B:232:LYS:NZ	2.29	0.47
1:B:419:GLU:CG	1:B:421:ARG:HH11	2.28	0.46
1:A:68:ILE:HD11	1:A:109:ALA:HA	1.98	0.46
1:B:419:GLU:HG2	1:B:421:ARG:HH11	1.78	0.45
1:A:258:LEU:HD22	5:A:951:HOH:O	2.17	0.44
1:A:370:HIS:CG	1:A:394:THR:HA	2.52	0.44
1:B:142:LEU:O	1:B:421:ARG:NH2	2.50	0.44
1:B:419:GLU:CG	1:B:421:ARG:NH1	2.77	0.44
1:A:59:LYS:CD	5:A:968:HOH:O	2.65	0.44
1:A:400:SER:HB2	1:B:401:GLU:HB3	1.98	0.44
1:A:149:PHE:O	1:A:168:MET:HA	2.18	0.43
1:B:370:HIS:CG	1:B:394:THR:HA	2.54	0.43
1:A:59:LYS:HD3	5:A:968:HOH:O	2.19	0.43
1:A:371:ARG:O	1:A:374:GLU:HG2	2.19	0.42
1:B:27:LYS:HE2	1:B:124:GLU:HA	2.01	0.41
1:A:293:ASP:HA	1:A:303:TRP:CH2	2.55	0.41
1:B:328:GLU:HG2	1:B:358:LEU:HD21	2.02	0.41
1:B:143:ILE:CD1	1:B:388:CYS:SG	3.09	0.41

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:334:LYS:NZ	1:B:237:GLU:OE2[1_556]	2.19	0.01

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	431/439 (98%)	419 (97%)	11 (3%)	1 (0%)	47 22
1	B	430/439 (98%)	422 (98%)	7 (2%)	1 (0%)	47 22
All	All	861/878 (98%)	841 (98%)	18 (2%)	2 (0%)	47 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	350/356 (98%)	338 (97%)	12 (3%)	37 7
1	B	349/356 (98%)	337 (97%)	12 (3%)	37 7
All	All	699/712 (98%)	675 (97%)	24 (3%)	37 7

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	54	GLN
1	A	59	LYS
1	A	88	LYS
1	A	101	ASN
1	A	215	ASN
1	A	273	ASP
1	A	284	ARG
1	A	325	LYS
1	A	337	ASN
1	A	344	ASN
1	A	370	HIS
1	B	97	ASP
1	B	101	ASN

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Mol	Chain	Res	Type
1	B	143	ILE
1	B	150	ASN
1	B	215	ASN
1	B	326	ARG
1	B	332	GLU
1	B	344	ASN
1	B	370	HIS
1	B	391	GLN
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	101	ASN
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	B	101	ASN
1	B	150	ASN
1	B	189	HIS
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 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	$\#\|Z\| > 2$
4	PEP	B	601	2	9,9,9	3.04	4 (44%)	11,13,13	0.96	0
3	2PG	A	601	2	9,10,10	1.57	2 (22%)	11,14,14	1.21	1 (9%)

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
4	PEP	B	601	2	-	1/9/9/9	-
3	2PG	A	601	2	-	2/11/11/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	PEP	C3-C2	7.72	1.53	1.31
3	A	601	2PG	O1-C1	3.07	1.31	1.22
3	A	601	2PG	O2-C1	-2.46	1.22	1.30
4	B	601	PEP	O2-C2	2.39	1.45	1.39
4	B	601	PEP	O1-C1	2.36	1.28	1.22
4	B	601	PEP	P-O2	2.13	1.62	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	2PG	P-O1P-C2	-2.73	116.77	123.04

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	PEP	C3-C2-O2-P
3	A	601	2PG	O1-C1-C2-C3
3	A	601	2PG	O2-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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^2)	Q<0.9
1	A	433/439 (98%)	-0.13	15 (3%)	44	43	6, 10, 26, 42	0
1	B	432/439 (98%)	-0.17	14 (3%)	47	46	6, 11, 23, 39	0
All	All	865/878 (98%)	-0.15	29 (3%)	45	44	6, 11, 24, 42	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	6.1
1	B	263	PRO	5.9
1	B	418	ASP	5.8
1	B	141	ASP	5.8
1	B	140	SER	4.8
1	A	264	THR	4.4
1	B	264	THR	3.7
1	B	267	SER	3.7
1	A	253	ASP	3.5
1	A	267	SER	3.3
1	A	266	PRO	3.2
1	A	419	GLU	3.1
1	B	419	GLU	2.9
1	A	54	GLN	2.9
1	A	418	ASP	2.9
1	B	421	ARG	2.9
1	B	266	PRO	2.9
1	B	262	SER	2.8
1	B	431	SER	2.8
1	A	125	ARG	2.6
1	B	432	VAL	2.6
1	A	263	PRO	2.4
1	A	140	SER	2.3
1	B	53	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	215	ASN	2.2
1	A	325	LYS	2.1
1	A	57	LEU	2.1
1	A	403	LEU	2.1
1	A	265	ASP	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 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^{th} 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^2)	Q<0.9
3	2PG	A	601	11/11	0.99	0.06	6,7,8,11	0
4	PEP	B	601	10/10	0.99	0.09	6,6,9,11	0
2	MG	B	599	1/1	1.00	0.06	7,7,7,7	0
2	MG	B	600	1/1	1.00	0.07	6,6,6,6	0
2	MG	A	599	1/1	1.00	0.07	7,7,7,7	0
2	MG	A	600	1/1	1.00	0.05	7,7,7,7	0

6.5 Other polymers (i)

There are no such residues in this entry.