



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:53 AM UTC

PDB ID : 3UJR / pdb_00003ujr
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

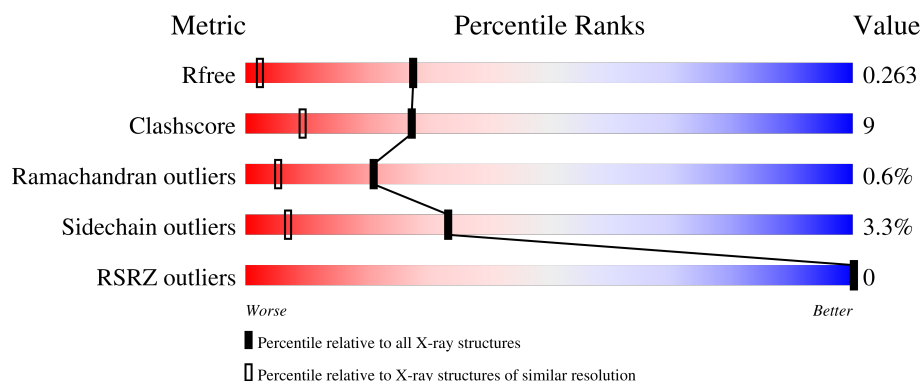
1 Overall quality at a glance

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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (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 ≥ 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	 79% 17% ..
1	B	443	 78% 17% ..

2 Entry composition

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
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			

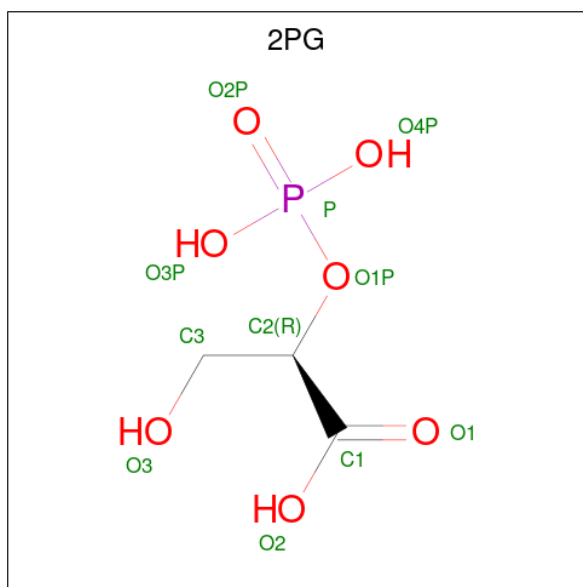
There are 20 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (CCD ID: 2PG) (formula: $C_3H_7O_7P$).



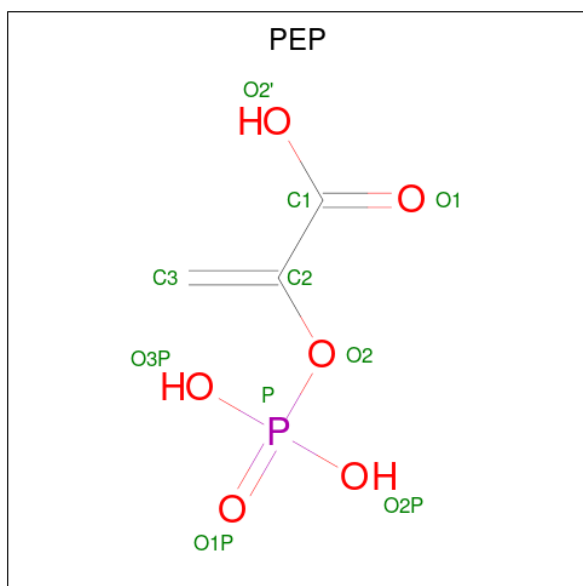
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			11	3	7	1		

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



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

- Molecule 5 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



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

- Molecule 6 is water.

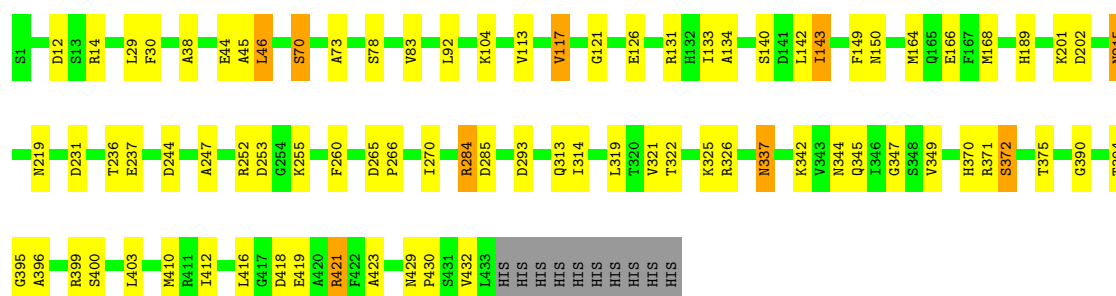
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	316	Total 316	O 316	0	0
6	B	278	Total 278	O 278	0	0

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.

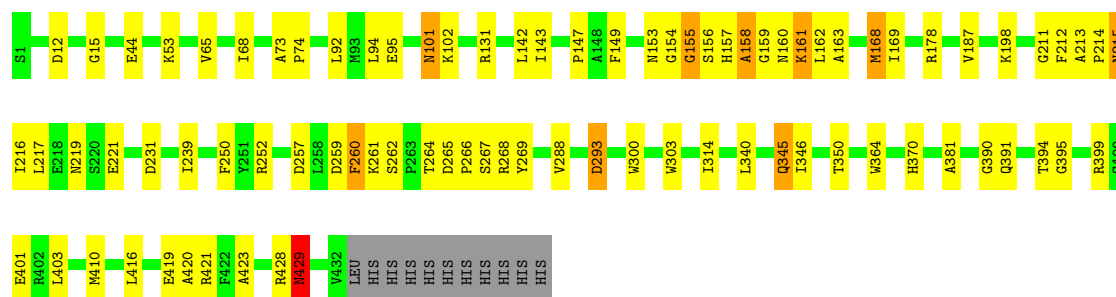
- Molecule 1: Gamma-enolase

Chain A: 



- Molecule 1: Gamma-enolase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 1.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.264 0.212 , 0.263	Depositor DCC
R_{free} test set	8909 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	5.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7247	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PEP, TRS, 2PG, MG

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	1.35	8/3369 (0.2%)	1.34	17/4558 (0.4%)
1	B	1.41	11/3361 (0.3%)	1.34	17/4547 (0.4%)
All	All	1.38	19/6730 (0.3%)	1.34	34/9105 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	ASP	C-O	-10.32	1.19	1.23
1	A	349	VAL	CA-CB	7.59	1.62	1.54
1	B	293	ASP	CA-CB	6.88	1.57	1.52
1	B	147	PRO	C-O	6.67	1.31	1.23
1	B	381	ALA	C-O	6.25	1.31	1.24
1	B	68	ILE	C-O	-5.77	1.17	1.24
1	A	412	ILE	CA-CB	5.64	1.61	1.54
1	B	169	ILE	CA-C	5.50	1.59	1.52
1	A	45	ALA	CA-CB	-5.45	1.44	1.53
1	A	347	GLY	C-O	-5.44	1.16	1.24
1	B	168	MET	C-O	5.36	1.30	1.23
1	A	395	GLY	N-CA	5.22	1.49	1.45
1	B	314	ILE	CA-CB	5.18	1.60	1.54
1	B	158	ALA	CA-C	-5.13	1.46	1.52
1	A	104	LYS	N-CA	5.12	1.52	1.46
1	A	70	SER	N-CA	5.11	1.52	1.46
1	B	288	VAL	C-O	5.03	1.29	1.24
1	B	350	THR	CA-CB	5.02	1.61	1.53
1	A	117	VAL	C-O	-5.01	1.18	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	GLY	N-CA-C	7.68	125.54	115.40
1	B	155	GLY	N-CA-C	7.27	124.33	112.84
1	B	395	GLY	N-CA-C	7.07	119.25	112.04
1	A	260	PHE	N-CA-C	6.62	119.32	111.71
1	B	300	TRP	N-CA-C	6.42	119.10	111.33
1	B	157	HIS	CA-C-N	-6.16	114.22	122.72
1	B	157	HIS	C-N-CA	-6.16	114.22	122.72
1	B	161	LYS	N-CA-C	6.07	120.69	113.16
1	A	429	ASN	CA-C-N	-6.00	113.78	120.45
1	A	429	ASN	C-N-CA	-6.00	113.78	120.45
1	B	346	ILE	N-CA-C	5.91	116.68	111.90
1	A	73	ALA	CA-C-N	-5.89	112.95	119.19
1	A	73	ALA	C-N-CA	-5.89	112.95	119.19
1	A	133	ILE	O-C-N	5.88	127.68	121.91
1	B	420	ALA	N-CA-C	5.78	118.09	109.59
1	A	403	LEU	N-CA-C	5.74	119.09	111.75
1	A	432	VAL	N-CA-C	5.63	120.32	113.00
1	B	429	ASN	CA-C-N	5.60	125.21	119.56
1	B	429	ASN	C-N-CA	5.60	125.21	119.56
1	B	428	ARG	CA-C-N	-5.55	116.85	122.74
1	B	428	ARG	C-N-CA	-5.55	116.85	122.74
1	A	293	ASP	CA-C-N	5.49	125.16	119.56
1	A	293	ASP	C-N-CA	5.49	125.16	119.56
1	B	345	GLN	N-CA-C	-5.47	106.11	112.89
1	A	375	THR	N-CA-C	-5.41	101.23	108.86
1	B	92	LEU	N-CA-C	-5.38	105.50	111.36
1	A	38	ALA	N-CA-C	-5.30	105.88	112.93
1	B	364	TRP	N-CA-C	5.23	118.22	110.48
1	A	371	ARG	CA-C-N	5.20	128.63	120.82
1	A	371	ARG	C-N-CA	5.20	128.63	120.82
1	B	212	PHE	N-CA-C	5.13	118.43	110.17
1	A	321	VAL	N-CA-C	5.10	119.95	109.34
1	A	410	MET	N-CA-C	5.06	116.79	111.28
1	A	247	ALA	N-CA-C	5.04	117.50	111.71

There are no chirality outliers.

There are no planarity outliers.

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	3314	0	3289	52	0
1	B	3306	0	3278	71	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	120	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 9.

All (120) 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	1.10	0.89
1:B:158:ALA:CB	1:B:261:LYS:HZ3	1.79	0.84
1:B:158:ALA:HB3	1:B:261:LYS:HZ2	1.01	0.82
1:A:215:ASN:H	1:A:215:ASN:HD22	1.29	0.81
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:B:158:ALA:CB	1:B:261:LYS:HZ2	1.90	0.76
1:A:231:ASP:OD2	1:A:236:THR:OG1	2.04	0.75
1:B:215:ASN:H	1:B:215:ASN:ND2	1.80	0.75
1:A:143:ILE:HD11	1:A:390:GLY:HA2	1.68	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:GLY:O	1:B:261:LYS:NZ	2.28	0.65
1:B:158:ALA:C	1:B:160:ASN:N	2.55	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:337:ASN:HD22	1:A:337:ASN:C	2.06	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:158:ALA:C	1:B:160:ASN:H	2.06	0.62
1:B:198:LYS:NZ	1:B:221:GLU:OE2	2.31	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: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:A:14:ARG:NH2	1:A:372:SER:HB3	2.16	0.59
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:A:29:LEU:C	1:A:29:LEU:HD23	2.29	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
1:B:154:GLY:C	1:B:158:ALA:HB2	2.32	0.55
1:B:156:SER:HA	1:B:260:PHE:CE1	2.42	0.55
1:B:213:ALA:O	1:B:214:PRO:C	2.49	0.54
1:A:70:SER:HB2	6:A:895:HOH:O	2.07	0.54
1:B:213:ALA:C	1:B:214:PRO:O	2.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:29:LEU:HD23	1:A:30:PHE:N	2.27	0.50
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:265:ASP:OD1	1:B:267:SER:OG	2.31	0.48
1:A:342:LYS:HZ3	3:A:503:2PG:H2	1.79	0.47
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:A:342:LYS:HZ1	3:A:503:2PG:C1	2.28	0.46
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:44:GLU:CD	1:B:345:GLN:HG2	2.42	0.44
1:B:65:VAL:HG12	6:B:761:HOH:O	2.17	0.44
1:B:12:ASP:OD1	1:B:12:ASP:C	2.61	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
1:B:252:ARG:NH2	1:B:260:PHE:HB2	2.33	0.44
1:B:429:ASN:CG	1:B:429:ASN:O	2.61	0.43
1:A:265:ASP:HA	1:A:266:PRO:HD3	1.81	0.43
1:A:253:ASP:CG	1:A:253:ASP:O	2.61	0.43
1:A:265:ASP:C	1:A:265:ASP:OD1	2.62	0.43
1:B:53:LYS:CG	6:B:719:HOH:O	2.66	0.43
1:A:83:VAL:HG23	1:A:121:GLY:HA2	2.01	0.43
1:A:252:ARG:O	1:A:253:ASP:C	2.62	0.43
1:A:44:GLU:CD	1:A:345:GLN:HG2	2.44	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:12:ASP:OD1	1:A:12:ASP:C	2.64	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 ⓘ

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%)	413 (96%)	17 (4%)	1 (0%)	43	19
1	B	430/443 (97%)	410 (95%)	16 (4%)	4 (1%)	14	2
All	All	861/886 (97%)	823 (96%)	33 (4%)	5 (1%)	21	5

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 ⓘ

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%)	24	4
1	B	349/360 (97%)	342 (98%)	7 (2%)	48	17
All	All	699/720 (97%)	676 (97%)	23 (3%)	33	7

All (23) 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	140	SER
1	A	143	ILE
1	A	201	LYS
1	A	202	ASP
1	A	215	ASN
1	A	237	GLU
1	A	284	ARG
1	A	325	LYS
1	A	337	ASN
1	A	344	ASN
1	A	372	SER
1	A	418	ASP
1	A	421	ARG
1	B	101	ASN
1	B	215	ASN

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Mol	Chain	Res	Type
1	B	216	ILE
1	B	391	GLN
1	B	403	LEU
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	189	HIS
1	A	205	ASN
1	A	215	ASN
1	A	219	ASN
1	A	337	ASN
1	A	360	GLN
1	A	426	ASN
1	B	101	ASN
1	B	157	HIS
1	B	215	ASN
1	B	345	GLN
1	B	362	ASN
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 oligosaccharides 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	1.54	2 (22%)	12,14,14	2.39	1 (8%)
4	TRS	A	504	-	7,7,7	0.39	0	9,9,9	1.19	1 (11%)
5	PEP	B	503	2	9,9,9	1.28	2 (22%)	11,13,13	1.50	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	-	-	4/9/9/9	-
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	2.78	1.30	1.22
3	A	503	2PG	P-O1P	2.35	1.63	1.59
5	B	503	PEP	O1-C1	2.16	1.27	1.22
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	2.98	122.44	110.83
4	A	504	TRS	C2-C-N	2.55	114.66	108.17
5	B	503	PEP	O2-C2-C3	-2.42	120.23	124.85
5	B	503	PEP	O2P-P-O2	-2.20	98.92	105.32

There are no chirality outliers.

All (8) 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
4	A	504	TRS	N-C-C2-O2
3	A	503	2PG	O2-C1-C2-C3
3	A	503	2PG	O1-C1-C2-C3
4	A	504	TRS	N-C-C1-O1

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 [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, 95th 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	433/443 (97%)	-1.26	0 100 100	2, 5, 14, 25	0
1	B	432/443 (97%)	-1.19	0 100 100	2, 6, 18, 29	5 (1%)
All	All	865/886 (97%)	-1.22	0 100 100	2, 5, 17, 29	5 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th 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
4	TRS	A	504	8/8	0.99	0.03	12,14,16,18	0
2	MG	A	502	1/1	1.00	0.01	2,2,2,2	0
2	MG	B	501	1/1	1.00	0.01	2,2,2,2	0
2	MG	B	502	1/1	1.00	0.02	3,3,3,3	0
3	2PG	A	503	11/11	1.00	0.02	2,2,5,6	0
2	MG	A	501	1/1	1.00	0.01	2,2,2,2	0
5	PEP	B	503	10/10	1.00	0.02	2,4,6,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.