wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:21 PM GMT

PDB ID	:	1JXA
Title	:	GLUCOSAMINE 6-PHOSPHATE SYNTHASE WITH GLUCOSE 6-PHOSPHATE
Authors	:	Teplyakov, A.; Obmolova, G.; Badet, B.; Badet-Denisot, M.A.
Deposited on	:	2001-09-06
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

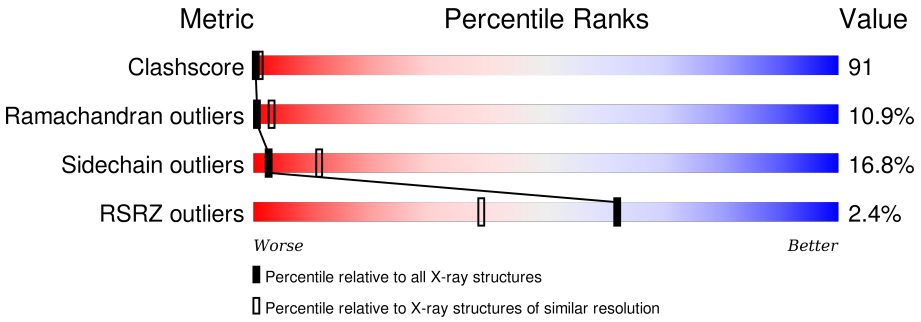
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 >=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 <=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	608	20% 54% 23%
1	B	608	17% 60% 20%
1	C	608	5% 21% 60% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14156 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.

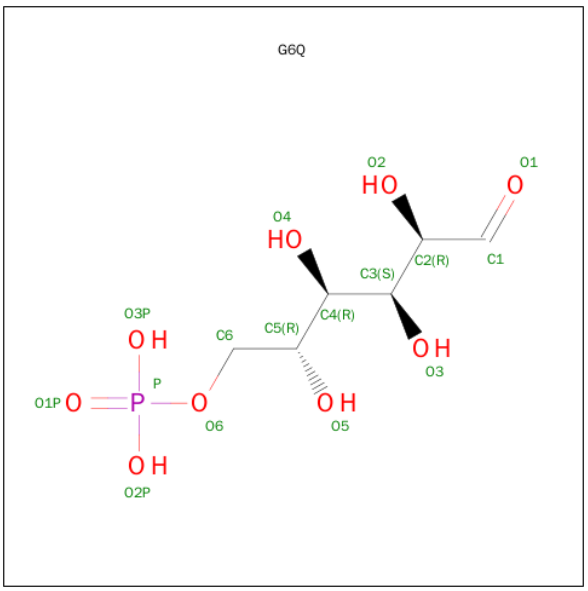
- Molecule 1 is a protein called glucosamine 6-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	B	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			
1	C	608	Total	C	N	O	S	0	0	0
			4695	2953	829	896	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	LYS	ARG	CONFLICT	UNP P17169
B	421	LYS	ARG	CONFLICT	UNP P17169
C	421	LYS	ARG	CONFLICT	UNP P17169

- Molecule 2 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is water.

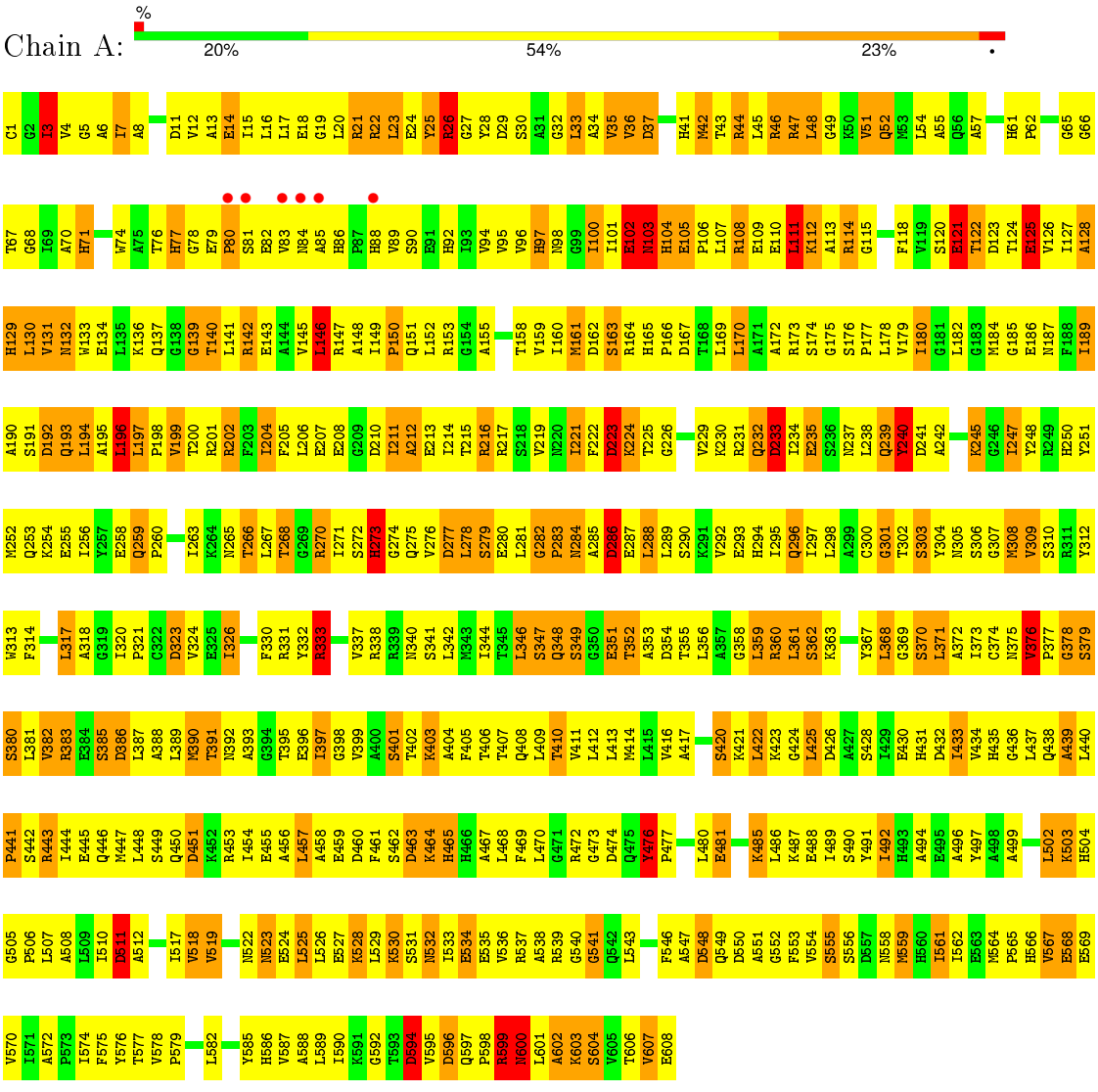
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	10	Total	O	0	0
			10	10		
3	C	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

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 (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.

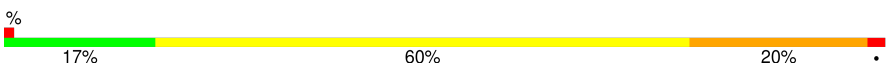
- Molecule 1: glucosamine 6-phosphate synthase

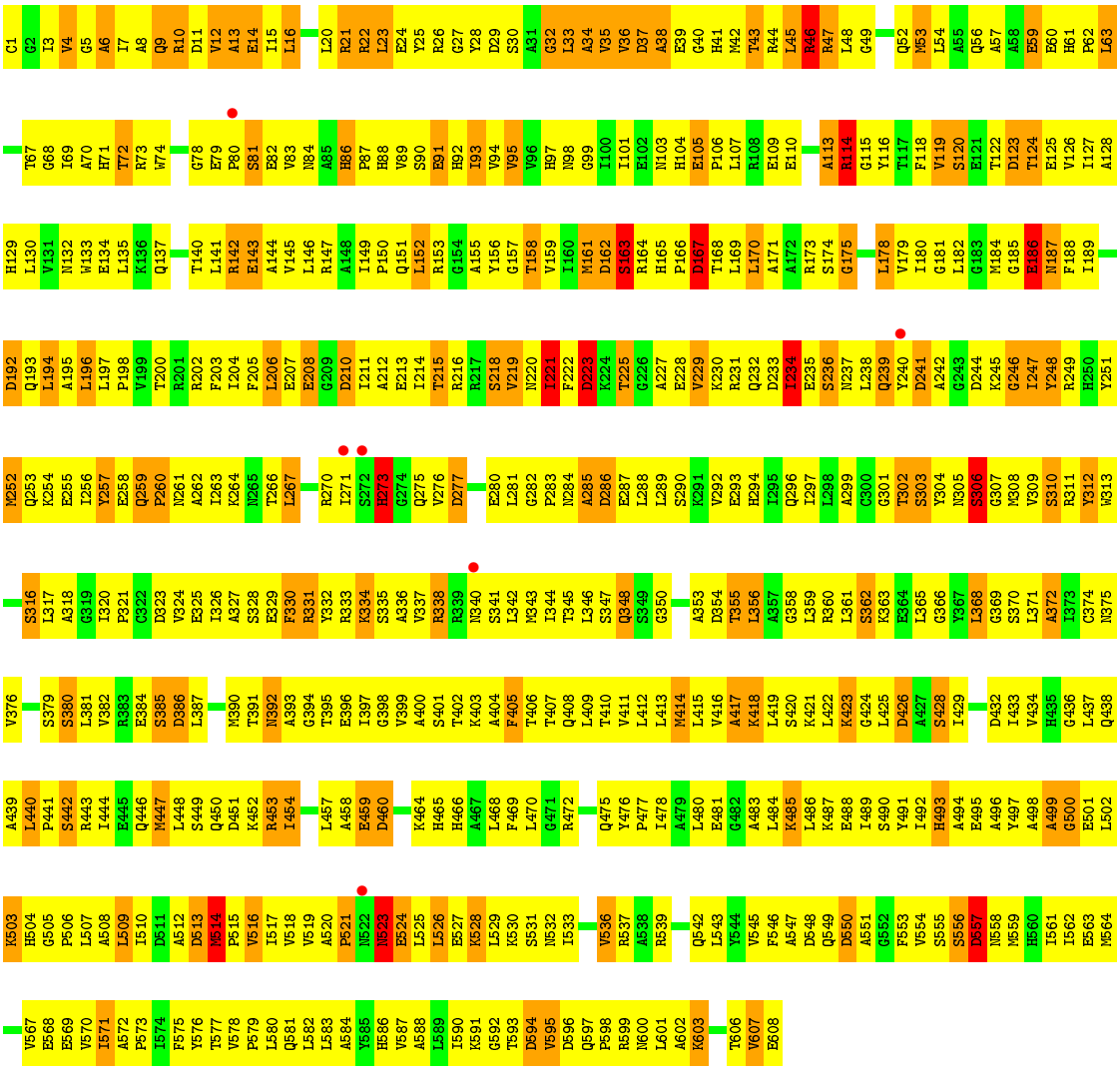
Chain A:



- Molecule 1: glucosamine 6-phosphate synthase

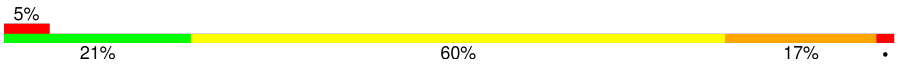
Chain B:

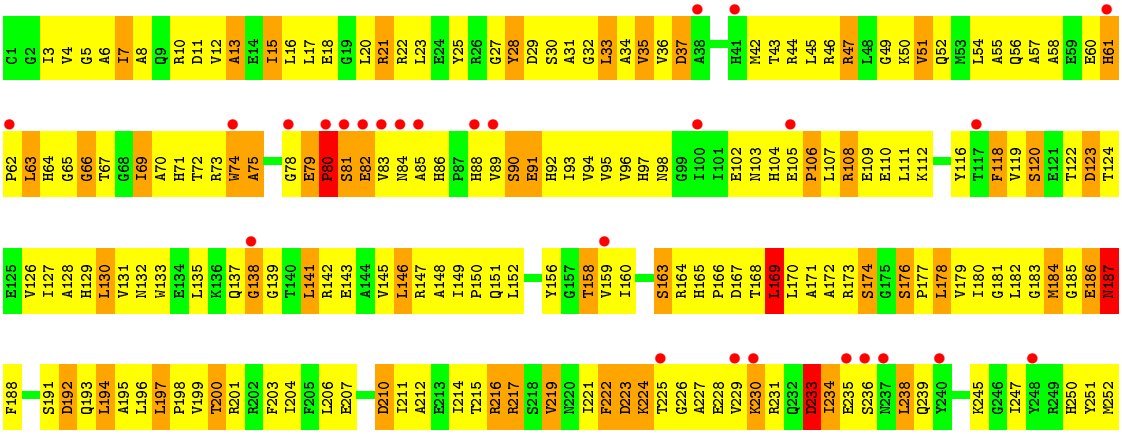


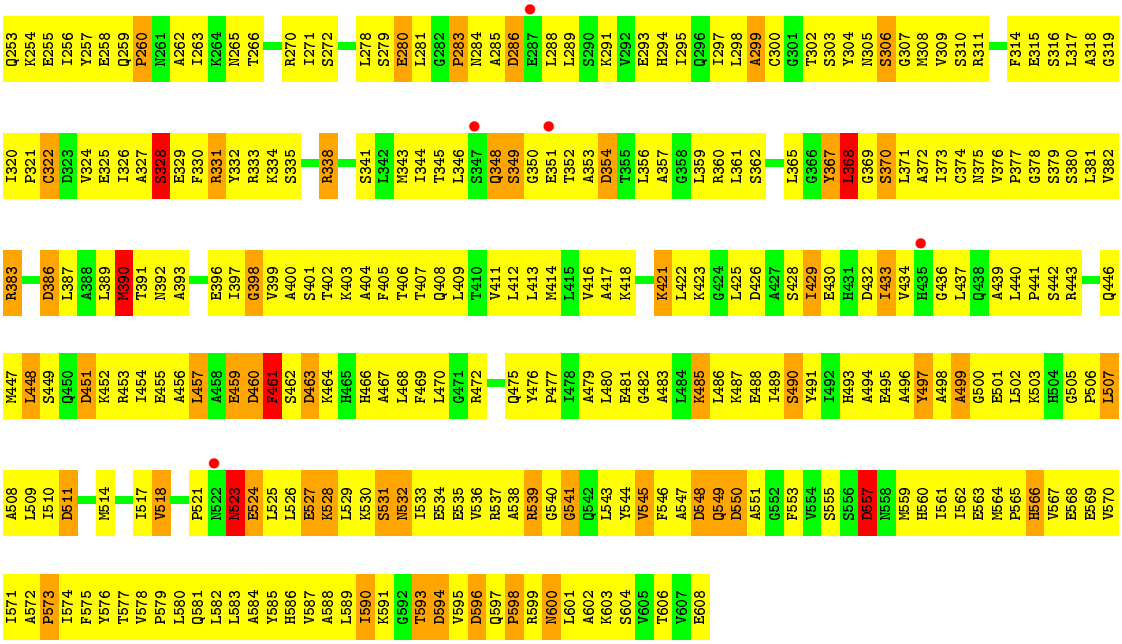


• Molecule 1: glucosamine 6-phosphate synthase

Chain C:






Q253 K254 E255 I256 Y257 E258 Q259 P260 N261 A262 I263 K264 N265 T266 R270 I271 S272 L278 S279 E280 L281 G282 P283 N284 A285 D286 E287 L288 L289 S290 K291 V292 E293 H294 I295 Q296 I297 L298 A299 G300 G301 T302 S303 Y304 N305 S306 G307 M308 V309 S310 R311 F314 E315 S316 L317 A318 G319
I320 P321 C322 D323 V324 E325 I326 A327 S328 E329 F330 R331 Y332 R333 K334 S335 R338 S341 L342 M343 I344 T345 L346 S347 Q348 S349 G350 E351 T352 A353 D354 T355 L356 A357 G358 L359 R360 L361 S362 L365 G366 Y367 L368 G369 S370 L371 A372 I373 C374 N375 V376 P377 G378 S379 S380 L381 V382
R383 D386 L387 A388 L389 M390 T391 N392 A393 E396 I397 G398 V399 A400 S401 T402 K403 A404 F405 T406 T407 Q408 L409 T410 V411 L412 L413 M414 L415 V416 A417 K418 K421 L422 K423 G424 L425 D426 A427 S428 I429 E430 H431 D432 I433 V434 H435 G436 L437 Q438 A439 L440 P441 S442 R443 Q446
M447 L448 S449 Q450 D451 K452 R453 I454 E455 A456 L457 A458 E459 D460 F461 S462 D463 K464 H465 H466 A467 L468 F469 L470 G471 R472 Q475 Y476 P477 I478 A479 L480 E481 G482 A483 I484 K485 L486 K487 E488 I489 S490 Y491 I492 H493 A494 E495 A496 Y497 A498 A499 G500 E501 L502 K503 H504 G505 P506 L507
A508 L509 I510 D511 M514 I517 V518 P521 N522 N523 E524 L525 L526 E527 K528 L529 K530 S531 N532 I533 E534 E535 V536 R537 A538 R539 G540 G541 Q542 L543 Y544 V545 F546 A547 D548 Q549 D550 A551 G552 F553 V554 S555 S556 D557 N558 M559 H560 I561 I562 E563 M564 P565 H566 V567 E568 E569 V570
I571 A572 P573 I574 F575 Y576 T577 V578 P579 L580 Q581 L582 L583 A584 Y585 H586 V587 A588 L589 I590 K591 G592 T593 D594 V595 D596 Q597 P598 R599 N600 L601 A602 K603 S604 V605 T606 V607 E608

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.40Å 112.40Å 185.10Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 19.97 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-3.10) 92.7 (19.97-3.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 3.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.280 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 83.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 45685 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14156	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: G6Q

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	0.82	1/4776 (0.0%)	1.34	47/6467 (0.7%)
1	B	0.67	0/4776	1.10	29/6467 (0.4%)
1	C	0.51	0/4776	0.90	18/6467 (0.3%)
All	All	0.68	1/14328 (0.0%)	1.13	94/19401 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	TYR	CD1-CE1	-5.16	1.31	1.39

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	323	ASP	CB-CG-OD2	9.78	127.10	118.30
1	A	22	ARG	NE-CZ-NH1	-8.83	115.88	120.30
1	B	47	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	142	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	B	114	ARG	NE-CZ-NH1	8.76	124.68	120.30

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	4695	0	4715	862	1
1	B	4695	0	4715	918	0
1	C	4695	0	4715	826	0
2	A	16	0	10	4	0
2	B	16	0	11	2	0
3	A	26	0	0	2	0
3	B	10	0	0	2	0
3	C	3	0	0	0	0
All	All	14156	0	14166	2564	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 91.

The worst 5 of 2564 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:100:ILE:CD1	1:A:100:ILE:CG1	1.76	1.63
1:A:304:TYR:CE1	1:A:326:ILE:HD13	1.47	1.48
1:A:304:TYR:CD1	1:A:326:ILE:CD1	2.18	1.26
1:B:484:LEU:O	1:B:485:LYS:HG2	1.27	1.25
1:B:223:ASP:OD2	1:B:225:THR:HG23	1.32	1.25

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:487:LYS:NZ	1:A:497:TYR:OH[2_555]	2.05	0.15

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	606/608 (100%)	417 (69%)	128 (21%)	61 (10%)	1 4
1	B	606/608 (100%)	423 (70%)	113 (19%)	70 (12%)	0 2
1	C	606/608 (100%)	374 (62%)	164 (27%)	68 (11%)	0 3
All	All	1818/1824 (100%)	1214 (67%)	405 (22%)	199 (11%)	0 3

5 of 199 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	71	HIS
1	A	77	HIS
1	A	103	ASN
1	A	111	LEU

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	500/500 (100%)	393 (79%)	107 (21%)	1 5
1	B	500/500 (100%)	422 (84%)	78 (16%)	3 14
1	C	500/500 (100%)	433 (87%)	67 (13%)	5 20
All	All	1500/1500 (100%)	1248 (83%)	252 (17%)	2 11

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	53	MET
1	B	232	GLN
1	C	461	PHE
1	B	86	HIS
1	B	170	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	HIS
1	B	375	ASN
1	C	438	GLN
1	B	187	ASN
1	B	250	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	G6Q	A	700	-	15,15,15	2.13	6 (40%)	18,21,21	2.85	11 (61%)
2	G6Q	B	701	1	15,15,15	1.38	3 (20%)	18,21,21	2.05	5 (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
2	G6Q	A	700	-	-	0/18/20/20	0/0/0/0
2	G6Q	B	701	1	-	0/18/20/20	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	G6Q	O5-C5	-3.19	1.36	1.43
2	A	700	G6Q	P-O2P	-2.96	1.44	1.54
2	B	701	G6Q	C3-C2	-2.63	1.48	1.53
2	B	701	G6Q	O4-C4	-2.44	1.37	1.43
2	A	700	G6Q	C3-C2	-2.33	1.49	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	G6Q	C3-C2-C1	-4.79	104.62	111.68
2	B	701	G6Q	O1-C1-C2	-4.56	112.30	125.60
2	A	700	G6Q	O1-C1-C2	-4.45	112.63	125.60
2	A	700	G6Q	O2-C2-C1	-4.26	100.05	110.22
2	A	700	G6Q	O3P-P-O1P	-4.12	97.30	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	G6Q	4	0
2	B	701	G6Q	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^{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	608/608 (100%)	-0.72	6 (0%)	84	69	9, 38, 101, 133	0
1	B	608/608 (100%)	-0.51	6 (0%)	84	69	19, 78, 125, 138	0
1	C	608/608 (100%)	0.08	32 (5%)	30	13	44, 113, 137, 151	0
All	All	1824/1824 (100%)	-0.38	44 (2%)	62	39	9, 79, 131, 151	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ASN	8.8
1	C	89	VAL	5.7
1	C	81	SER	5.7
1	B	240	TYR	4.9
1	A	85	ALA	4.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	G6Q	B	701	16/16	0.94	0.17	0.78	62,73,81,84	0
2	G6Q	A	700	16/16	0.96	0.13	0.38	25,31,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.