Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 10:51 PM EST

PDB ID	:	3UJS
Title	:	Asymmetric complex of human neuron specific enolase-6-PGA/PEP
Authors	:	Qin, J.; Chai, G.; Brewer, J.; Lovelace, L.; Lebioda, L.
Deposited on	:	2011-11-08
Resolution	:	1.65 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 (i)) were used in the production of this report:

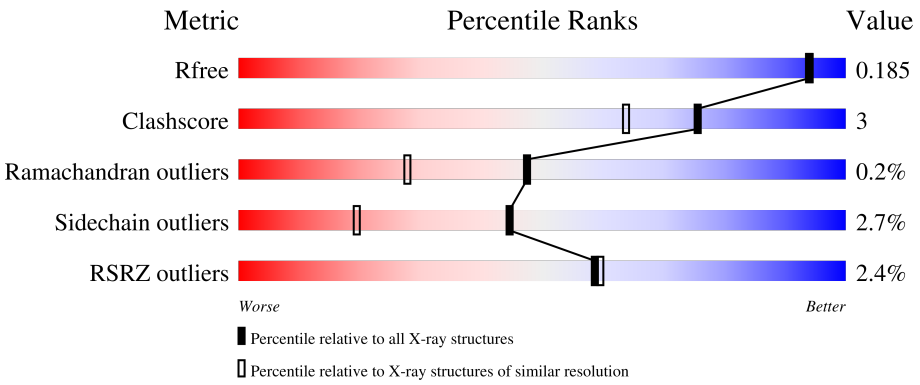
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	443	3% 88% 8% • •
1	B	443	% 87% 9% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7359 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	3251	2058	558	622	13	0	0	0
1	B	433	3269	2068	556	632	13	0	0	0

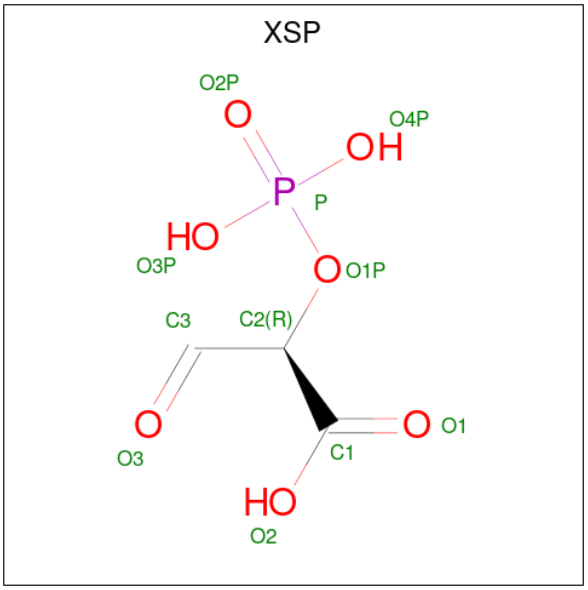
There are 20 discrepancies between the modelled and reference sequences:

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).

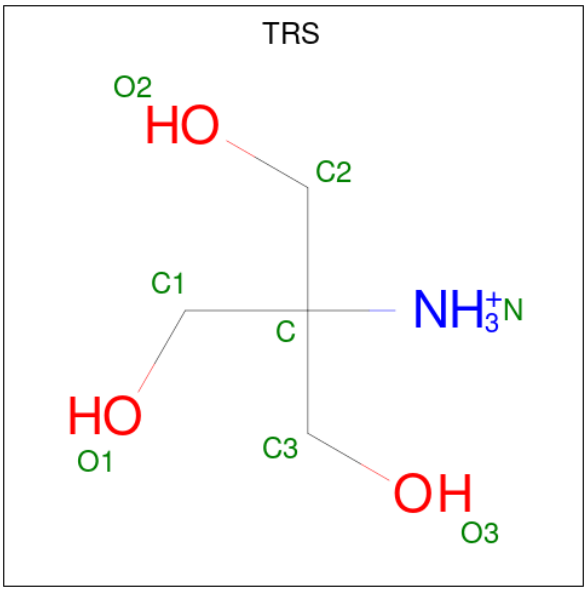
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
			Total	Mg		
2	B	2	2	2	0	0

- Molecule 3 is (2R)-3-oxo-2-(phosphonooxy)propanoic acid (three-letter code: XSP) (formula: $C_3H_5O_7P$).



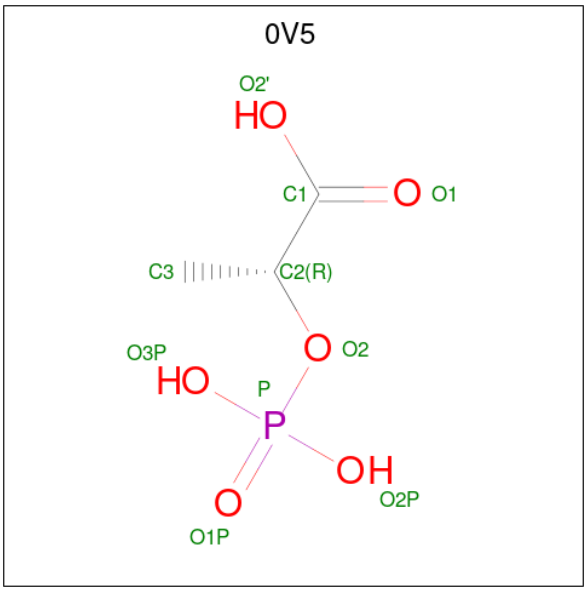
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	11	3	7	1	0	0

- 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 (2R)-2-(phosphonooxy)propanoic acid (three-letter code: 0V5) (formula: $C_3H_7O_6P$).



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

- Molecule 6 is water.

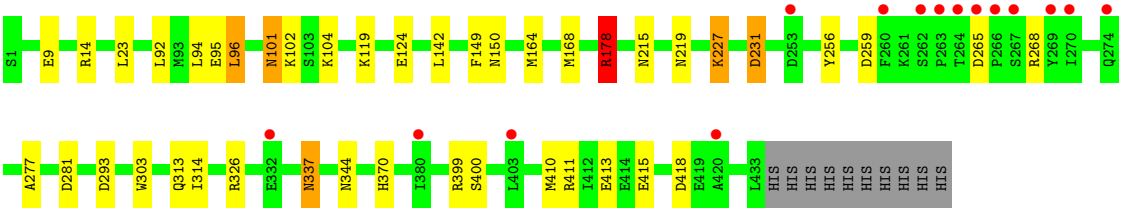
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	381	381	381	0	0
			Total	O		
6	B	425	425	425	0	0

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.

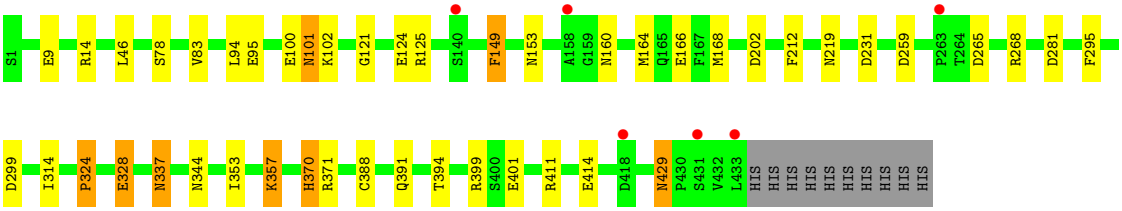
- Molecule 1: Gamma-enolase

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	114.45Å 119.82Å 68.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.84 – 1.65 43.84 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.84-1.65) 99.3 (43.84-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.20 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.135 , 0.185 0.134 , 0.185	Depositor DCC
R_{free} test set	5744 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, 0V5, MG, XSP

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	1.27	8/3306 (0.2%)	1.06	10/4478 (0.2%)
1	B	1.34	13/3324 (0.4%)	1.06	11/4502 (0.2%)
All	All	1.31	21/6630 (0.3%)	1.06	21/8980 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	415	GLU	CB-CG	9.07	1.69	1.52
1	B	212	PHE	CE1-CZ	6.67	1.50	1.37
1	A	124	GLU	CG-CD	6.21	1.61	1.51
1	B	231	ASP	CB-CG	6.16	1.64	1.51
1	A	124	GLU	CD-OE2	6.10	1.32	1.25
1	B	328	GLU	CG-CD	5.90	1.60	1.51
1	A	119	LYS	CD-CE	5.88	1.66	1.51
1	B	414	GLU	CD-OE2	-5.74	1.19	1.25
1	B	9	GLU	CB-CG	-5.64	1.41	1.52
1	B	95	GLU	CG-CD	5.50	1.60	1.51
1	B	100	GLU	CG-CD	5.47	1.60	1.51
1	B	295	PHE	CE1-CZ	5.46	1.47	1.37
1	B	124	GLU	CD-OE1	5.37	1.31	1.25
1	A	9	GLU	CB-CG	-5.32	1.42	1.52
1	B	388	CYS	CB-SG	-5.31	1.73	1.81
1	B	357	LYS	CE-NZ	5.26	1.62	1.49
1	B	149	PHE	CE1-CZ	5.26	1.47	1.37
1	A	415	GLU	CG-CD	-5.23	1.44	1.51
1	A	277	ALA	CA-CB	5.22	1.63	1.52
1	B	357	LYS	CD-CE	5.06	1.64	1.51
1	A	256	TYR	CE2-CZ	5.05	1.45	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	14	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	357	LYS	CD-CE-NZ	8.50	131.24	111.70
1	A	178	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	96	LEU	CB-CG-CD2	7.50	123.75	111.00
1	A	104	LYS	CD-CE-NZ	-7.19	95.16	111.70
1	A	231	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	299	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	371	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	281	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	411	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	B	14	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	14	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	78	SER	CA-CB-OG	-5.82	95.48	111.20
1	B	411	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	231	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	259	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	281	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	259	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	411	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	326	ARG	NE-CZ-NH1	-5.01	117.80	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	3251	0	3201	21	0
1	B	3269	0	3220	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	3	0	0
4	A	8	0	12	0	0
5	B	10	0	6	1	0
6	A	381	0	0	3	3
6	B	425	0	0	5	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7359	0	6442	40	3

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 3.

All (40) 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:357:LYS:HD2	6:B:932:HOH:O	1.34	1.27
1:A:178:ARG:HD3	1:A:413:GLU:OE1	1.49	1.10
1:B:353:ILE:HG22	1:B:357:LYS:HE2	1.50	0.91
1:B:314:ILE:H	1:B:337:ASN:HD21	1.34	0.73
1:A:101:ASN:H	1:A:101:ASN:HD22	1.42	0.64
1:B:101:ASN:HD22	1:B:101:ASN:H	1.46	0.63
1:B:314:ILE:H	1:B:337:ASN:ND2	1.97	0.63
1:A:314:ILE:H	1:A:337:ASN:HD21	1.48	0.60
1:B:265:ASP:O	1:B:268:ARG:HG2	2.03	0.57
1:A:314:ILE:H	1:A:337:ASN:ND2	2.03	0.56
1:A:227:LYS:HE2	1:A:231:ASP:OD2	2.07	0.55
1:B:166:GLU:OE2	5:B:602:0V5:H4	2.07	0.54
1:B:337:ASN:C	1:B:337:ASN:HD22	2.10	0.54
1:A:215:ASN:CB	1:B:202:ASP:OD2	2.57	0.53
1:A:418:ASP:HA	6:A:1033:HOH:O	2.07	0.53
1:B:125:ARG:HD2	6:B:1070:HOH:O	2.07	0.53
1:B:328:GLU:HG3	6:B:1039:HOH:O	2.10	0.52
1:B:429:ASN:ND2	6:B:1046:HOH:O	2.44	0.51
1:A:95:GLU:CG	6:A:883:HOH:O	2.60	0.50
1:A:313:GLN:HA	1:A:337:ASN:HD21	1.76	0.50
1:B:324:PRO:HG2	6:B:1104:HOH:O	2.12	0.49
1:A:149:PHE:O	1:A:168:MET:HA	2.13	0.48
1:B:429:ASN:HD22	1:B:429:ASN:N	2.12	0.46
1:A:142:LEU:N	6:A:895:HOH:O	2.47	0.46
1:A:101:ASN:HD22	1:A:101:ASN:N	2.10	0.46
1:A:164:MET:H	1:A:219:ASN:HD21	1.63	0.45
1:A:265:ASP:O	1:A:268:ARG:HG2	2.18	0.44
1:B:94:LEU:HD22	1:B:102:LYS:HE3	1.99	0.44
1:A:293:ASP:HA	1:A:303:TRP:CH2	2.52	0.44
1:B:164:MET:H	1:B:219:ASN:HD21	1.65	0.44
1:A:178:ARG:HD2	1:A:410:MET:HA	2.00	0.44
1:B:83:VAL:HG23	1:B:121:GLY:HA2	2.00	0.43
1:A:23:LEU:C	1:A:23:LEU:HD23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PHE:O	1:B:168:MET:HA	2.18	0.43
1:A:92:LEU:C	1:A:92:LEU:HD23	2.40	0.41
1:A:94:LEU:CD2	1:A:102:LYS:HE3	2.50	0.41
1:A:400:SER:HB2	1:B:401:GLU:HB3	2.02	0.41
1:B:429:ASN:HD22	1:B:429:ASN:H	1.68	0.41
1:A:337:ASN:HD22	1:A:337:ASN:C	2.24	0.40
1:B:370:HIS:CG	1:B:394:THR:HA	2.56	0.40

All (3) 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)
6:A:948:HOH:O	6:B:765:HOH:O[1_556]	1.87	0.33
6:A:1040:HOH:O	6:B:996:HOH:O[1_556]	1.97	0.23
6:A:870:HOH:O	6:B:728:HOH:O[3_545]	2.09	0.11

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%)	419 (97%)	11 (3%)	1 (0%)	47 28
1	B	431/443 (97%)	422 (98%)	8 (2%)	1 (0%)	47 28
All	All	862/886 (97%)	841 (98%)	19 (2%)	2 (0%)	47 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	ARG
1	A	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	329/360 (91%)	321 (98%)	8 (2%)	49	23
1	B	334/360 (93%)	324 (97%)	10 (3%)	41	15
All	All	663/720 (92%)	645 (97%)	18 (3%)	44	19

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	A	101	ASN
1	A	150	ASN
1	A	178	ARG
1	A	227	LYS
1	A	337	ASN
1	A	344	ASN
1	A	370	HIS
1	B	46	LEU
1	B	101	ASN
1	B	153	ASN
1	B	160	ASN
1	B	324	PRO
1	B	337	ASN
1	B	344	ASN
1	B	370	HIS
1	B	391	GLN
1	B	429	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	139	ASN
1	A	150	ASN
1	A	153	ASN

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Mol	Chain	Res	Type
1	A	219	ASN
1	A	309	ASN
1	A	337	ASN
1	A	426	ASN
1	B	91	ASN
1	B	101	ASN
1	B	160	ASN
1	B	219	ASN
1	B	337	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	$\#\|Z\| > 2$
5	0V5	B	602	2	8,9,9	1.39	2 (25%)	11,13,13	1.89	4 (36%)
3	XSP	A	602	2	10,10,10	2.49	3 (30%)	8,14,14	1.55	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TRS	A	603	-	7,7,7	0.63	0	9,9,9	1.09	1 (11%)

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
5	0V5	B	602	2	-	3/9/9/9	-
3	XSP	A	602	2	-	2/7/11/11	-
4	TRS	A	603	-	-	0/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	XSP	O3-C3	5.39	1.41	1.19
3	A	602	XSP	O1P-C2	4.27	1.51	1.45
5	B	602	0V5	P-O2	2.47	1.64	1.59
5	B	602	0V5	C2-C1	2.11	1.55	1.52
3	A	602	XSP	O1-C1	2.08	1.28	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	XSP	P-O1P-C2	-3.60	112.80	123.06
5	B	602	0V5	C3-C2-C1	3.18	114.53	109.28
5	B	602	0V5	O2'-C1-O1	-2.89	117.53	124.09
5	B	602	0V5	O2-C2-C1	2.83	116.26	111.04
5	B	602	0V5	O3P-P-O2P	2.33	116.53	107.64
4	A	603	TRS	C2-C-C1	-2.13	104.20	110.81

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	XSP	O2-C1-C2-C3
3	A	602	XSP	O1-C1-C2-C3
5	B	602	0V5	O1-C1-C2-C3
5	B	602	0V5	O2'-C1-C2-C3
5	B	602	0V5	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	0V5	1	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%)	-0.20	15 (3%)	44	45	9, 19, 33, 46	0
1	B	433/443 (97%)	-0.43	6 (1%)	75	79	9, 16, 29, 51	0
All	All	866/886 (97%)	-0.32	21 (2%)	59	59	9, 17, 32, 51	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	LEU	5.6
1	A	264	THR	3.6
1	A	263	PRO	3.5
1	A	420	ALA	3.5
1	B	263	PRO	3.3
1	A	269	TYR	3.2
1	A	270	ILE	3.2
1	A	260	PHE	3.1
1	A	332	GLU	3.1
1	A	267	SER	3.0
1	B	158	ALA	2.7
1	A	266	PRO	2.7
1	A	265	ASP	2.6
1	B	140	SER	2.5
1	B	418	ASP	2.5
1	A	403	LEU	2.4
1	A	253	ASP	2.2
1	A	262	SER	2.2
1	A	380	ILE	2.2
1	B	431	SER	2.1
1	A	274	GLN	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, 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	603	8/8	0.86	0.21	28,34,36,36	0
3	XSP	A	602	11/11	0.99	0.06	14,16,27,30	0
2	MG	A	601	1/1	0.99	0.05	17,17,17,17	0
5	0V5	B	602	10/10	0.99	0.08	12,14,17,21	0
2	MG	A	600	1/1	1.00	0.05	16,16,16,16	0
2	MG	B	600	1/1	1.00	0.06	12,12,12,12	0
2	MG	B	601	1/1	1.00	0.03	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.