wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:19 PM GMT

PDB ID	:	4HY3
Title	:	Crystal structure of a phosphoglycerate oxidoreductase from rhizobium etli
Authors	:	Kumaran, D.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2012-11-12
Resolution	:	2.80 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:

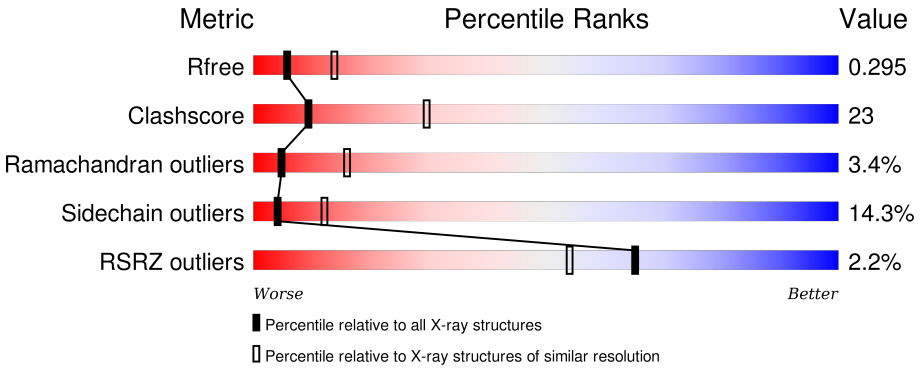
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	365	% 50% 32% 6% • 11%
1	B	365	2% 49% 31% 7% • 13%
1	C	365	5% 45% 30% 8% • 18%
1	D	365	59% 24% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9794 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 phosphoglycerate oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	Se	0	0	0
			2464	1560	432	461	1	10			
1	B	319	Total	C	N	O	S	Se	0	0	0
			2431	1540	427	453	1	10			
1	C	301	Total	C	N	O	Se		0	0	0
			2292	1459	398	426	9				
1	D	321	Total	C	N	O	S	Se	0	0	0
			2451	1551	432	457	1	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	EXPRESSION TAG	UNP Q2K273
A	-20	HIS	-	EXPRESSION TAG	UNP Q2K273
A	-19	HIS	-	EXPRESSION TAG	UNP Q2K273
A	-18	HIS	-	EXPRESSION TAG	UNP Q2K273
A	-17	HIS	-	EXPRESSION TAG	UNP Q2K273
A	-16	HIS	-	EXPRESSION TAG	UNP Q2K273
A	-15	HIS	-	EXPRESSION TAG	UNP Q2K273
A	-14	SER	-	EXPRESSION TAG	UNP Q2K273
A	-13	SER	-	EXPRESSION TAG	UNP Q2K273
A	-12	GLY	-	EXPRESSION TAG	UNP Q2K273
A	-11	VAL	-	EXPRESSION TAG	UNP Q2K273
A	-10	ASP	-	EXPRESSION TAG	UNP Q2K273
A	-9	LEU	-	EXPRESSION TAG	UNP Q2K273
A	-8	GLY	-	EXPRESSION TAG	UNP Q2K273
A	-7	THR	-	EXPRESSION TAG	UNP Q2K273
A	-6	GLU	-	EXPRESSION TAG	UNP Q2K273
A	-5	ASN	-	EXPRESSION TAG	UNP Q2K273
A	-4	LEU	-	EXPRESSION TAG	UNP Q2K273
A	-3	TYR	-	EXPRESSION TAG	UNP Q2K273
A	-2	PHE	-	EXPRESSION TAG	UNP Q2K273
A	-1	GLN	-	EXPRESSION TAG	UNP Q2K273

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q2K273
B	-21	MSE	-	EXPRESSION TAG	UNP Q2K273
B	-20	HIS	-	EXPRESSION TAG	UNP Q2K273
B	-19	HIS	-	EXPRESSION TAG	UNP Q2K273
B	-18	HIS	-	EXPRESSION TAG	UNP Q2K273
B	-17	HIS	-	EXPRESSION TAG	UNP Q2K273
B	-16	HIS	-	EXPRESSION TAG	UNP Q2K273
B	-15	HIS	-	EXPRESSION TAG	UNP Q2K273
B	-14	SER	-	EXPRESSION TAG	UNP Q2K273
B	-13	SER	-	EXPRESSION TAG	UNP Q2K273
B	-12	GLY	-	EXPRESSION TAG	UNP Q2K273
B	-11	VAL	-	EXPRESSION TAG	UNP Q2K273
B	-10	ASP	-	EXPRESSION TAG	UNP Q2K273
B	-9	LEU	-	EXPRESSION TAG	UNP Q2K273
B	-8	GLY	-	EXPRESSION TAG	UNP Q2K273
B	-7	THR	-	EXPRESSION TAG	UNP Q2K273
B	-6	GLU	-	EXPRESSION TAG	UNP Q2K273
B	-5	ASN	-	EXPRESSION TAG	UNP Q2K273
B	-4	LEU	-	EXPRESSION TAG	UNP Q2K273
B	-3	TYR	-	EXPRESSION TAG	UNP Q2K273
B	-2	PHE	-	EXPRESSION TAG	UNP Q2K273
B	-1	GLN	-	EXPRESSION TAG	UNP Q2K273
B	0	SER	-	EXPRESSION TAG	UNP Q2K273
C	-21	MSE	-	EXPRESSION TAG	UNP Q2K273
C	-20	HIS	-	EXPRESSION TAG	UNP Q2K273
C	-19	HIS	-	EXPRESSION TAG	UNP Q2K273
C	-18	HIS	-	EXPRESSION TAG	UNP Q2K273
C	-17	HIS	-	EXPRESSION TAG	UNP Q2K273
C	-16	HIS	-	EXPRESSION TAG	UNP Q2K273
C	-15	HIS	-	EXPRESSION TAG	UNP Q2K273
C	-14	SER	-	EXPRESSION TAG	UNP Q2K273
C	-13	SER	-	EXPRESSION TAG	UNP Q2K273
C	-12	GLY	-	EXPRESSION TAG	UNP Q2K273
C	-11	VAL	-	EXPRESSION TAG	UNP Q2K273
C	-10	ASP	-	EXPRESSION TAG	UNP Q2K273
C	-9	LEU	-	EXPRESSION TAG	UNP Q2K273
C	-8	GLY	-	EXPRESSION TAG	UNP Q2K273
C	-7	THR	-	EXPRESSION TAG	UNP Q2K273
C	-6	GLU	-	EXPRESSION TAG	UNP Q2K273
C	-5	ASN	-	EXPRESSION TAG	UNP Q2K273
C	-4	LEU	-	EXPRESSION TAG	UNP Q2K273
C	-3	TYR	-	EXPRESSION TAG	UNP Q2K273

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	EXPRESSION TAG	UNP Q2K273
C	-1	GLN	-	EXPRESSION TAG	UNP Q2K273
C	0	SER	-	EXPRESSION TAG	UNP Q2K273
D	-21	MSE	-	EXPRESSION TAG	UNP Q2K273
D	-20	HIS	-	EXPRESSION TAG	UNP Q2K273
D	-19	HIS	-	EXPRESSION TAG	UNP Q2K273
D	-18	HIS	-	EXPRESSION TAG	UNP Q2K273
D	-17	HIS	-	EXPRESSION TAG	UNP Q2K273
D	-16	HIS	-	EXPRESSION TAG	UNP Q2K273
D	-15	HIS	-	EXPRESSION TAG	UNP Q2K273
D	-14	SER	-	EXPRESSION TAG	UNP Q2K273
D	-13	SER	-	EXPRESSION TAG	UNP Q2K273
D	-12	GLY	-	EXPRESSION TAG	UNP Q2K273
D	-11	VAL	-	EXPRESSION TAG	UNP Q2K273
D	-10	ASP	-	EXPRESSION TAG	UNP Q2K273
D	-9	LEU	-	EXPRESSION TAG	UNP Q2K273
D	-8	GLY	-	EXPRESSION TAG	UNP Q2K273
D	-7	THR	-	EXPRESSION TAG	UNP Q2K273
D	-6	GLU	-	EXPRESSION TAG	UNP Q2K273
D	-5	ASN	-	EXPRESSION TAG	UNP Q2K273
D	-4	LEU	-	EXPRESSION TAG	UNP Q2K273
D	-3	TYR	-	EXPRESSION TAG	UNP Q2K273
D	-2	PHE	-	EXPRESSION TAG	UNP Q2K273
D	-1	GLN	-	EXPRESSION TAG	UNP Q2K273
D	0	SER	-	EXPRESSION TAG	UNP Q2K273

- Molecule 2 is water.

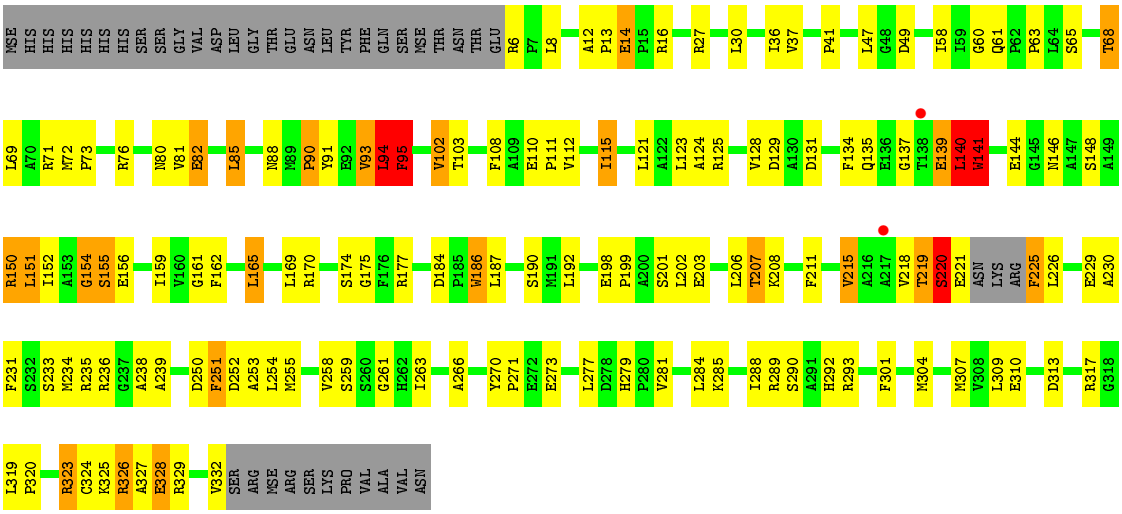
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	36	Total O 36 36	0	0
2	C	37	Total O 37 37	0	0
2	D	54	Total O 54 54	0	0

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.

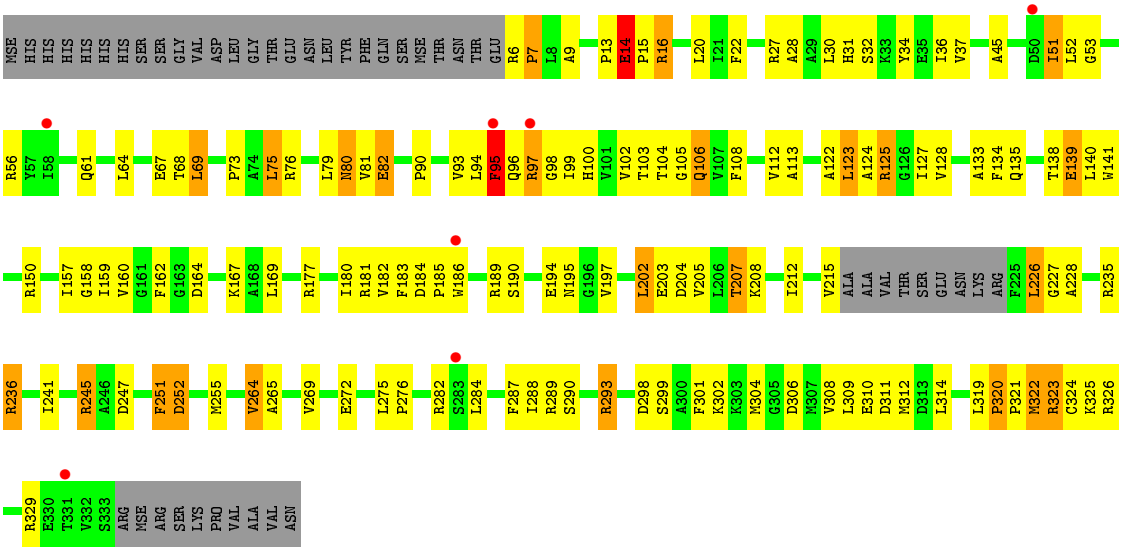
- Molecule 1: phosphoglycerate oxidoreductase

Chain A:



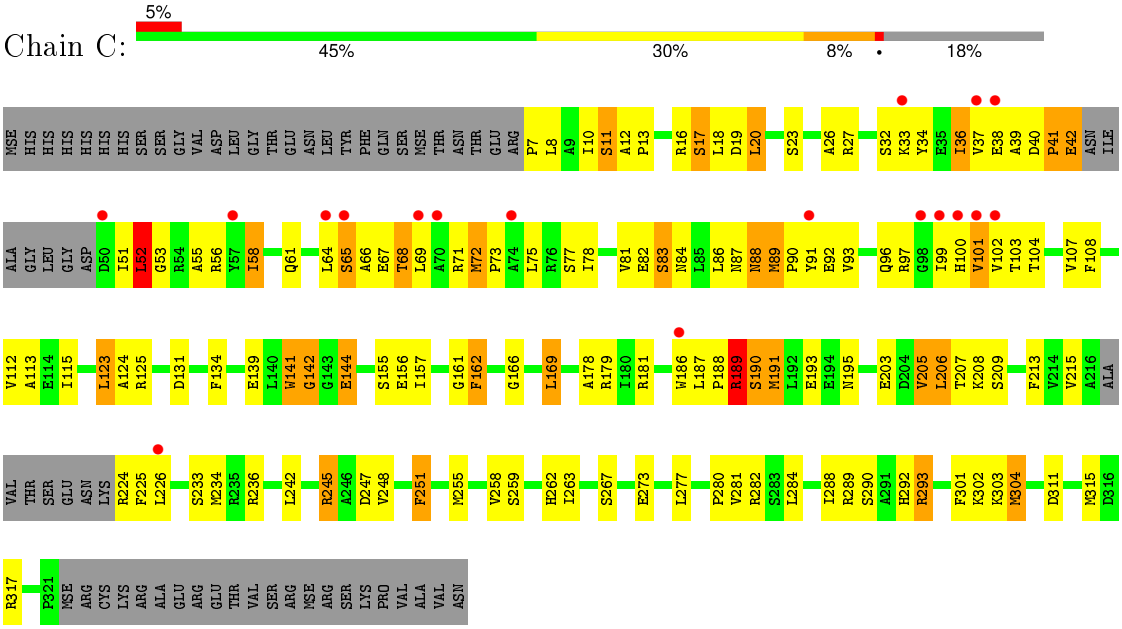
- Molecule 1: phosphoglycerate oxidoreductase

Chain B:



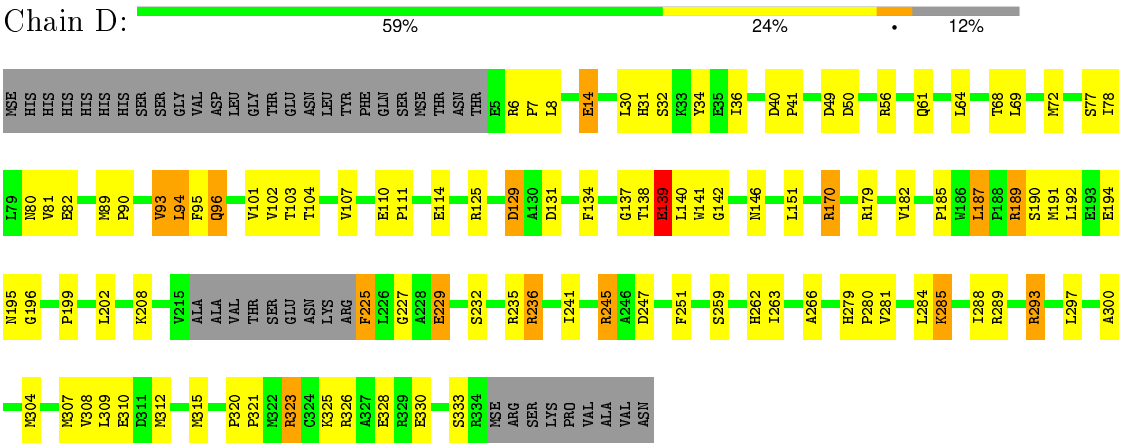
• Molecule 1: phosphoglycerate oxidoreductase

Chain C:



• Molecule 1: phosphoglycerate oxidoreductase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.73Å 121.12Å 106.65Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	104.55 – 2.80 44.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (104.55-2.80) 98.9 (44.94-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.97 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.291 0.210 , 0.295	Depositor DCC
R_{free} test set	1890 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 37426 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9794	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.62	2/2499 (0.1%)	0.87	4/3366 (0.1%)
1	B	0.54	1/2466 (0.0%)	0.75	0/3320
1	C	0.58	2/2327 (0.1%)	0.81	0/3135
1	D	0.73	2/2486 (0.1%)	0.94	3/3346 (0.1%)
All	All	0.62	7/9778 (0.1%)	0.85	7/13167 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	ARG	C-N	6.73	1.49	1.34
1	C	186	TRP	CD2-CE2	5.54	1.48	1.41
1	A	186	TRP	CD2-CE2	5.47	1.48	1.41
1	D	141	TRP	CD2-CE2	5.45	1.47	1.41
1	C	141	TRP	CD2-CE2	5.25	1.47	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	236	ARG	O-C-N	-6.49	112.17	123.20
1	D	236	ARG	CA-C-N	6.00	128.20	116.20
1	A	27	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	94	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	27	ARG	CG-CD-NE	-5.46	100.34	111.80

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	2464	0	2473	120	0
1	B	2431	0	2441	122	0
1	C	2292	0	2299	120	0
1	D	2451	0	2460	104	0
2	A	29	0	0	5	0
2	B	36	0	0	6	0
2	C	37	0	0	10	0
2	D	54	0	0	18	0
All	All	9794	0	9673	438	0

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 23.

The worst 5 of 438 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:D:208:LYS:HE3	2:D:442:HOH:O	1.29	1.31
1:C:234:MSE:HE1	1:C:263:ILE:HD13	1.28	1.15
1:B:14:GLU:HB3	1:B:15:PRO:HD3	1.21	1.15
1:B:14:GLU:HB3	1:B:15:PRO:CD	1.76	1.13
1:C:68:THR:HA	1:C:71:ARG:HD3	1.31	1.11

There are no symmetry-related clashes.

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	320/365 (88%)	279 (87%)	31 (10%)	10 (3%)	5 17
1	B	315/365 (86%)	264 (84%)	41 (13%)	10 (3%)	5 17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	295/365 (81%)	239 (81%)	40 (14%)	16 (5%)	2 7
1	D	317/365 (87%)	293 (92%)	18 (6%)	6 (2%)	10 32
All	All	1247/1460 (85%)	1075 (86%)	130 (10%)	42 (3%)	5 16

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	GLU
1	B	75	LEU
1	B	95	PHE
1	B	236	ARG
1	C	65	SER

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	256/281 (91%)	214 (84%)	42 (16%)	3 8
1	B	253/281 (90%)	220 (87%)	33 (13%)	5 15
1	C	238/281 (85%)	202 (85%)	36 (15%)	3 10
1	D	255/281 (91%)	223 (88%)	32 (12%)	6 17
All	All	1002/1124 (89%)	859 (86%)	143 (14%)	4 12

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	226	LEU
1	C	38	GLU
1	D	229	GLU
1	B	251	PHE
1	B	293	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	HIS
1	B	195	ASN
1	C	195	ASN
1	B	84	ASN
1	C	100	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	314/365 (86%)	-0.26	2 (0%) 90 86	15, 43, 71, 90	0
1	B	309/365 (84%)	0.20	7 (2%) 64 52	32, 64, 91, 113	0
1	C	292/365 (80%)	0.14	18 (6%) 24 15	23, 60, 109, 142	0
1	D	311/365 (85%)	-0.35	0 100 100	14, 32, 58, 74	0
All	All	1226/1460 (83%)	-0.07	27 (2%) 65 54	14, 49, 93, 142	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	TYR	3.7
1	B	331	THR	3.6
1	C	186	TRP	3.4
1	C	37	VAL	3.3
1	C	98	GLY	3.2

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

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.