



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2018 – 01:00 PM EST

PDB ID : 5YP4
Title : Crystal structure of dipeptidyl peptidase IV (DPP IV) with Lys-Pro from Pseudoxanthomonas mexicana WO24
Authors : Roppongi, S.; Suzuki, Y.; Tateoka, C.; Fuimoto, M.; Morisawa, S.; Iizuka, I.; Nakamura, A.; Honma, N.; Shida, Y.; Ogasawara, W.; Tanaka, N.; Sakamoto, Y.; Nonaka, T.
Deposited on : 2017-11-01
Resolution : 1.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

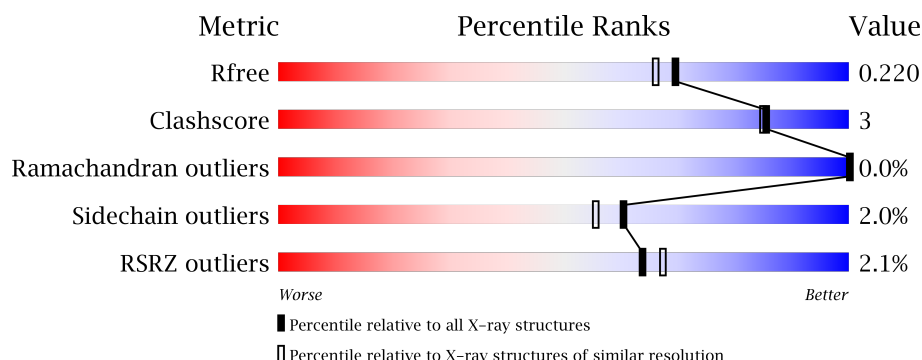
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 $\leq 5\%$. 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	745	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	745	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>..</div> </div> </div>
1	C	745	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	D	745	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	803	-	-	-	X
2	GOL	A	804	-	-	-	X
2	GOL	A	806	-	-	-	X
2	GOL	B	804	-	-	-	X
2	GOL	B	807	-	-	-	X
2	GOL	B	808	-	-	-	X
2	GOL	B	810	-	-	-	X
2	GOL	B	811	-	-	-	X
2	GOL	D	803	-	-	-	X
2	GOL	D	804	-	-	-	X
2	GOL	D	806	-	-	-	X
3	LYS	A	801	-	-	-	X
3	LYS	B	801	-	-	-	X
3	LYS	C	801	-	-	-	X
3	LYS	D	801	-	-	-	X
4	PRO	A	802	-	-	-	X
4	PRO	D	802	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25338 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 Dipeptidyl aminopeptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5660	3580	994	1076	10			
1	B	724	Total	C	N	O	S	0	0	0
			5660	3580	994	1076	10			
1	C	687	Total	C	N	O	S	0	1	0
			5379	3419	937	1013	10			
1	D	714	Total	C	N	O	S	0	0	0
			5571	3523	981	1057	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ILE	MET	see sequence details	UNP Q6F3I7
B	12	ILE	MET	see sequence details	UNP Q6F3I7
C	12	ILE	MET	see sequence details	UNP Q6F3I7
D	12	ILE	MET	see sequence details	UNP Q6F3I7

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



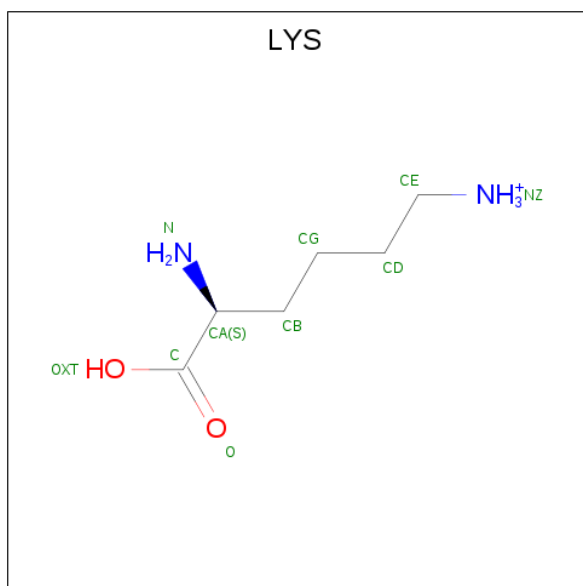
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

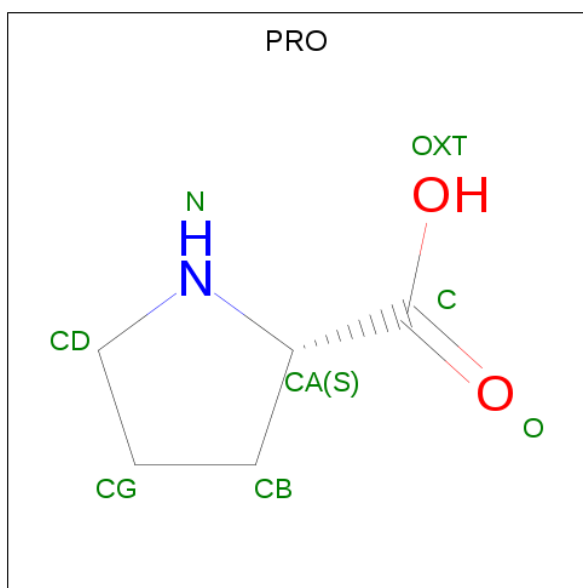
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	2	1		
3	B	1	Total	C	N	O	0	0
			9	6	2	1		
3	C	1	Total	C	N	O	0	0
			9	6	2	1		
3	D	1	Total	C	N	O	0	0
			9	6	2	1		

- Molecule 4 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	5	1	1		
4	B	1	Total	C	N	O	0	0
			7	5	1	1		
4	C	1	Total	C	N	O	0	0
			8	5	1	2		
4	D	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	817	Total	O	0	0
			817	817		
5	B	685	Total	O	0	0
			685	685		
5	C	611	Total	O	0	0
			611	611		
5	D	764	Total	O	0	0
			764	764		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

Residue Type	Count
ALA	1
ARG	1
ASP	1
ASN	1
GLU	1
LEU	1
PHE	1
PRO	1
SER	1
THR	1
TRP	1
VAL	1
ALA	1
THR	1
ALA	1
LEU	1
PRO	1
ALA	1
ALA	1
HIS	1
A22	1
A34	1
P35	1
L36	1
S37	1
T42	1
I46	1
R52	1
L56	1
R61	1
D62	1
L68	1
I73	1
T78	1
R79	1
I107	1
A108	1
A109	1
D121	1
D137	1
S141	1
G142	1
R143	1
D144	1
H154	1
G152	1
N175	1
G193	1
E209	1
Y241	1
P245	1
D246	1
R279	1
D286	1
R297	1
Q307	1
S308	1
R309	1
L321	1
R327	1
R351	1
P352	1
L353	1
E357	1
L390	1
R403	1
L416	1
R437	1
V443	1
R484	1
T494	1
L504	1
Q533	1
T534	1
V535	1
T536	1
R537	1
A538	1
N539	1
P540	1
G541	1
P546	1
T560	1
T566	1
P567	1
R568	1
L577	1
L590	1
D603	1
R606	1
W612	1
S613	1
M614	1
G636	1
A637	1
D646	1
T647	1
H648	1
R652	1
F670	1
I684	1
H685	1
K699	1
M714	1
R724	1
R731	1
Y732	1
R733	1
E736	1
R741	1
K744	1
P745	1

Chain B:

89%

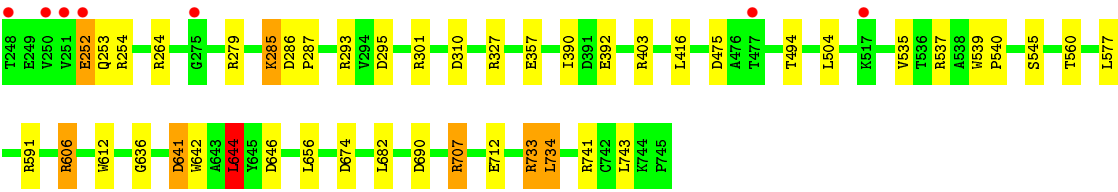
7%

Chain C:

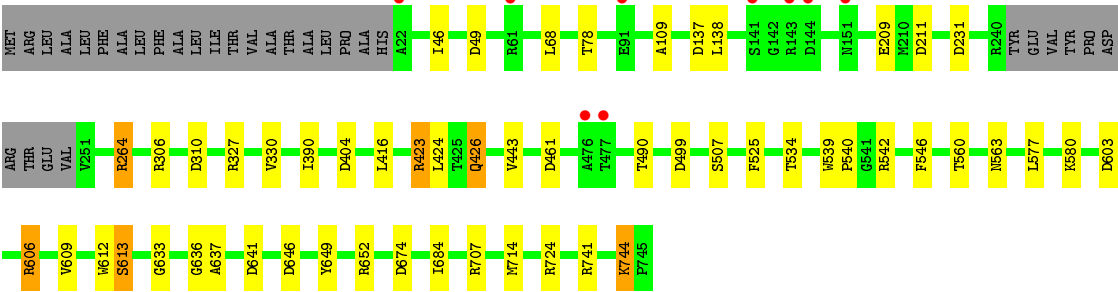
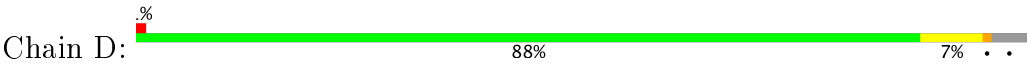
4% 84% 7% 8%

MET ARG ARG ARG ALA ILE ALA PHE ALA LEU PHE ALA LEU ILE THR VAL ALA THR LEU PRO ALA HIS A22 E28 D49 R52 K59 ASP ARG D62 R63 R64 R65 E70 D83 S84 S85 R86 R87 R88 R89 GLY GLU VAL LEU SER ASP GLU LYS ARG ARG GLU

ARG GLN ARG ARG ILE ALA ALA L110 W118 SER PRO ASP GLY LYS A124 L129 Y136 ASP LEU THR LYS SER GLY ARG ASP A145 V146 L149 T150 ASN GLY G153 G154 F155 P159 S169 R174 I179 A182 S183 R191 F204 E208 V237 Q238 Y241



● Molecule 1: Dipeptidyl aminopeptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	88.66Å 104.49Å 112.84Å 67.42° 68.83° 65.46°	Depositor
Resolution (Å)	40.00 – 1.90 49.31 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.00-1.90) 86.2 (49.31-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.164 , 0.213 0.173 , 0.220	Depositor DCC
R_{free} test set	12222 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25338	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.77% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	1.02	5/5799 (0.1%)	1.06	28/7887 (0.4%)
1	B	0.94	0/5799	1.01	26/7887 (0.3%)
1	C	0.95	4/5515 (0.1%)	1.02	29/7501 (0.4%)
1	D	0.95	0/5706	1.01	19/7757 (0.2%)
All	All	0.97	9/22819 (0.0%)	1.03	102/31032 (0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	392	GLU	CD-OE2	6.16	1.32	1.25
1	A	736	GLU	CD-OE2	-5.40	1.19	1.25
1	A	37	SER	CB-OG	-5.36	1.35	1.42
1	C	642	TRP	CB-CG	-5.33	1.40	1.50
1	C	545	SER	CB-OG	-5.25	1.35	1.42

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	606	ARG	NE-CZ-NH2	-16.71	111.94	120.30
1	A	606	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	D	606	ARG	NE-CZ-NH2	-13.25	113.67	120.30
1	D	606	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	C	301	ARG	NE-CZ-NH2	-11.63	114.48	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	5660	0	5521	39	0
1	B	5660	0	5521	26	0
1	C	5379	0	5251	30	0
1	D	5571	0	5441	21	0
2	A	24	0	32	3	0
2	B	60	0	80	5	0
2	C	12	0	16	1	0
2	D	30	0	40	0	0
3	A	9	0	12	0	0
3	B	9	0	12	0	0
3	C	9	0	12	0	0
3	D	9	0	12	0	0
4	A	7	0	7	0	0
4	B	7	0	7	0	0
4	C	8	0	7	0	0
4	D	7	0	7	0	0
5	A	817	0	0	10	0
5	B	685	0	0	5	0
5	C	611	0	0	8	0
5	D	764	0	0	5	0
All	All	25338	0	21978	117	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 3.

The worst 5 of 117 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:744:LYS:HB2	5:A:1318:HOH:O	1.18	1.29
1:D:744:LYS:HB2	5:D:1357:HOH:O	1.20	1.27
1:D:211:ASP:HB2	5:D:1501:HOH:O	1.53	1.07
1:A:744:LYS:CB	5:A:1318:HOH:O	1.84	0.91
1:A:648:HIS:HD2	1:A:652:ARG:HH21	1.20	0.88

There are no symmetry-related clashes.

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	722/745 (97%)	697 (96%)	25 (4%)	0	100	100
1	B	722/745 (97%)	694 (96%)	28 (4%)	0	100	100
1	C	676/745 (91%)	655 (97%)	21 (3%)	0	100	100
1	D	710/745 (95%)	685 (96%)	24 (3%)	1 (0%)	55	45
All	All	2830/2980 (95%)	2731 (96%)	98 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	613	SER

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	587/602 (98%)	574 (98%)	13 (2%)	57	51
1	B	587/602 (98%)	573 (98%)	14 (2%)	54	47
1	C	558/602 (93%)	549 (98%)	9 (2%)	68	65
1	D	577/602 (96%)	566 (98%)	11 (2%)	62	57
All	All	2309/2408 (96%)	2262 (98%)	47 (2%)	60	55

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	426	GLN
1	B	584	VAL
1	D	563	ASN
1	B	546	PHE
1	C	191	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	426	GLN
1	B	648	HIS
1	D	64	ASN
1	B	64	ASN
1	D	105	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

29 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
3	LYS	A	801	4	8,8,9	0.66	0	5,8,10	1.18	1 (20%)
4	PRO	A	802	1,3	6,7,8	1.32	1 (16%)	7,8,10	1.78	1 (14%)
2	GOL	A	803	-	5,5,5	0.54	0	5,5,5	0.61	0
2	GOL	A	804	-	5,5,5	0.42	0	5,5,5	1.10	0
2	GOL	A	805	-	5,5,5	1.12	0	5,5,5	0.77	0
2	GOL	A	806	-	5,5,5	0.35	0	5,5,5	0.45	0
3	LYS	B	801	4	8,8,9	0.73	0	5,8,10	1.41	1 (20%)
4	PRO	B	802	1,3	6,7,8	0.54	0	7,8,10	2.04	1 (14%)
2	GOL	B	803	-	5,5,5	0.30	0	5,5,5	1.25	0
2	GOL	B	804	-	5,5,5	0.41	0	5,5,5	0.52	0
2	GOL	B	805	-	5,5,5	0.29	0	5,5,5	0.88	0
2	GOL	B	806	-	5,5,5	0.67	0	5,5,5	1.37	1 (20%)
2	GOL	B	807	-	5,5,5	1.09	0	5,5,5	2.07	3 (60%)
2	GOL	B	808	-	5,5,5	0.28	0	5,5,5	1.14	1 (20%)
2	GOL	B	809	-	5,5,5	0.16	0	5,5,5	0.50	0
2	GOL	B	810	-	5,5,5	0.32	0	5,5,5	0.41	0
2	GOL	B	811	-	5,5,5	0.46	0	5,5,5	1.75	2 (40%)
2	GOL	B	812	-	5,5,5	0.26	0	5,5,5	0.88	0
3	LYS	C	801	4	8,8,9	1.59	1 (12%)	5,8,10	1.17	0
4	PRO	C	802	3	5,8,8	0.63	0	6,10,10	1.11	0
2	GOL	C	803	-	5,5,5	0.69	0	5,5,5	0.55	0
2	GOL	C	804	-	5,5,5	0.40	0	5,5,5	0.76	0
3	LYS	D	801	4	8,8,9	0.54	0	5,8,10	1.60	1 (20%)
4	PRO	D	802	1,3	6,7,8	0.36	0	7,8,10	2.45	1 (14%)
2	GOL	D	803	-	5,5,5	0.26	0	5,5,5	0.20	0
2	GOL	D	804	-	5,5,5	0.92	0	5,5,5	1.18	1 (20%)
2	GOL	D	805	-	5,5,5	0.45	0	5,5,5	0.73	0
2	GOL	D	806	-	5,5,5	0.39	0	5,5,5	0.42	0
2	GOL	D	807	-	5,5,5	0.33	0	5,5,5	0.54	0

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	LYS	A	801	4	-	0/5/7/9	0/0/0/0
4	PRO	A	802	1,3	-	0/0/9/11	0/1/1/1
2	GOL	A	803	-	-	0/4/4/4	0/0/0/0
2	GOL	A	804	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	805	-	-	0/4/4/4	0/0/0/0
2	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	LYS	B	801	4	-	0/5/7/9	0/0/0/0
4	PRO	B	802	1,3	-	0/0/9/11	0/1/1/1
2	GOL	B	803	-	-	0/4/4/4	0/0/0/0
2	GOL	B	804	-	-	0/4/4/4	0/0/0/0
2	GOL	B	805	-	-	0/4/4/4	0/0/0/0
2	GOL	B	806	-	-	0/4/4/4	0/0/0/0
2	GOL	B	807	-	-	0/4/4/4	0/0/0/0
2	GOL	B	808	-	-	0/4/4/4	0/0/0/0
2	GOL	B	809	-	-	0/4/4/4	0/0/0/0
2	GOL	B	810	-	-	0/4/4/4	0/0/0/0
2	GOL	B	811	-	-	0/4/4/4	0/0/0/0
2	GOL	B	812	-	-	0/4/4/4	0/0/0/0
3	LYS	C	801	4	-	0/5/7/9	0/0/0/0
4	PRO	C	802	3	-	0/0/11/11	0/1/1/1
2	GOL	C	803	-	-	0/4/4/4	0/0/0/0
2	GOL	C	804	-	-	0/4/4/4	0/0/0/0
3	LYS	D	801	4	-	0/5/7/9	0/0/0/0
4	PRO	D	802	1,3	-	0/0/9/11	0/1/1/1
2	GOL	D	803	-	-	0/4/4/4	0/0/0/0
2	GOL	D	804	-	-	0/4/4/4	0/0/0/0
2	GOL	D	805	-	-	0/4/4/4	0/0/0/0
2	GOL	D	806	-	-	0/4/4/4	0/0/0/0
2	GOL	D	807	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	PRO	CA-C	3.08	1.54	1.50
3	C	801	LYS	CA-C	4.13	1.55	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	802	PRO	CB-CA-C	-6.23	104.13	112.70
4	B	802	PRO	CB-CA-C	-5.11	105.67	112.70
4	A	802	PRO	CB-CA-C	-4.31	106.77	112.70
2	B	807	GOL	O3-C3-C2	-3.27	93.59	110.07
3	D	801	LYS	O-C-CA	-3.06	116.57	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	GOL	3	0
2	B	808	GOL	2	0
2	B	810	GOL	1	0
2	B	811	GOL	2	0
2	C	803	GOL	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	724/745 (97%)	-0.30	12 (1%) 70 73	9, 18, 35, 79	0
1	B	724/745 (97%)	-0.19	11 (1%) 74 77	11, 21, 39, 70	0
1	C	687/745 (92%)	-0.17	27 (3%) 40 44	11, 20, 46, 75	0
1	D	714/745 (95%)	-0.29	9 (1%) 77 80	9, 19, 37, 79	0
All	All	2849/2980 (95%)	-0.24	59 (2%) 64 67	9, 20, 40, 79	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	745	PRO	5.8
1	B	152	GLY	5.4
1	D	143	ARG	4.5
1	C	250	VAL	4.4
1	A	143	ARG	4.2

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 carbohydrates 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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	B	810	6/6	0.79	0.27	11.20	32,44,50,53	0
3	LYS	A	801	9/10	0.93	0.21	6.63	16,16,27,28	0
2	GOL	D	803	6/6	0.93	0.15	6.28	23,35,40,47	0
2	GOL	B	808	6/6	0.84	0.20	6.22	37,48,51,52	0
2	GOL	B	804	6/6	0.90	0.13	6.06	30,33,36,37	0
2	GOL	D	804	6/6	0.90	0.20	4.81	26,28,37,44	0
3	LYS	D	801	9/10	0.94	0.22	4.59	14,15,24,27	0
3	LYS	C	801	9/10	0.92	0.16	3.74	18,25,36,38	0
2	GOL	B	811	6/6	0.89	0.15	3.60	23,29,33,38	0
2	GOL	A	806	6/6	0.88	0.21	3.46	38,42,46,52	0
2	GOL	A	804	6/6	0.90	0.14	3.25	32,34,37,41	0
2	GOL	A	803	6/6	0.82	0.17	3.24	27,35,54,54	0
2	GOL	B	807	6/6	0.86	0.19	3.20	25,28,32,36	0
4	PRO	D	802	7/8	0.95	0.17	3.02	13,14,15,16	0
2	GOL	D	806	6/6	0.81	0.25	2.68	32,34,36,44	0
3	LYS	B	801	9/10	0.97	0.16	2.60	15,18,34,39	0
4	PRO	A	802	7/8	0.91	0.15	2.46	14,14,15,16	0
2	GOL	D	805	6/6	0.91	0.17	1.58	43,50,51,54	0
4	PRO	C	802	8/8	0.91	0.11	1.45	19,21,22,23	0
2	GOL	B	803	6/6	0.85	0.15	1.18	39,41,46,47	0
2	GOL	A	805	6/6	0.95	0.10	0.98	19,21,22,22	0
2	GOL	C	803	6/6	0.93	0.10	0.84	21,24,28,30	0
2	GOL	D	807	6/6	0.93	0.11	0.40	29,36,39,45	0
2	GOL	B	812	6/6	0.93	0.11	0.17	32,36,37,38	0
4	PRO	B	802	7/8	0.96	0.10	-0.78	14,15,16,16	0
2	GOL	B	809	6/6	0.87	0.19	-	40,50,54,57	0
2	GOL	C	804	6/6	0.77	0.19	-	38,41,45,49	0
2	GOL	B	805	6/6	0.84	0.22	-	39,47,51,58	0
2	GOL	B	806	6/6	0.74	0.26	-	47,48,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.