Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 01:24 AM JST

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 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:

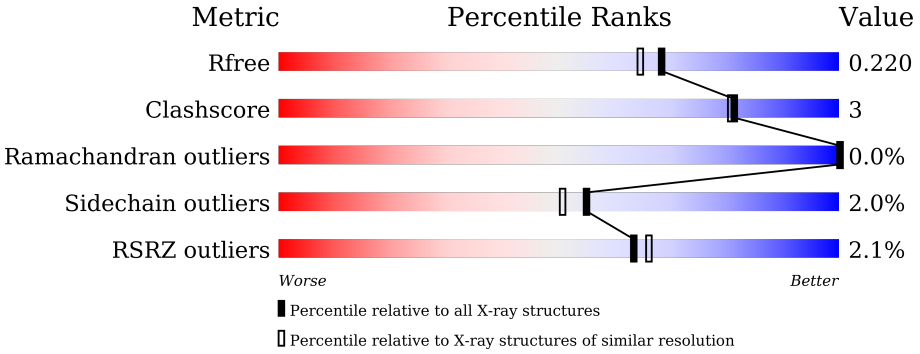
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	745	2% 87% 9% • •
1	B	745	% 89% 7% • •
1	C	745	4% 84% 7% • 8%
1	D	745	% 88% 7% • •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	807	-	X	-	-

2 Entry composition (i)

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.

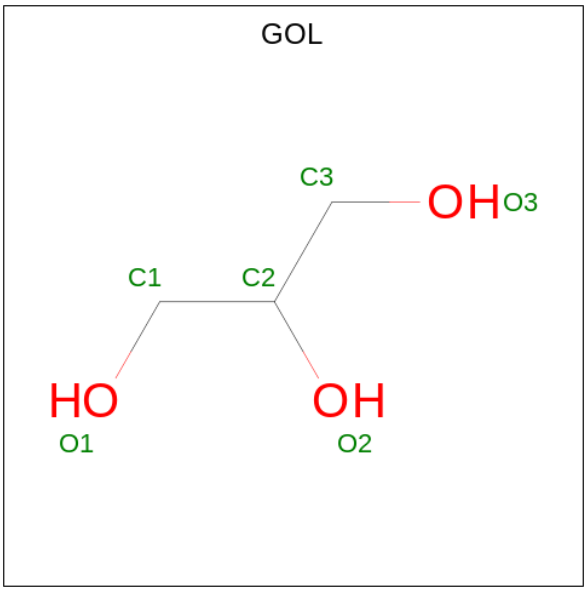
- Molecule 1 is a protein called Dipeptidyl aminopeptidase 4.

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

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: $C_3H_8O_3$).



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

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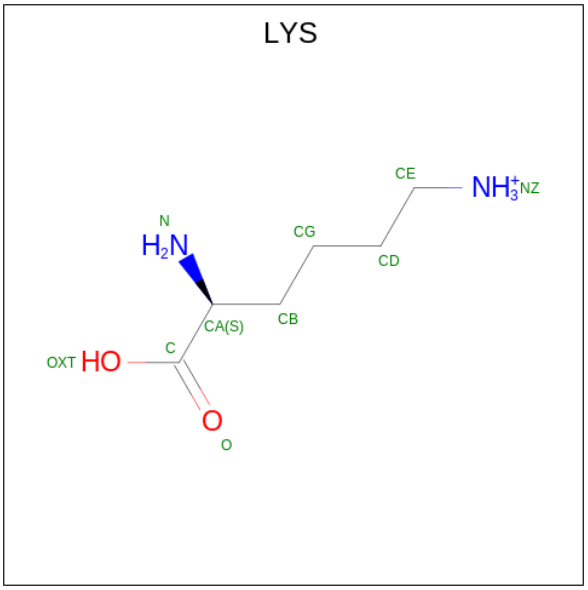
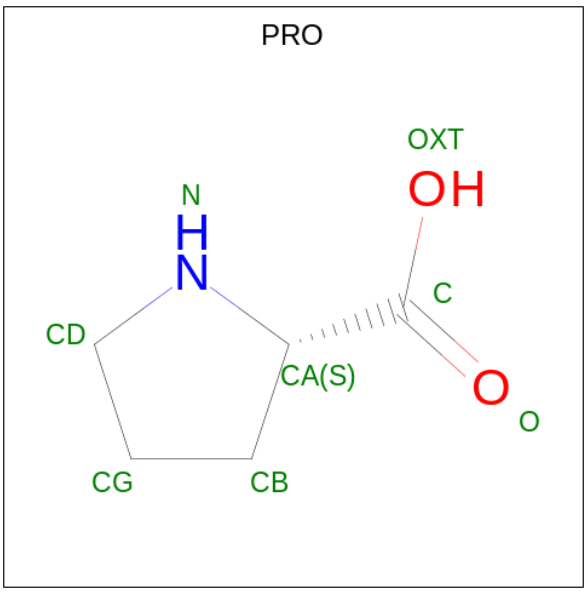
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	C	1	6	3	3		0	0
			Total	C	O			
2	C	1	6	3	3		0	0
			Total	C	O			
2	D	1	6	3	3		0	0
			Total	C	O			
2	D	1	6	3	3		0	0
			Total	C	O			
2	D	1	6	3	3		0	0
			Total	C	O			
2	D	1	6	3	3		0	0
			Total	C	O			
2	D	1	6	3	3		0	0

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



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

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



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

- Molecule 5 is water.

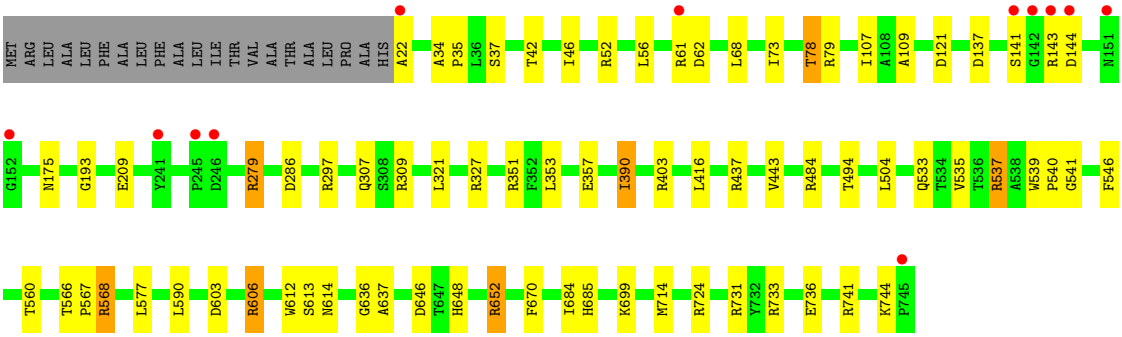
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	817	817	817	0	0
5	B	685	685	685	0	0
5	C	611	611	611	0	0
5	D	764	764	764	0	0

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.

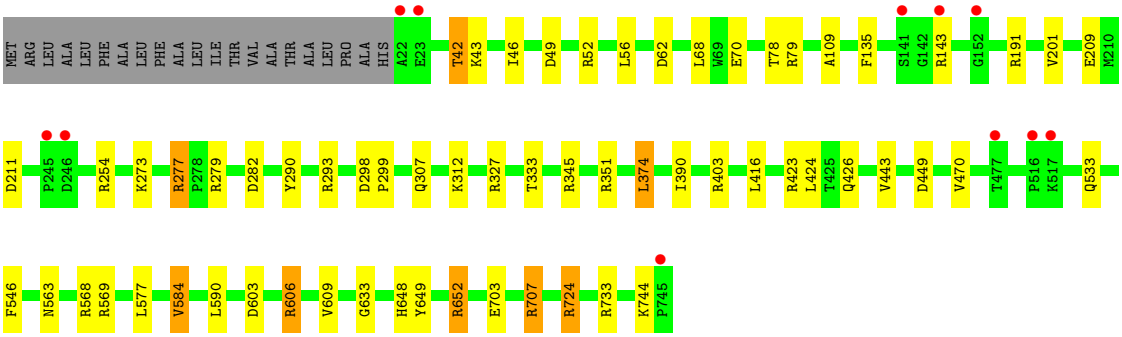
• Molecule 1: Dipeptidyl aminopeptidase 4

Chain A:



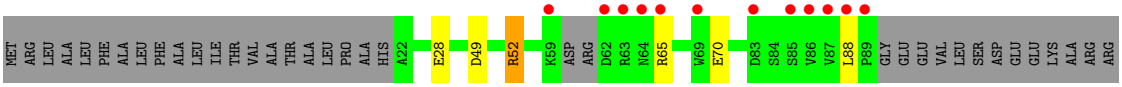
• Molecule 1: Dipeptidyl aminopeptidase 4

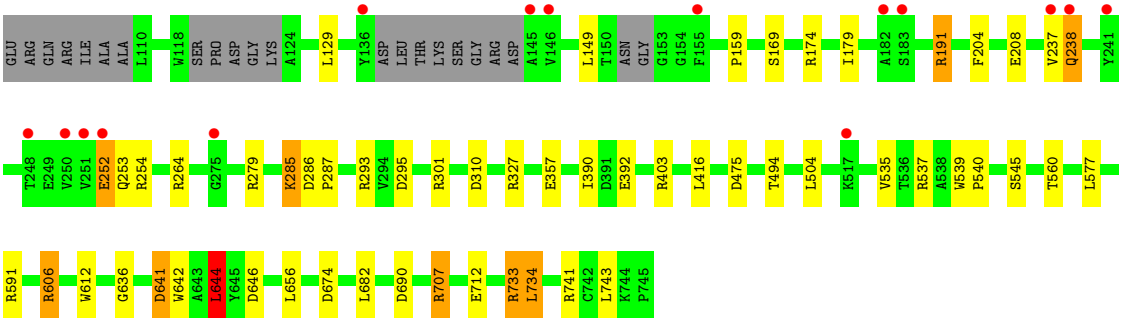
Chain B:



• Molecule 1: Dipeptidyl aminopeptidase 4

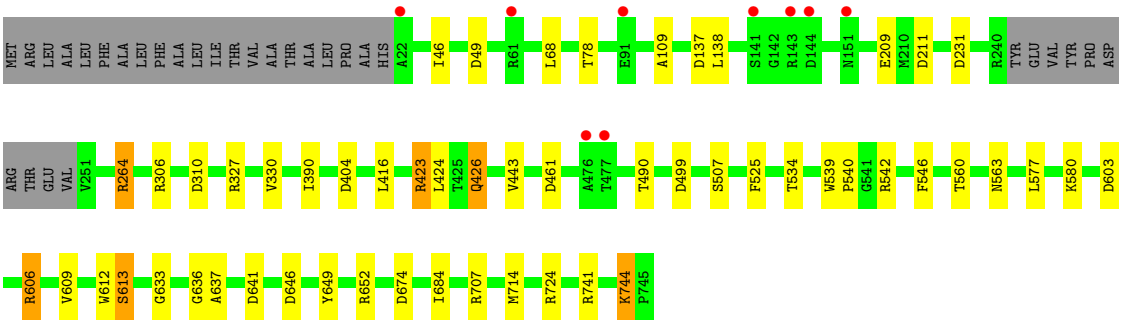
Chain C:





- Molecule 1: Dipeptidyl aminopeptidase 4

Chain D:



4 Data and refinement statistics (i)

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) 94.2 (49.31-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	12223 reflections (4.99%)	wwPDB-VP
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 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: 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%)

All (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
1	A	357	GLU	CD-OE2	5.22	1.31	1.25
1	A	541	GLY	C-O	5.19	1.31	1.23
1	A	606	ARG	CD-NE	-5.18	1.37	1.46
1	C	357	GLU	CD-OE1	5.01	1.31	1.25

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	C	301	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	B	724	ARG	NE-CZ-NH1	-10.01	115.30	120.30
1	A	351	ARG	NE-CZ-NH2	-9.30	115.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	ASP	CB-CG-OD1	8.99	126.39	118.30
1	A	537	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C	310	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	568	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	C	591	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	327	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	590	LEU	CA-CB-CG	-7.42	98.25	115.30
1	D	499	ASP	CB-CG-OD1	7.29	124.86	118.30
1	C	537	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	B	49	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	652	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	724	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	286	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	733	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	568	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	C	606	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	644	LEU	CA-CB-CG	6.94	131.27	115.30
1	B	351	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	591	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	D	264	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	A	484	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	B	606	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	606	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	C	174	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	C	174	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	62	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	403	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	C	641	ASP	CB-CG-OD1	6.53	124.17	118.30
1	D	423	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	D	641	ASP	CB-CG-OD1	6.44	124.10	118.30
1	B	584	VAL	CG1-CB-CG2	6.37	121.08	110.90
1	D	741	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	B	724	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	C	403	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	423	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	590	LEU	CA-CB-CG	-6.12	101.22	115.30
1	B	652	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	49	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	461	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	741	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	C	254	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	327	ARG	NE-CZ-NH2	-6.04	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	569	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	606	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	707	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	52	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	707	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	68	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	403	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	731	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	264	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	D	652	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	309	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	52	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	137	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	68	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	297	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	403	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	52	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	D	49	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	403	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	293	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	65	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	52	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	327	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	327	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	137	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	306	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	327	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	282	ASP	CB-CG-OD1	5.36	123.13	118.30
1	D	330	VAL	CB-CA-C	-5.34	101.25	111.40
1	D	310	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	733	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	327	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	295	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	537	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	542	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	143	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	537	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	254	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	707	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	345	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	404	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	68	LEU	CA-CB-CG	5.15	127.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	733	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	736	GLU	CG-CD-OE2	-5.13	108.05	118.30
1	C	295	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	475	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	121	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	286	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	279	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	724	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	52	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	B	282	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:22:ALA:N	5:A:901:HOH:O	2.06	0.88
1:C:712:GLU:OE2	1:C:741[B]:ARG:NH2	2.11	0.83
1:A:603:ASP:OD2	1:A:606:ARG:HD3	1.80	0.82
1:A:648:HIS:CD2	1:A:652:ARG:HH21	1.98	0.81
1:D:525:PHE:O	1:D:560:THR:HG23	1.83	0.77
1:B:648:HIS:HD2	1:B:652:ARG:HH21	1.34	0.75
1:D:674:ASP:OD1	1:D:707:ARG:NH1	2.20	0.74
1:B:109:ALA:HB2	1:B:724:ARG:HD3	1.70	0.74
1:B:277:ARG:NH1	5:B:902:HOH:O	2.23	0.70
1:B:648:HIS:CD2	1:B:652:ARG:HH21	2.11	0.69
1:B:293:ARG:HD2	2:B:808:GOL:H11	1.73	0.69
1:A:62:ASP:OD1	5:A:902:HOH:O	2.12	0.68
1:A:175:ASN:HD21	1:A:193:GLY:H	1.39	0.68
1:A:307:GLN:NE2	1:A:648:HIS:HE1	1.95	0.64
1:D:109:ALA:HB2	1:D:724:ARG:HD2	1.81	0.63
1:B:293:ARG:HD2	2:B:808:GOL:C1	2.30	0.61
1:A:109:ALA:HB3	2:A:803:GOL:H31	1.83	0.60
1:D:744:LYS:CB	5:D:1357:HOH:O	2.03	0.59
1:A:603:ASP:OD2	1:A:606:ARG:CD	2.50	0.59
1:C:641:ASP:O	1:C:644:LEU:HD12	2.04	0.58
1:A:744:LYS:CG	5:A:1318:HOH:O	2.34	0.57
1:B:603:ASP:OD2	1:B:606:ARG:HD3	2.05	0.57
1:D:603:ASP:OD2	1:D:606:ARG:HD3	2.04	0.57
1:B:70:GLU:OE2	1:B:79:ARG:NH1	2.39	0.56
1:B:201:VAL:HB	2:B:811:GOL:H32	1.86	0.56
1:A:307:GLN:HE22	1:A:648:HIS:HE1	1.52	0.56
1:C:690:ASP:HB3	5:C:1343:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:HB1	1:A:35:PRO:HD2	1.87	0.55
1:A:606:ARG:HD2	5:A:974:HOH:O	2.07	0.55
1:B:211:ASP:HB2	5:B:1341:HOH:O	2.06	0.55
1:C:208:GLU:OE1	5:C:901:HOH:O	2.18	0.55
1:A:670:PHE:CZ	1:A:699:LYS:HG2	2.42	0.54
1:C:149:LEU:HB3	1:C:179:ILE:HD13	1.90	0.54
1:B:42:THR:HG23	1:B:43:LYS:HG3	1.89	0.53
1:B:46:ILE:HD11	1:B:443:VAL:HG23	1.90	0.53
1:C:204:PHE:CE1	1:C:208:GLU:HG3	2.44	0.53
1:A:279:ARG:NH2	1:A:321:LEU:O	2.42	0.53
1:B:744:LYS:HB2	1:C:285:LYS:HD3	1.91	0.52
1:B:298:ASP:HB2	1:B:299:PRO:CD	2.40	0.52
1:B:307:GLN:OE1	1:B:648:HIS:HE1	1.92	0.51
2:B:811:GOL:H11	5:B:1114:HOH:O	2.11	0.51
1:C:612:TRP:CE3	1:C:636:GLY:HA3	2.46	0.51
1:D:231:ASP:HB3	1:D:264:ARG:HB2	1.93	0.51
1:C:238:GLN:HE21	1:C:253:GLN:HE21	1.60	0.49
1:C:88:LEU:HD11	1:C:129:LEU:HD13	1.95	0.49
1:B:42:THR:HG22	1:B:56:LEU:HB2	1.95	0.49
1:C:238:GLN:HE21	1:C:253:GLN:NE2	2.10	0.49
1:D:46:ILE:HD11	1:D:443:VAL:HG23	1.94	0.49
1:A:648:HIS:HD2	1:A:652:ARG:NH2	2.01	0.48
1:C:264:ARG:NH2	1:C:287:PRO:HB3	2.28	0.48
1:C:494:THR:HA	1:C:504:LEU:O	2.14	0.47
1:D:423:ARG:NH2	1:D:426:GLN:NE2	2.62	0.47
1:A:613:SER:HA	1:A:637:ALA:O	2.15	0.47
1:B:390:ILE:HD11	1:B:416:LEU:HD21	1.96	0.47
1:C:535:VAL:HG22	1:C:560:THR:HG23	1.96	0.47
1:C:734:LEU:HD13	5:C:913:HOH:O	2.14	0.46
1:A:107:ILE:HA	2:A:803:GOL:H32	1.97	0.46
1:A:539:TRP:CD2	1:A:540:PRO:HD2	2.50	0.46
1:C:28:GLU:OE2	1:C:733:ARG:NH2	2.49	0.46
1:C:734:LEU:HD22	5:D:1286:HOH:O	2.15	0.46
1:B:733:ARG:HD2	5:B:1187:HOH:O	2.15	0.46
1:C:656:LEU:HB3	5:C:1340:HOH:O	2.16	0.46
1:B:312:LYS:O	1:B:333:THR:HA	2.15	0.46
1:C:674:ASP:OD1	1:C:707:ARG:NE	2.45	0.46
1:A:109:ALA:CB	2:A:803:GOL:H31	2.44	0.45
1:D:534:THR:HB	1:D:560:THR:HG21	1.98	0.45
1:B:374:LEU:HD11	5:B:931:HOH:O	2.16	0.45
1:B:449:ASP:OD2	2:B:810:GOL:O1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:803:GOL:H32	5:C:1389:HOH:O	2.16	0.45
1:C:237:VAL:CG1	1:C:252:GLU:HG3	2.47	0.45
1:D:613:SER:HA	1:D:637:ALA:O	2.17	0.45
1:C:52:ARG:HD3	1:C:70:GLU:OE1	2.17	0.45
1:D:612:TRP:CE3	1:D:636:GLY:HA3	2.52	0.45
1:C:390:ILE:CD1	1:C:416:LEU:HD21	2.46	0.44
1:B:609:VAL:O	1:B:633:GLY:HA2	2.17	0.44
1:C:644:LEU:HD23	5:C:1344:HOH:O	2.17	0.44
1:A:353:LEU:HD11	1:A:390:ILE:HG12	2.00	0.44
1:A:537:ARG:NE	5:A:910:HOH:O	2.42	0.43
1:A:494:THR:HA	1:A:504:LEU:O	2.18	0.43
1:A:61:ARG:HG2	5:A:1245:HOH:O	2.17	0.43
1:D:534:THR:OG1	1:D:560:THR:CG2	2.67	0.43
1:C:286:ASP:HA	1:C:287:PRO:HD2	1.88	0.43
1:A:42:THR:HG22	1:A:56:LEU:HB2	2.01	0.43
1:A:603:ASP:CG	1:A:606:ARG:HD3	2.38	0.42
1:C:539:TRP:CD2	1:C:540:PRO:HD2	2.54	0.42
1:B:209:GLU:CD	1:B:649:TYR:HB2	2.40	0.42
1:A:78:THR:HG21	5:A:1311:HOH:O	2.19	0.42
1:C:682:LEU:HD21	1:C:734:LEU:HD12	2.02	0.42
1:A:209:GLU:OE2	1:A:646:ASP:OD2	2.38	0.42
1:C:191:ARG:NH2	5:C:929:HOH:O	2.52	0.42
1:A:46:ILE:HD11	1:A:443:VAL:HG23	2.02	0.42
1:D:609:VAL:O	1:D:633:GLY:HA2	2.20	0.42
1:C:741[A]:ARG:NH2	5:C:913:HOH:O	2.42	0.41
1:A:307:GLN:HE22	1:A:648:HIS:CE1	2.35	0.41
1:A:535:VAL:HG22	1:A:560:THR:HG23	2.01	0.41
1:A:684:ILE:HA	1:A:714:MET:O	2.19	0.41
1:D:534:THR:OG1	1:D:560:THR:HG22	2.20	0.41
1:A:614:ASN:ND2	5:A:943:HOH:O	2.53	0.41
1:D:209:GLU:CD	1:D:649:TYR:HB2	2.41	0.41
1:A:34:ALA:HB1	1:A:35:PRO:CD	2.50	0.41
1:A:612:TRP:CE3	1:A:636:GLY:HA3	2.56	0.41
1:D:490:THR:CG2	1:D:507:SER:HB2	2.50	0.41
1:B:703:GLU:OE2	1:B:707:ARG:NE	2.47	0.41
1:D:580:LYS:HE2	5:D:1304:HOH:O	2.19	0.41
1:D:539:TRP:CD2	1:D:540:PRO:HD2	2.55	0.41
1:B:290:TYR:HB2	1:B:307:GLN:HB3	2.02	0.41
1:C:159:PRO:HA	1:C:169:SER:O	2.20	0.41
1:D:684:ILE:HA	1:D:714:MET:O	2.20	0.41
1:A:566:THR:HB	1:A:567:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:GLN:OE1	1:B:568:ARG:HD3	2.21	0.40
1:A:533:GLN:OE1	1:A:568:ARG:HD3	2.22	0.40
1:C:606:ARG:HD2	1:C:743:LEU:O	2.22	0.40

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	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%)	51	42
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 (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	587/602 (98%)	574 (98%)	13 (2%)	52	47
1	B	587/602 (98%)	573 (98%)	14 (2%)	49	43
1	C	558/602 (93%)	549 (98%)	9 (2%)	62	60
1	D	577/602 (96%)	566 (98%)	11 (2%)	57	53
All	All	2309/2408 (96%)	2262 (98%)	47 (2%)	55	51

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	78	THR
1	A	79	ARG
1	A	141	SER
1	A	143	ARG
1	A	144	ASP
1	A	279	ARG
1	A	390	ILE
1	A	416	LEU
1	A	437	ARG
1	A	546	PHE
1	A	577	LEU
1	A	685	HIS
1	B	42	THR
1	B	78	THR
1	B	135	PHE
1	B	191	ARG
1	B	273	LYS
1	B	277	ARG
1	B	374	LEU
1	B	424	LEU
1	B	426	GLN
1	B	470	VAL
1	B	546	PHE
1	B	563	ASN
1	B	577	LEU
1	B	584	VAL
1	C	191	ARG
1	C	238	GLN
1	C	252	GLU
1	C	279	ARG
1	C	285	LYS
1	C	577	LEU

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Mol	Chain	Res	Type
1	C	644	LEU
1	C	646	ASP
1	C	734	LEU
1	D	78	THR
1	D	138	LEU
1	D	390	ILE
1	D	416	LEU
1	D	424	LEU
1	D	426	GLN
1	D	546	PHE
1	D	563	ASN
1	D	577	LEU
1	D	646	ASP
1	D	744	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	175	ASN
1	A	238	GLN
1	A	307	GLN
1	A	519	GLN
1	A	614	ASN
1	A	648	HIS
1	B	64	ASN
1	B	426	GLN
1	B	614	ASN
1	B	648	HIS
1	C	238	GLN
1	C	253	GLN
1	C	548	ASN
1	C	614	ASN
1	D	64	ASN
1	D	105	GLN
1	D	426	GLN
1	D	548	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)

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	$\#\|Z\| > 2$
2	GOL	A	805	-	5,5,5	1.13	0	5,5,5	0.78	0
2	GOL	D	806	-	5,5,5	0.41	0	5,5,5	0.40	0
2	GOL	B	803	-	5,5,5	0.28	0	5,5,5	1.29	0
2	GOL	A	806	-	5,5,5	0.36	0	5,5,5	0.47	0
2	GOL	B	806	-	5,5,5	0.69	0	5,5,5	1.41	1 (20%)
2	GOL	C	803	-	5,5,5	0.70	0	5,5,5	0.57	0
2	GOL	B	807	-	5,5,5	0.93	0	5,5,5	2.18	3 (60%)
3	LYS	B	801	4	7,8,9	0.55	0	3,8,10	0.78	0
2	GOL	B	810	-	5,5,5	0.35	0	5,5,5	0.42	0
2	GOL	B	809	-	5,5,5	0.15	0	5,5,5	0.53	0
2	GOL	D	807	-	5,5,5	0.32	0	5,5,5	0.54	0
2	GOL	D	803	-	5,5,5	0.22	0	5,5,5	0.23	0
2	GOL	B	812	-	5,5,5	0.26	0	5,5,5	0.92	0
2	GOL	D	804	-	5,5,5	0.83	0	5,5,5	1.27	1 (20%)
4	PRO	D	802	3,1	5,7,8	0.26	0	7,8,10	2.42	1 (14%)
3	LYS	A	801	4	7,8,9	0.64	0	3,8,10	0.78	0
4	PRO	A	802	3,1	5,7,8	0.45	0	7,8,10	1.78	1 (14%)
4	PRO	B	802	3,1	5,7,8	0.31	0	7,8,10	2.02	1 (14%)
2	GOL	C	804	-	5,5,5	0.40	0	5,5,5	0.79	0
2	GOL	B	805	-	5,5,5	0.32	0	5,5,5	0.93	0
4	PRO	C	802	3	8,8,8	0.88	1 (12%)	10,10,10	1.47	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	LYS	D	801	4	7,8,9	0.56	0	3,8,10	0.89	0
2	GOL	A	804	-	5,5,5	0.46	0	5,5,5	1.14	0
2	GOL	D	805	-	5,5,5	0.45	0	5,5,5	0.77	0
2	GOL	A	803	-	5,5,5	0.54	0	5,5,5	0.65	0
2	GOL	B	811	-	5,5,5	0.47	0	5,5,5	1.81	2 (40%)
2	GOL	B	808	-	5,5,5	0.31	0	5,5,5	1.18	1 (20%)
3	LYS	C	801	4	7,8,9	0.71	0	3,8,10	0.61	0
2	GOL	B	804	-	5,5,5	0.42	0	5,5,5	0.56	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
2	GOL	A	805	-	-	1/4/4/4	-
2	GOL	D	806	-	-	1/4/4/4	-
2	GOL	B	803	-	-	2/4/4/4	-
2	GOL	A	806	-	-	2/4/4/4	-
2	GOL	B	806	-	-	2/4/4/4	-
2	GOL	C	803	-	-	0/4/4/4	-
2	GOL	B	807	-	-	4/4/4/4	-
3	LYS	B	801	4	-	0/6/7/9	-
2	GOL	B	810	-	-	2/4/4/4	-
2	GOL	B	809	-	-	3/4/4/4	-
2	GOL	D	807	-	-	3/4/4/4	-
2	GOL	D	803	-	-	4/4/4/4	-
2	GOL	B	812	-	-	2/4/4/4	-
2	GOL	D	804	-	-	2/4/4/4	-
4	PRO	D	802	3,1	-	0/0/9/11	0/1/1/1
3	LYS	A	801	4	-	0/6/7/9	-
4	PRO	A	802	3,1	-	0/0/9/11	0/1/1/1
4	PRO	B	802	3,1	-	0/0/9/11	0/1/1/1
2	GOL	C	804	-	-	2/4/4/4	-
2	GOL	B	805	-	-	2/4/4/4	-
4	PRO	C	802	3	-	0/4/11/11	0/1/1/1
3	LYS	D	801	4	-	0/6/7/9	-
2	GOL	A	804	-	-	2/4/4/4	-
2	GOL	D	805	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	803	-	-	3/4/4/4	-
2	GOL	B	811	-	-	1/4/4/4	-
2	GOL	B	808	-	-	0/4/4/4	-
3	LYS	C	801	4	-	0/6/7/9	-
2	GOL	B	804	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	802	PRO	OXT-C	-2.01	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	-3.46	93.59	110.20
4	C	802	PRO	OXT-C-O	-3.15	116.93	124.09
2	B	811	GOL	C3-C2-C1	-2.71	101.16	111.70
2	D	804	GOL	O2-C2-C3	-2.52	98.03	109.12
2	B	808	GOL	O1-C1-C2	2.51	122.23	110.20
2	B	806	GOL	O3-C3-C2	2.41	121.74	110.20
2	B	807	GOL	O2-C2-C1	2.19	118.78	109.12
2	B	807	GOL	C3-C2-C1	-2.18	103.22	111.70
2	B	811	GOL	O2-C2-C1	2.17	118.68	109.12

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	806	GOL	O1-C1-C2-C3
2	B	803	GOL	C1-C2-C3-O3
2	B	803	GOL	O2-C2-C3-O3
2	B	804	GOL	O1-C1-C2-C3
2	B	807	GOL	O1-C1-C2-C3
2	B	809	GOL	O1-C1-C2-O2
2	B	809	GOL	O1-C1-C2-C3
2	B	812	GOL	C1-C2-C3-O3
2	C	804	GOL	O1-C1-C2-C3
2	D	804	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	D	807	GOL	C1-C2-C3-O3
2	B	805	GOL	O2-C2-C3-O3
2	B	806	GOL	O2-C2-C3-O3
2	A	803	GOL	O1-C1-C2-C3
2	B	805	GOL	C1-C2-C3-O3
2	B	806	GOL	C1-C2-C3-O3
2	B	807	GOL	C1-C2-C3-O3
2	B	810	GOL	O1-C1-C2-C3
2	D	803	GOL	O1-C1-C2-C3
2	D	803	GOL	C1-C2-C3-O3
2	D	805	GOL	O1-C1-C2-C3
2	A	806	GOL	O1-C1-C2-O2
2	B	804	GOL	O1-C1-C2-O2
2	B	807	GOL	O1-C1-C2-O2
2	B	807	GOL	O2-C2-C3-O3
2	B	810	GOL	O1-C1-C2-O2
2	D	803	GOL	O2-C2-C3-O3
2	D	804	GOL	O2-C2-C3-O3
2	D	807	GOL	O2-C2-C3-O3
2	B	812	GOL	O2-C2-C3-O3
2	C	804	GOL	O1-C1-C2-O2
2	D	805	GOL	O1-C1-C2-O2
2	A	804	GOL	O2-C2-C3-O3
2	A	803	GOL	O1-C1-C2-O2
2	A	803	GOL	C1-C2-C3-O3
2	A	804	GOL	C1-C2-C3-O3
2	A	805	GOL	O1-C1-C2-C3
2	B	809	GOL	C1-C2-C3-O3
2	B	811	GOL	C1-C2-C3-O3
2	D	803	GOL	O1-C1-C2-O2
2	D	807	GOL	O1-C1-C2-O2
2	D	806	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	803	GOL	1	0
2	B	810	GOL	1	0
2	A	803	GOL	3	0
2	B	811	GOL	2	0
2	B	808	GOL	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	724/745 (97%)	-0.30	12 (1%)	70	72	9, 18, 35, 79	0
1	B	724/745 (97%)	-0.19	11 (1%)	73	76	11, 21, 39, 70	0
1	C	687/745 (92%)	-0.16	27 (3%)	39	42	11, 20, 46, 75	0
1	D	714/745 (95%)	-0.29	9 (1%)	77	79	9, 19, 37, 79	0
All	All	2849/2980 (95%)	-0.24	59 (2%)	63	66	9, 20, 40, 79	0

All (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	4.6
1	C	250	VAL	4.4
1	A	143	ARG	4.3
1	A	141	SER	4.2
1	A	151	ASN	4.1
1	C	145	ALA	4.0
1	B	141	SER	3.8
1	C	62	ASP	3.8
1	C	241	TYR	3.7
1	C	63	ARG	3.7
1	C	85	SER	3.7
1	A	745	PRO	3.7
1	C	146	VAL	3.5
1	C	136	TYR	3.4
1	C	182	ALA	3.3
1	C	88	LEU	3.3
1	D	141	SER	3.2
1	A	144	ASP	3.2
1	A	241	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	151	ASN	3.1
1	B	143	ARG	3.1
1	C	86	VAL	3.1
1	A	61	ARG	2.9
1	A	245	PRO	2.9
1	B	516	PRO	2.8
1	D	22	ALA	2.7
1	D	477	THR	2.7
1	C	89	PRO	2.7
1	C	59	LYS	2.6
1	A	152	GLY	2.6
1	C	83	ASP	2.5
1	C	237	VAL	2.5
1	D	144	ASP	2.5
1	B	22	ALA	2.5
1	C	155	PHE	2.5
1	C	64	ASN	2.4
1	B	477	THR	2.4
1	A	142	GLY	2.4
1	C	275	GLY	2.4
1	B	23	GLU	2.3
1	C	252	GLU	2.3
1	C	183	SER	2.3
1	B	245	PRO	2.3
1	C	517	LYS	2.3
1	B	517	LYS	2.2
1	C	248	THR	2.2
1	C	251	VAL	2.2
1	B	246	ASP	2.2
1	C	87	VAL	2.2
1	C	238	GLN	2.1
1	A	22	ALA	2.1
1	C	65	ARG	2.1
1	D	91	GLU	2.1
1	D	61	ARG	2.0
1	C	69	TRP	2.0
1	D	476	ALA	2.0
1	A	246	ASP	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
2	GOL	B	806	6/6	0.71	0.26	47,48,56,59	0
2	GOL	C	804	6/6	0.79	0.19	38,41,45,49	0
2	GOL	B	810	6/6	0.80	0.27	32,44,50,53	0
2	GOL	D	806	6/6	0.82	0.24	32,34,36,44	0
2	GOL	A	803	6/6	0.84	0.17	27,35,54,54	0
2	GOL	B	805	6/6	0.84	0.23	39,47,51,58	0
2	GOL	B	808	6/6	0.85	0.20	37,48,51,52	0
2	GOL	B	803	6/6	0.85	0.15	39,41,46,47	0
2	GOL	B	807	6/6	0.86	0.19	25,28,32,36	0
2	GOL	B	809	6/6	0.88	0.19	40,50,54,57	0
2	GOL	A	806	6/6	0.88	0.20	38,42,46,52	0
2	GOL	A	804	6/6	0.89	0.14	32,34,37,41	0
2	GOL	B	811	6/6	0.89	0.15	23,29,33,38	0
2	GOL	B	804	6/6	0.90	0.13	30,33,36,37	0
2	GOL	D	805	6/6	0.91	0.17	43,50,51,54	0
2	GOL	D	804	6/6	0.91	0.19	26,28,37,44	0
3	LYS	C	801	9/10	0.91	0.16	18,25,36,38	0
4	PRO	A	802	7/8	0.91	0.15	14,14,15,16	0
4	PRO	C	802	8/8	0.92	0.11	19,21,22,23	0
2	GOL	D	803	6/6	0.93	0.15	23,35,40,47	0
2	GOL	D	807	6/6	0.93	0.11	29,36,39,45	0
3	LYS	A	801	9/10	0.93	0.20	16,16,27,28	0
2	GOL	B	812	6/6	0.94	0.11	32,36,37,38	0
2	GOL	C	803	6/6	0.94	0.11	21,24,28,30	0
2	GOL	A	805	6/6	0.95	0.09	19,21,22,22	0
3	LYS	D	801	9/10	0.95	0.22	14,15,24,27	0
4	PRO	D	802	7/8	0.95	0.16	13,14,15,16	0
4	PRO	B	802	7/8	0.96	0.09	14,15,16,16	0
3	LYS	B	801	9/10	0.97	0.16	15,18,34,39	0

6.5 Other polymers (i)

There are no such residues in this entry.