



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:13 AM UTC

PDB ID : 1JSL / pdb_00001jsl
Title : Crystal structure of Erwinia chrysanthemi L-asparaginase complexed with 6-HYDROXY-D-NORLEUCINE
Authors : Aghaiypour, K.; Wlodawer, A.; Lubkowski, J.
Deposited on : 2001-08-17
Resolution : 1.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

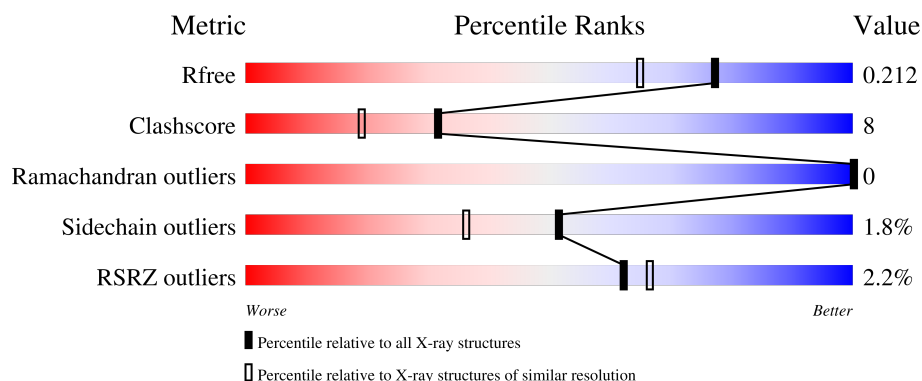
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 $\leq 5\%$. 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	327	 2% 80% 17% ..
1	B	327	 3% 80% 18% ..
1	C	327	 2% 86% 12% ..
1	D	327	 2% 85% 13% ..

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
3	1PE	A	2501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11215 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.

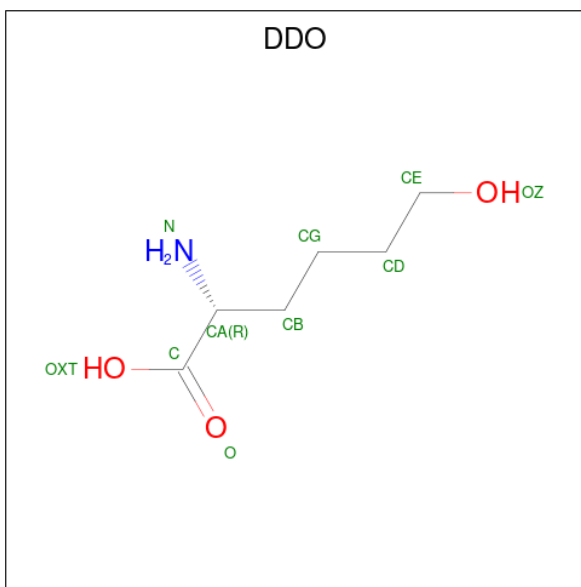
- Molecule 1 is a protein called L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	9	0
			2510	1578	440	482	10			
1	B	324	Total	C	N	O	S	0	8	0
			2503	1570	438	486	9			
1	C	324	Total	C	N	O	S	0	6	0
			2492	1564	440	479	9			
1	D	324	Total	C	N	O	S	0	4	0
			2472	1551	435	477	9			

There are 16 discrepancies between the modelled and reference sequences:

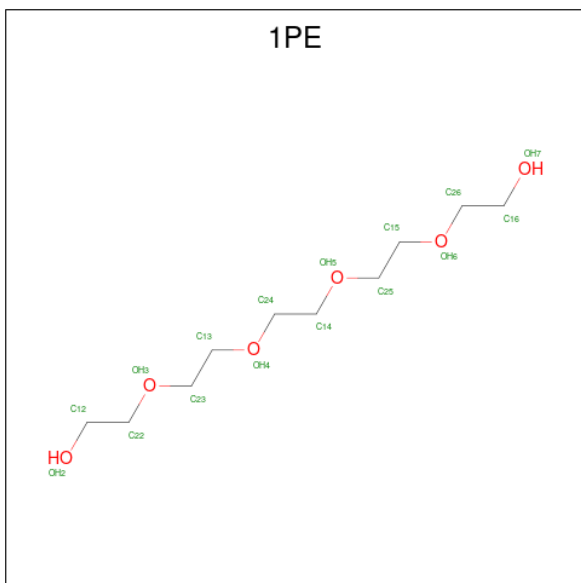
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	ILE	LEU	variant	UNP P06608
A	178	ARG	LYS	variant	UNP P06608
A	267	LEU	MET	variant	UNP P06608
A	274	MET	ILE	variant	UNP P06608
B	156	ILE	LEU	variant	UNP P06608
B	178	ARG	LYS	variant	UNP P06608
B	267	LEU	MET	variant	UNP P06608
B	274	MET	ILE	variant	UNP P06608
C	156	ILE	LEU	variant	UNP P06608
C	178	ARG	LYS	variant	UNP P06608
C	267	LEU	MET	variant	UNP P06608
C	274	MET	ILE	variant	UNP P06608
D	156	ILE	LEU	variant	UNP P06608
D	178	ARG	LYS	variant	UNP P06608
D	267	LEU	MET	variant	UNP P06608
D	274	MET	ILE	variant	UNP P06608

- Molecule 2 is 6-HYDROXY-D-NORLEUCINE (CCD ID: DDO) (formula: $C_6H_{13}NO_3$).



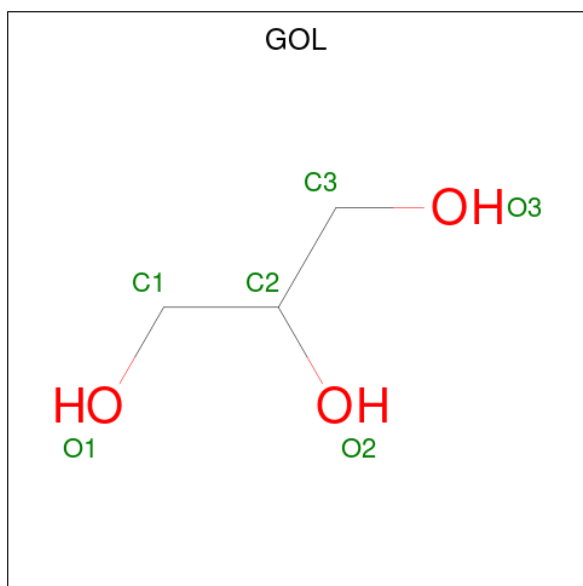
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	B	1	Total	C	N	O	0	0
			10	6	1	3		
2	C	1	Total	C	N	O	0	0
			10	6	1	3		
2	D	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

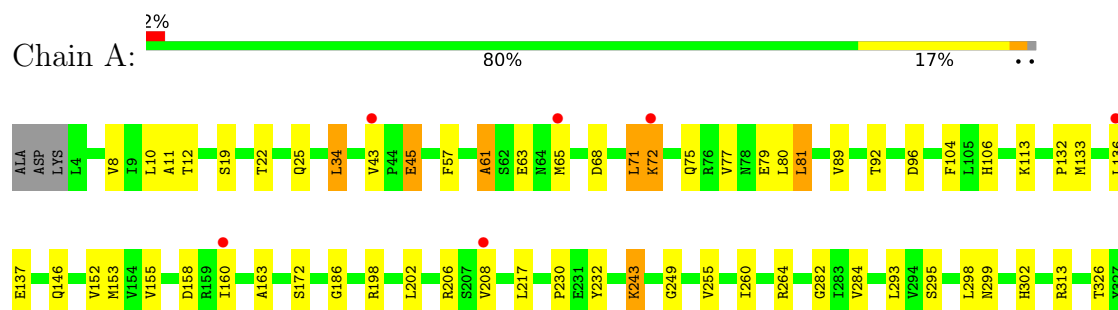
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	297	Total	O	0	1
			299	299		
5	B	273	Total	O	0	0
			273	273		
5	C	296	Total	O	0	0
			296	296		
5	D	293	Total	O	0	2
			296	296		

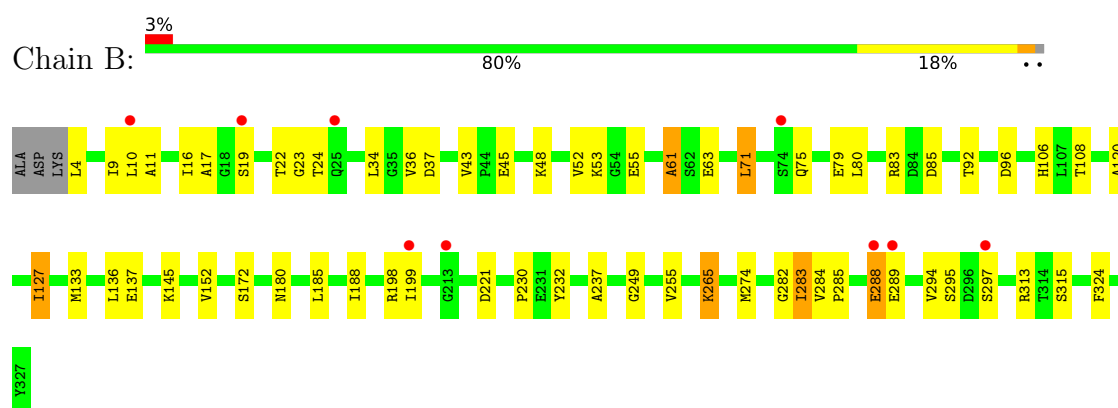
3 Residue-property plots

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.

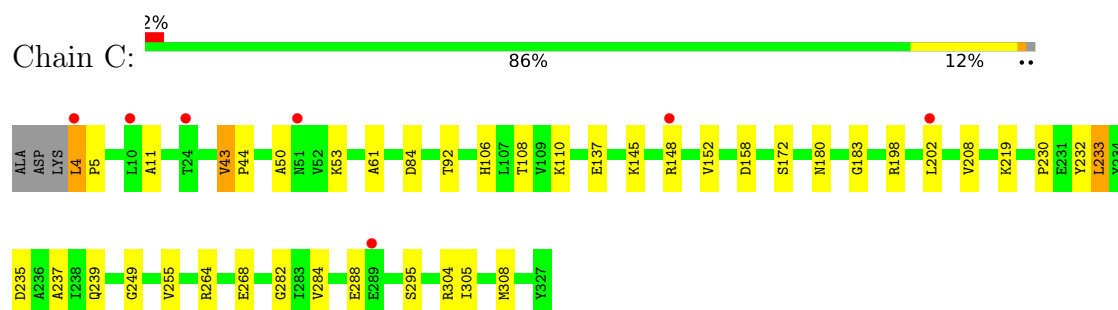
• Molecule 1: L-asparaginase



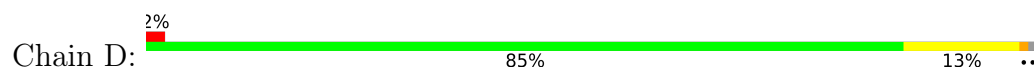
• Molecule 1: L-asparaginase

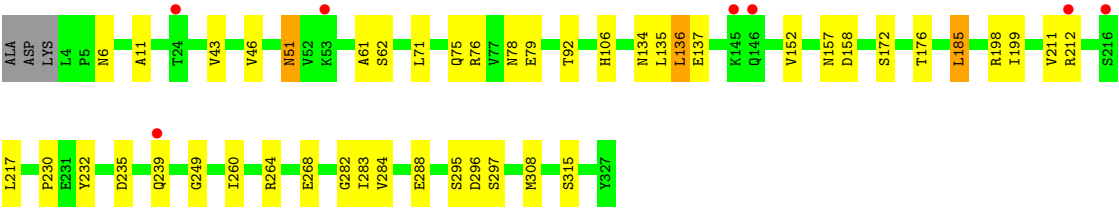


• Molecule 1: L-asparaginase



• Molecule 1: L-asparaginase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.15Å 90.39Å 127.37Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 87.0 (20.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.212 0.186 , 0.212	Depositor DCC
R_{free} test set	1465 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: 1PE, DDO, 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	0.38	0/2546	0.93	10/3454 (0.3%)
1	B	0.38	0/2539	0.94	12/3443 (0.3%)
1	C	0.38	0/2528	0.95	12/3429 (0.3%)
1	D	0.39	0/2508	0.94	10/3400 (0.3%)
All	All	0.38	0/10121	0.94	44/13726 (0.3%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	284	VAL	N-CA-C	-11.39	96.28	107.55
1	B	284	VAL	N-CA-C	-10.76	96.90	107.55
1	A	284	VAL	N-CA-C	-10.18	97.48	107.55
1	C	284	VAL	N-CA-C	-9.01	98.63	107.55
1	A	249	GLY	N-CA-C	7.94	122.71	112.54
1	C	249	GLY	N-CA-C	7.50	123.99	112.51
1	C	282	GLY	N-CA-C	7.22	122.28	112.17
1	A	282	GLY	N-CA-C	7.21	122.27	112.17
1	D	282	GLY	N-CA-C	6.83	121.72	112.17
1	D	249	GLY	N-CA-C	6.74	122.81	112.51
1	C	43	VAL	CA-C-N	6.59	127.12	119.47
1	C	43	VAL	C-N-CA	6.59	127.12	119.47
1	B	249	GLY	N-CA-C	6.30	123.00	112.85
1	B	172	SER	N-CA-C	6.20	122.99	113.19
1	A	61	ALA	N-CA-C	-6.01	100.70	110.20
1	A	172	SER	N-CA-C	6.00	122.67	113.19
1	C	255	VAL	N-CA-C	5.81	116.48	108.12
1	B	282	GLY	N-CA-C	5.79	122.67	112.83
1	B	96	ASP	N-CA-C	5.78	118.04	111.11
1	B	295	SER	N-CA-C	5.72	119.89	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	SER	N-CA-C	5.68	122.89	114.09
1	D	61	ALA	N-CA-C	-5.67	101.25	110.20
1	D	51	ASN	N-CA-C	-5.66	99.31	108.41
1	A	243	LYS	N-CA-C	-5.62	106.59	113.50
1	C	61	ALA	N-CA-C	-5.62	101.32	110.20
1	B	283	ILE	N-CA-C	5.60	116.36	108.36
1	C	295	SER	N-CA-C	5.59	119.81	113.15
1	B	180	ASN	N-CA-C	5.43	117.62	111.11
1	A	198	ARG	N-CA-C	-5.42	99.58	108.41
1	D	172	SER	N-CA-C	5.40	122.45	114.09
1	D	198	ARG	N-CA-C	-5.40	99.64	108.76
1	A	96	ASP	N-CA-C	5.37	117.55	111.11
1	A	295	SER	N-CA-C	5.35	119.44	113.02
1	C	198	ARG	N-CA-C	-5.35	100.18	108.90
1	A	255	VAL	N-CA-C	5.26	115.48	108.11
1	C	180	ASN	N-CA-C	5.23	117.38	111.11
1	B	198	ARG	N-CA-C	-5.20	99.98	108.76
1	B	315	SER	N-CA-C	-5.15	105.88	113.61
1	B	108	THR	N-CA-C	5.13	120.39	113.72
1	D	176	THR	N-CA-C	5.11	116.85	111.28
1	C	108	THR	N-CA-C	5.08	120.33	113.72
1	D	296	ASP	CB-CA-C	-5.08	110.74	116.63
1	D	295	SER	N-CA-C	5.07	119.10	113.02
1	B	61	ALA	N-CA-C	-5.02	101.77	109.76

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	2510	0	2558	62	0
1	B	2503	0	2535	47	0
1	C	2492	0	2534	28	0
1	D	2472	0	2513	30	0
2	A	10	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	10	1	0
2	C	10	0	10	0	0
2	D	10	0	10	2	0
3	A	16	0	22	7	0
4	C	12	0	14	1	0
4	D	6	0	7	1	0
5	A	299	0	0	8	0
5	B	273	0	0	6	0
5	C	296	0	0	4	0
5	D	296	0	0	4	0
All	All	11215	0	10223	164	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 8.

All (164) 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)
2:A:2401:DDO:HE1	5:A:2508[C]:HOH:O	1.30	1.27
1:A:153:MET:HB3	1:A:160[B]:ILE:HD11	1.17	1.15
1:A:43[B]:VAL:HB	1:A:136[B]:LEU:HD11	1.49	0.94
1:A:243:LYS:HZ3	3:A:2501:1PE:H131	1.33	0.93
1:A:153:MET:CB	1:A:160[B]:ILE:HD11	2.02	0.90
1:A:153:MET:HB3	1:A:160[B]:ILE:CD1	2.04	0.88
1:A:133:MET:HA	1:B:127:ILE:HD11	1.60	0.84
1:D:260:ILE:O	1:D:264:ARG:HG2	1.79	0.82
1:A:243:LYS:HZ2	3:A:2501:1PE:H162	1.46	0.81
1:A:243:LYS:NZ	3:A:2501:1PE:H162	2.01	0.75
1:B:185:LEU:HD21	1:B:199[A]:ILE:HG23	1.69	0.75
1:A:136[B]:LEU:HD22	1:B:127:ILE:HD13	1.70	0.73
1:A:160[B]:ILE:HG22	1:A:186:GLY:O	1.89	0.73
1:A:160[B]:ILE:HG22	1:A:186:GLY:C	2.14	0.73
1:A:155:VAL:HG22	1:A:160[B]:ILE:HD13	1.72	0.71
1:C:232:TYR:CE2	1:C:233:LEU:HD13	2.28	0.69
1:A:264:ARG:HH21	1:A:264:ARG:HG3	1.58	0.69
1:A:155:VAL:CG2	1:A:160[B]:ILE:HD13	2.22	0.69
1:A:243:LYS:NZ	3:A:2501:1PE:H131	2.07	0.69
1:A:43[B]:VAL:CB	1:A:136[B]:LEU:HD11	2.26	0.64
1:D:212:ARG:HD2	5:D:2765:HOH:O	1.98	0.64
1:A:8[A]:VAL:CG2	1:A:89:VAL:HG22	2.28	0.64
1:B:145:LYS:HD3	1:B:145:LYS:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PRO:O	1:A:136[B]:LEU:HD13	1.98	0.63
1:B:53:LYS:HE3	5:B:2589:HOH:O	1.99	0.63
1:B:19:SER:OG	1:B:34[A]:LEU:HD21	1.98	0.63
1:B:288:GLU:OE2	1:B:289[B]:GLU:HG2	2.01	0.61
1:A:10:LEU:HD22	1:A:57:PHE:HB2	1.83	0.61
1:A:243:LYS:HZ3	3:A:2501:1PE:C13	2.11	0.60
1:B:45:GLU:O	1:B:48:LYS:HG3	2.03	0.59
1:C:305:ILE:HA	1:C:308:MET:HE2	1.85	0.59
1:A:163:ALA:O	1:A:302:HIS:HE1	1.84	0.58
1:C:145:LYS:HD3	1:C:148:ARG:NH2	2.18	0.58
1:A:75:GLN:O	1:A:79:GLU:HG3	2.04	0.57
1:A:208[A]:VAL:HG12	1:A:313:ARG:CZ	2.35	0.56
1:A:11:ALA:HA	1:A:92:THR:OG1	2.05	0.56
1:B:133:MET:HB3	5:B:2612:HOH:O	2.04	0.56
1:A:230:PRO:HB2	1:A:232:TYR:CD1	2.41	0.56
1:B:288:GLU:HG3	5:B:2526:HOH:O	2.05	0.56
1:B:265:LYS:N	1:B:265:LYS:HE3	2.20	0.56
1:A:22:THR:HG23	1:A:25:GLN:H	1.71	0.55
1:C:4[B]:LEU:HG	1:C:50:ALA:HA	1.88	0.55
1:D:11:ALA:HA	1:D:92:THR:OG1	2.06	0.55
1:B:137:GLU:HB3	1:B:188:ILE:HD13	1.89	0.55
1:C:230:PRO:HB2	1:C:232:TYR:CD1	2.42	0.55
1:C:230:PRO:HG2	1:C:233:LEU:HD22	1.89	0.55
1:A:298:LEU:HD12	1:A:302:HIS:HB3	1.88	0.55
1:B:71:LEU:O	1:B:75:GLN:HG3	2.07	0.55
1:B:288:GLU:OE2	1:B:289[A]:GLU:HG3	2.07	0.55
1:C:219:LYS:HD3	5:C:2776:HOH:O	2.06	0.54
1:A:71:LEU:O	1:A:75:GLN:HG3	2.07	0.54
1:D:78:ASN:HB3	1:D:212:ARG:HH11	1.72	0.54
1:A:136[B]:LEU:HD22	1:B:127:ILE:CD1	2.37	0.54
1:D:76:ARG:NH2	1:D:79:GLU:OE2	2.41	0.54
1:B:45:GLU:HB3	1:B:48:LYS:HE3	1.90	0.54
1:A:264:ARG:HG3	1:A:264:ARG:NH2	2.21	0.54
1:C:235:ASP:O	1:C:239:GLN:HG3	2.07	0.53
1:B:22:THR:HG22	1:B:23:GLY:N	2.23	0.53
1:B:288:GLU:HA	5:B:2544:HOH:O	2.08	0.53
1:A:8[A]:VAL:HG22	1:A:89:VAL:HG22	1.91	0.52
1:D:6:ASN:HD22	1:D:51:ASN:HB2	1.74	0.52
1:A:160[B]:ILE:O	1:A:160[B]:ILE:HG23	2.10	0.52
1:A:133:MET:CA	1:B:127:ILE:HD11	2.37	0.51
1:A:264:ARG:HD3	5:A:2715:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ARG:O	1:D:268:GLU:HG3	2.10	0.51
2:D:2404:DDO:HE1	5:D:2613[B]:HOH:O	2.09	0.51
1:D:288:GLU:HG2	5:D:2686:HOH:O	2.10	0.51
1:B:43:VAL:HG13	1:B:43:VAL:O	2.10	0.51
1:A:43[A]:VAL:HG13	1:A:43[A]:VAL:O	2.11	0.51
1:C:137:GLU:OE1	1:C:158:ASP:OD1	2.28	0.51
1:B:283:ILE:HD13	1:B:297[B]:SER:OG	2.09	0.51
1:B:313:ARG:HH21	1:B:313:ARG:HG2	1.76	0.51
1:C:11:ALA:HA	1:C:92:THR:OG1	2.11	0.51
1:A:22:THR:HG22	5:A:2683:HOH:O	2.10	0.50
1:A:299:ASN:OD1	1:A:302:HIS:HD2	1.93	0.50
1:B:288:GLU:H	1:B:288:GLU:CD	2.17	0.50
1:C:202[A]:LEU:HD21	5:C:2842:HOH:O	2.09	0.50
1:A:326[A]:THR:HG23	5:A:2539:HOH:O	2.10	0.50
1:C:304:ARG:O	1:C:308:MET:HG3	2.12	0.50
2:A:2401:DDO:CE	5:A:2508[C]:HOH:O	2.15	0.49
1:B:10[A]:LEU:HD23	1:B:55:GLU:HB3	1.94	0.49
1:D:185:LEU:HD11	1:D:199:ILE:HG23	1.95	0.49
1:D:235:ASP:O	1:D:239:GLN:HG2	2.12	0.49
1:A:260:ILE:O	1:A:264:ARG:HG2	2.13	0.49
1:A:133:MET:HE2	1:B:127:ILE:HG12	1.93	0.49
1:B:34[A]:LEU:N	1:B:34[A]:LEU:HD22	2.28	0.49
3:A:2501:1PE:H152	5:A:2628:HOH:O	2.13	0.48
5:B:2545:HOH:O	1:C:183:GLY:HA2	2.12	0.48
1:D:283[B]:ILE:HD13	1:D:297:SER:HB3	1.95	0.48
1:B:45:GLU:O	1:B:48:LYS:HE3	2.14	0.48
1:D:43:VAL:O	1:D:43:VAL:HG13	2.14	0.48
1:D:71:LEU:O	1:D:75:GLN:HG3	2.13	0.48
1:C:264:ARG:O	1:C:268:GLU:HG3	2.14	0.48
1:D:43:VAL:CG2	1:D:136:LEU:HG	2.43	0.48
1:B:22:THR:HG22	1:B:24:THR:H	1.78	0.47
1:D:230:PRO:HB2	1:D:232:TYR:CD1	2.48	0.47
1:D:134:ASN:ND2	1:D:157:ASN:H	2.13	0.47
1:A:81:LEU:HG	1:A:113:LYS:HB2	1.95	0.47
1:B:11:ALA:HA	1:B:92:THR:OG1	2.15	0.47
2:B:2402:DDO:OZ	2:B:2402:DDO:HB2	2.14	0.47
1:A:146:GLN:NE2	1:A:146:GLN:HA	2.29	0.47
1:D:137:GLU:OE1	1:D:158:ASP:OD1	2.33	0.47
1:C:4[A]:LEU:N	1:C:4[A]:LEU:HD23	2.31	0.46
1:A:45:GLU:CD	5:A:2556:HOH:O	2.58	0.46
1:A:68:ASP:O	1:A:72[A]:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8[A]:VAL:HG21	1:A:80:LEU:HD13	1.98	0.46
1:A:61:ALA:HB1	1:A:63:GLU:OE1	2.16	0.46
1:A:243:LYS:HZ1	3:A:2501:1PE:H142	1.79	0.46
1:A:104:PHE:CE1	1:A:217:LEU:HD11	2.51	0.46
1:C:110:LYS:NZ	5:C:2744:HOH:O	2.47	0.46
1:D:315:SER:H	4:D:2602:GOL:H32	1.81	0.46
1:A:232:TYR:OH	1:C:237:ALA:HA	2.17	0.45
1:D:185:LEU:HD11	1:D:199:ILE:CG2	2.46	0.45
1:C:43:VAL:HG13	1:C:43:VAL:O	2.16	0.45
1:D:106:HIS:HA	1:D:152:VAL:HG23	1.99	0.45
1:A:146:GLN:HA	1:A:146:GLN:HE21	1.81	0.45
1:B:221:ASP:OD1	1:D:232:TYR:OH	2.27	0.45
1:B:237:ALA:HA	1:D:232:TYR:OH	2.17	0.45
1:B:230:PRO:HB2	1:B:232:TYR:CD1	2.52	0.45
1:A:19:SER:HB3	1:A:34:LEU:HD11	2.00	0.44
1:B:288:GLU:CD	1:B:288:GLU:N	2.75	0.44
1:C:208:VAL:O	1:C:208:VAL:HG22	2.16	0.44
1:A:160[B]:ILE:HG23	1:A:186:GLY:N	2.32	0.44
1:B:83:ARG:HB3	1:B:85:ASP:OD1	2.18	0.44
1:C:233:LEU:HD12	1:C:233:LEU:HA	1.87	0.44
1:A:77:VAL:HG12	1:A:81:LEU:HD22	1.99	0.43
1:D:43:VAL:HG11	1:D:135:LEU:HD23	1.99	0.43
1:A:12:THR:HB	1:A:65[A]:MET:CE	2.49	0.43
1:B:145:LYS:H	1:B:145:LYS:CD	2.30	0.43
1:B:61:ALA:HB1	1:B:63:GLU:OE1	2.17	0.43
1:D:211:VAL:HG22	5:D:2788:HOH:O	2.18	0.43
1:A:22:THR:HG23	1:A:25:GLN:N	2.33	0.43
1:D:217:LEU:HB2	1:D:308:MET:HE2	2.00	0.43
1:C:84:ASP:HB2	4:C:2603:GOL:H31	2.01	0.43
1:A:106:HIS:HA	1:A:152:VAL:HG23	2.01	0.42
1:B:145:LYS:HD3	1:B:145:LYS:N	2.32	0.42
1:D:62:SER:OG	2:D:2404:DDO:O	2.21	0.42
1:A:34:LEU:CD1	1:A:34:LEU:N	2.83	0.42
1:A:137:GLU:OE1	1:A:158:ASP:OD1	2.38	0.42
1:B:22:THR:HG23	5:B:2619:HOH:O	2.20	0.42
1:C:5:PRO:HG2	1:C:50:ALA:HB2	2.01	0.42
1:B:36:VAL:HG13	1:B:37:ASP:N	2.34	0.42
1:B:285:PRO:O	1:B:294:VAL:HG11	2.19	0.42
1:C:43:VAL:N	1:C:44:PRO:HD3	2.35	0.42
1:C:264:ARG:HA	1:C:264:ARG:HD3	1.91	0.42
1:C:106:HIS:HA	1:C:152:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:OD1	1:A:302:HIS:CD2	2.72	0.41
1:C:264:ARG:HH21	1:C:264:ARG:HG3	1.86	0.41
1:B:17:ALA:C	1:B:34[A]:LEU:HD23	2.45	0.41
1:D:43:VAL:HG21	1:D:136:LEU:HG	2.03	0.41
1:D:217:LEU:CB	1:D:308:MET:HE2	2.51	0.41
1:A:202:LEU:HG	1:A:326[A]:THR:HG22	2.03	0.41
1:C:53:LYS:NZ	5:C:2824:HOH:O	2.53	0.41
1:D:283[A]:ILE:N	1:D:283[A]:ILE:HD12	2.36	0.41
1:C:145:LYS:HD3	1:C:145:LYS:HA	1.91	0.41
1:B:75:GLN:O	1:B:79:GLU:HG3	2.21	0.40
1:A:206:ARG:NH1	5:A:2717:HOH:O	2.54	0.40
1:B:106:HIS:HA	1:B:152:VAL:HG23	2.03	0.40
1:B:16:ILE:HA	1:B:120:ALA:HB3	2.03	0.40
1:B:313:ARG:HG2	1:B:313:ARG:NH2	2.35	0.40
1:A:22:THR:HG22	1:A:25:GLN:HB2	2.04	0.40
1:B:9:ILE:HD12	1:B:52:VAL:HG11	2.03	0.40
1:B:274:MET:HE3	1:B:324:PHE:CE2	2.56	0.40
1:D:43:VAL:HG22	1:D:46:VAL:HG13	2.03	0.40

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	331/327 (101%)	324 (98%)	7 (2%)	0	100	100
1	B	330/327 (101%)	323 (98%)	7 (2%)	0	100	100
1	C	327/327 (100%)	320 (98%)	7 (2%)	0	100	100
1	D	326/327 (100%)	320 (98%)	6 (2%)	0	100	100
All	All	1314/1308 (100%)	1287 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	271/264 (103%)	264 (97%)	7 (3%)	40	23
1	B	270/264 (102%)	262 (97%)	8 (3%)	36	19
1	C	268/264 (102%)	264 (98%)	4 (2%)	57	43
1	D	266/264 (101%)	264 (99%)	2 (1%)	73	65
All	All	1075/1056 (102%)	1054 (98%)	21 (2%)	51	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	45	GLU
1	A	71	LEU
1	A	72[A]	LYS
1	A	72[B]	LYS
1	A	81	LEU
1	A	293	LEU
1	B	4	LEU
1	B	71	LEU
1	B	80	LEU
1	B	127	ILE
1	B	136	LEU
1	B	255	VAL
1	B	265	LYS
1	B	288	GLU
1	C	4[A]	LEU
1	C	4[B]	LEU
1	C	233	LEU
1	C	288	GLU
1	D	136	LEU
1	D	185	LEU

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	146	GLN
1	A	180	ASN
1	A	191	ASN
1	A	227	GLN
1	A	281	ASN
1	A	302	HIS
1	B	180	ASN
1	C	41	ASN
1	C	180	ASN
1	C	191	ASN
1	C	227	GLN
1	C	239	GLN
1	C	281	ASN
1	D	6	ASN
1	D	51	ASN
1	D	134	ASN
1	D	146	GLN
1	D	180	ASN
1	D	191	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	DDO	A	2401	1	8,9,9	0.65	0	7,10,10	0.38	0
4	GOL	C	2601	-	5,5,5	0.28	0	5,5,5	2.13	2 (40%)
2	DDO	C	2403	1	8,9,9	0.64	0	7,10,10	0.51	0
4	GOL	D	2602	-	5,5,5	0.26	0	5,5,5	2.23	1 (20%)
2	DDO	B	2402	1	8,9,9	0.68	0	7,10,10	0.39	0
3	1PE	A	2501	-	15,15,15	0.33	0	14,14,14	0.49	0
4	GOL	C	2603	-	5,5,5	0.29	0	5,5,5	2.13	1 (20%)
2	DDO	D	2404	1	8,9,9	0.63	0	7,10,10	0.45	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	DDO	A	2401	1	-	3/9/9/9	-
4	GOL	C	2601	-	-	2/4/4/4	-
2	DDO	C	2403	1	-	3/9/9/9	-
4	GOL	D	2602	-	-	2/4/4/4	-
2	DDO	B	2402	1	-	2/9/9/9	-
3	1PE	A	2501	-	-	5/13/13/13	-
4	GOL	C	2603	-	-	3/4/4/4	-
2	DDO	D	2404	1	-	3/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2602	GOL	C3-C2-C1	4.40	127.92	111.80
4	C	2603	GOL	C3-C2-C1	3.97	126.37	111.80
4	C	2601	GOL	C3-C2-C1	3.91	126.14	111.80
4	C	2601	GOL	O2-C2-C3	2.12	117.96	109.18

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2401	DDO	O-C-CA-N
2	B	2402	DDO	O-C-CA-N
2	C	2403	DDO	O-C-CA-N
2	D	2404	DDO	O-C-CA-N
4	C	2603	GOL	C1-C2-C3-O3
4	D	2602	GOL	O1-C1-C2-O2
2	B	2402	DDO	OXT-C-CA-N
2	A	2401	DDO	OXT-C-CA-N
2	C	2403	DDO	OXT-C-CA-N
2	D	2404	DDO	OXT-C-CA-N
4	C	2601	GOL	O1-C1-C2-O2
4	C	2603	GOL	O1-C1-C2-O2
3	A	2501	1PE	OH5-C14-C24-OH4
4	D	2602	GOL	O2-C2-C3-O3
4	C	2601	GOL	O2-C2-C3-O3
2	C	2403	DDO	CE-CD-CG-CB
3	A	2501	1PE	C15-C25-OH5-C14
4	C	2603	GOL	O2-C2-C3-O3
2	D	2404	DDO	CE-CD-CG-CB
3	A	2501	1PE	C16-C26-OH6-C15
2	A	2401	DDO	CE-CD-CG-CB
3	A	2501	1PE	C13-C23-OH3-C22
3	A	2501	1PE	OH4-C13-C23-OH3

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	DDO	2	0
4	D	2602	GOL	1	0
2	B	2402	DDO	1	0
3	A	2501	1PE	7	0
4	C	2603	GOL	1	0
2	D	2404	DDO	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	324/327 (99%)	-0.11	6 (1%) 66 71	3, 17, 29, 34	13 (4%)
1	B	324/327 (99%)	-0.06	9 (2%) 55 59	3, 16, 30, 34	12 (3%)
1	C	324/327 (99%)	-0.17	7 (2%) 62 66	4, 16, 27, 33	11 (3%)
1	D	324/327 (99%)	-0.18	7 (2%) 62 66	3, 16, 28, 37	9 (2%)
All	All	1296/1308 (99%)	-0.13	29 (2%) 62 66	3, 17, 29, 37	45 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	THR	5.7
1	A	160[A]	ILE	5.5
1	D	24	THR	5.4
1	A	136[A]	LEU	4.5
1	B	10[A]	LEU	4.3
1	B	213	GLY	4.0
1	C	4[A]	LEU	3.9
1	A	72[A]	LYS	3.6
1	C	51[A]	ASN	3.5
1	D	239	GLN	2.9
1	C	202[A]	LEU	2.8
1	D	212	ARG	2.7
1	B	289[A]	GLU	2.7
1	D	216[A]	SER	2.6
1	B	297[A]	SER	2.6
1	B	288	GLU	2.6
1	B	74[A]	SER	2.5
1	D	53[A]	LYS	2.5
1	B	25	GLN	2.4
1	A	43[A]	VAL	2.3
1	A	65[A]	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	289	GLU	2.2
1	D	145	LYS	2.2
1	B	19	SER	2.2
1	B	199[A]	ILE	2.1
1	C	10[A]	LEU	2.1
1	C	148	ARG	2.1
1	D	146	GLN	2.0
1	A	208[A]	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	GOL	C	2603	6/6	0.73	0.13	39,39,40,40	0
3	1PE	A	2501	16/16	0.81	0.16	29,32,37,38	0
4	GOL	D	2602	6/6	0.85	0.14	25,28,28,29	0
2	DDO	C	2403	10/10	0.87	0.10	20,21,22,22	0
2	DDO	A	2401	10/10	0.89	0.09	18,19,21,21	0
2	DDO	D	2404	10/10	0.91	0.09	17,19,20,21	0
2	DDO	B	2402	10/10	0.91	0.09	21,22,24,24	0
4	GOL	C	2601	6/6	0.93	0.07	17,17,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.