Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 03:57 AM EDT

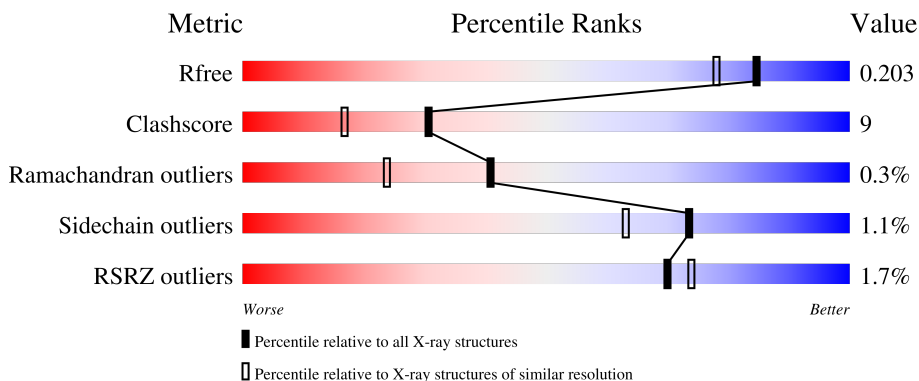|		
PDB ID	:	1JSR
Title	:	CRYSTAL STRUCTURE OF ERWINIA CHRYSANTHEMI L-ASPARAGINASE COMPLEXED WITH 6-HYDROXY-L-NORLEUCINE
Authors	:	Aghaiypour, K.; Wlodawer, A.; Lubkowski, J.
Deposited on	:	2001-08-17
Resolution	:	1.70 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
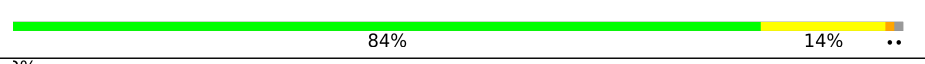*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.203
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		1.1%
RSRZ outliers		1.7%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 <=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	% / 83% / 15% / ••
1	B	327	4% / 83% / 15% / ••
1	C	327	84% / 14% / ••
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
2	LDO	B	2402	-	-	X	-
3	1PE	A	2501	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11357 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	13	0
			2539	1595	443	492	9			
1	B	324	Total	C	N	O	S	0	15	0
			2567	1610	453	493	11			
1	C	324	Total	C	N	O	S	0	11	0
			2536	1590	452	485	9			
1	D	324	Total	C	N	O	S	0	14	0
			2550	1596	450	494	10			

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-L-NORLEUCINE (three-letter code: LDO) (formula: $C_6H_{13}NO_3$).

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

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
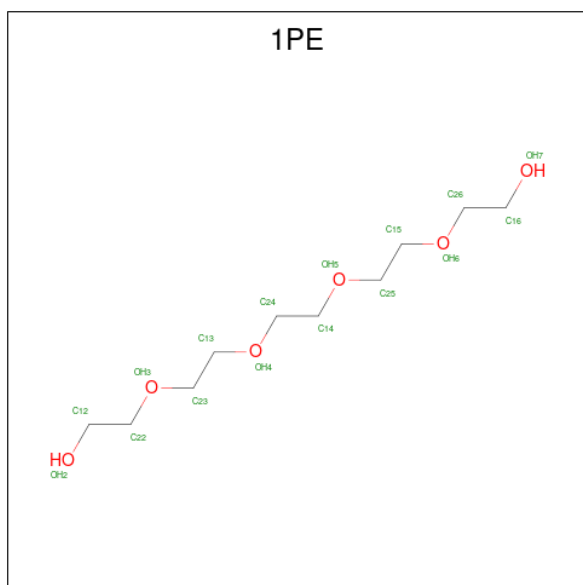
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 16	C 10	O 6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	272	Total 273	O 273	0	1
5	B	251	Total 251	O 251	0	0
5	C	278	Total 279	O 279	0	1
5	D	282	Total 282	O 282	0	0

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
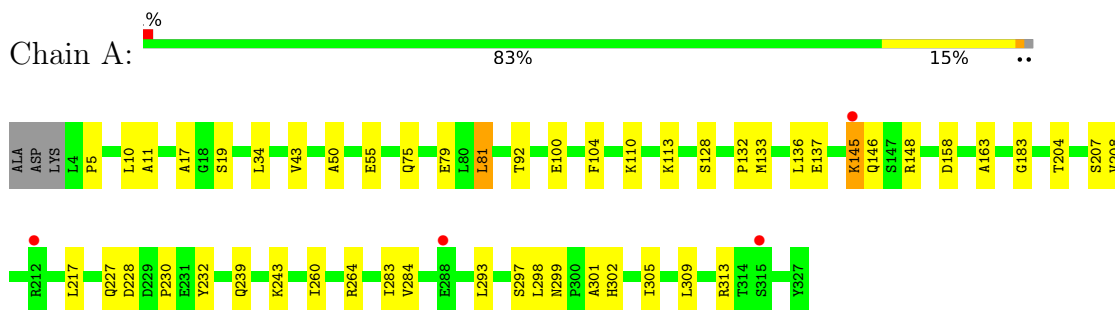
Chain A:

- Molecule 1: L-asparaginase

Chain B:

- Molecule 1: L-asparaginase

Chain C:

- Molecule 1: L-asparaginase

Chain D:
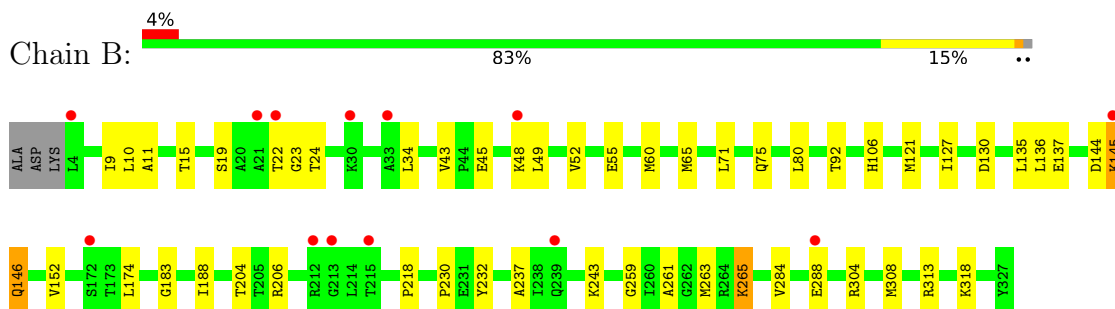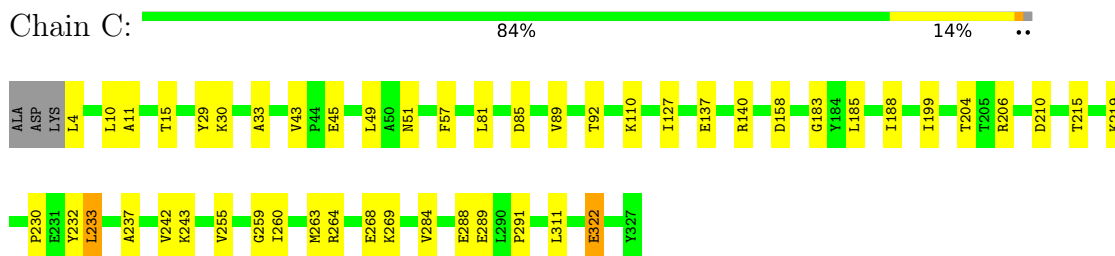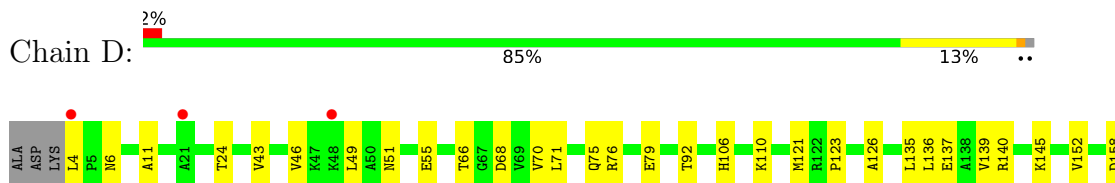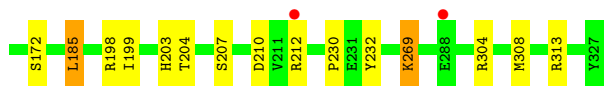
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.06Å 90.36Å 127.41Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.96 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 89.8 (19.96-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.182 , 0.209 0.173 , 0.203	Depositor DCC
R_{free} test set	2701 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	11.6	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11357	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LDO, 1PE, 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	0.31	0/2575	0.64	1/3494 (0.0%)
1	B	0.32	0/2603	0.65	1/3524 (0.0%)
1	C	0.31	0/2572	0.65	1/3486 (0.0%)
1	D	0.32	0/2586	0.64	0/3506
All	All	0.31	0/10336	0.64	3/14010 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	VAL	N-CA-C	-5.10	97.22	111.00
1	C	284	VAL	N-CA-C	-5.10	97.24	111.00
1	A	284	VAL	N-CA-C	-5.08	97.29	111.00

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	2539	0	2576	56	0
1	B	2567	0	2610	48	0
1	C	2536	0	2583	41	0
1	D	2550	0	2579	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	10	3	0
2	B	10	0	10	7	0
2	C	10	0	10	2	0
2	D	10	0	10	0	0
3	A	16	0	22	7	0
4	C	18	0	21	3	0
4	D	6	0	7	0	0
5	A	273	0	0	4	0
5	B	251	0	0	6	0
5	C	279	0	0	6	0
5	D	282	0	0	12	0
All	All	11357	0	10438	190	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 9.

All (190) 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:C:2403:LDO:HE1	5:C:2613[B]:HOH:O	1.17	1.27
1:A:243:LYS:HZ3	3:A:2501:1PE:H131	1.29	0.98
2:A:2401:LDO:CE	5:A:2507[B]:HOH:O	2.10	0.97
1:B:206[B]:ARG:HA	1:B:206[B]:ARG:HE	1.36	0.91
1:A:43[B]:VAL:HB	1:A:136[B]:LEU:HD11	1.52	0.90
1:A:145:LYS:HE2	1:A:146:GLN:HG2	1.57	0.87
2:A:2401:LDO:HE1	5:A:2507[B]:HOH:O	1.73	0.87
2:C:2403:LDO:CE	5:C:2613[B]:HOH:O	1.90	0.79
1:B:22:THR:HG22	1:B:24:THR:H	1.48	0.78
1:A:243:LYS:NZ	3:A:2501:1PE:H131	1.99	0.77
1:B:15:THR:OG1	2:B:2402:LDO:CG	2.33	0.76
1:A:136[B]:LEU:HD22	1:B:127[B]:ILE:HD13	1.67	0.75
1:D:43:VAL:HG21	1:D:136[B]:LEU:HG	1.69	0.75
1:C:185:LEU:HD21	1:C:199[B]:ILE:HG23	1.70	0.73
1:D:269:LYS:HA	1:D:269:LYS:HE3	1.70	0.73
2:A:2401:LDO:HE2	5:A:2507[B]:HOH:O	1.81	0.72
1:B:206[B]:ARG:HA	1:B:206[B]:ARG:NE	2.04	0.72
1:D:212:ARG:HD2	5:D:1229:HOH:O	1.90	0.71
1:B:60[A]:MET:HE1	1:B:65:MET:HB2	1.71	0.70
1:D:313:ARG:NH1	5:D:987:HOH:O	2.24	0.69
1:A:136[B]:LEU:HD22	1:B:127[B]:ILE:CD1	2.23	0.67
1:D:185:LEU:HD11	1:D:199:ILE:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:O	1:A:264:ARG:HG2	1.94	0.67
1:C:232:TYR:CE2	1:C:233:LEU:HD13	2.29	0.67
1:B:145:LYS:HD3	1:B:145:LYS:H	1.59	0.66
1:A:104:PHE:CE1	1:A:217:LEU:HD11	2.31	0.65
1:C:215[A]:THR:HG21	4:C:2601:GOL:O2	1.97	0.64
1:A:100[A]:GLU:CD	1:A:301:ALA:HB1	2.17	0.64
1:C:10:LEU:HD22	1:C:57:PHE:HB2	1.78	0.64
1:C:110:LYS:HZ1	1:C:210:ASP:HA	1.62	0.64
1:B:19:SER:HB2	1:B:34[B]:LEU:HD21	1.80	0.63
1:A:145:LYS:N	1:A:145:LYS:HD3	2.13	0.63
1:A:298[B]:LEU:HD12	1:A:302:HIS:HB3	1.81	0.63
1:A:104:PHE:CE1	1:A:309[B]:LEU:HD21	2.34	0.62
1:D:145:LYS:H	1:D:145:LYS:HE2	1.63	0.62
1:B:71[B]:LEU:O	1:B:75:GLN:HG3	1.99	0.62
1:D:199:ILE:HD11	1:D:203:HIS:CD2	2.34	0.61
1:A:264:ARG:HH21	1:A:264:ARG:HG3	1.64	0.61
1:D:145:LYS:H	1:D:145:LYS:CE	2.13	0.61
1:B:45:GLU:O	1:B:48[B]:LYS:HG3	2.00	0.61
1:B:237:ALA:HA	1:D:232:TYR:OH	2.02	0.60
1:B:71[A]:LEU:O	1:B:75:GLN:HG3	1.99	0.60
1:B:137:GLU:HB3	1:B:188:ILE:HD13	1.84	0.60
1:A:133:MET:HA	1:B:127[B]:ILE:HD11	1.84	0.59
1:D:43:VAL:CG2	1:D:136[B]:LEU:HG	2.32	0.59
1:B:43:VAL:HG13	1:B:43:VAL:O	2.03	0.59
1:D:46[B]:VAL:HG12	1:D:136[B]:LEU:HD23	1.84	0.59
1:A:145:LYS:HD3	1:A:145:LYS:H	1.67	0.58
1:A:305:ILE:O	1:A:309[B]:LEU:HD23	2.03	0.58
1:A:34:LEU:HD12	1:A:34:LEU:N	2.18	0.58
1:A:43[A]:VAL:HG13	1:A:43[A]:VAL:O	2.04	0.57
1:A:132:PRO:O	1:A:136[B]:LEU:HD13	2.04	0.57
1:A:163:ALA:O	1:A:302:HIS:HE1	1.87	0.56
1:D:68:ASP:OD1	5:D:964:HOH:O	2.18	0.56
1:B:15:THR:CB	2:B:2402:LDO:CD	2.81	0.56
1:C:230:PRO:HB2	1:C:232:TYR:CD1	2.41	0.56
1:C:30:LYS:HG3	1:C:33:ALA:HB2	1.87	0.55
1:B:218:PRO:HB3	1:B:243[A]:LYS:HD3	1.87	0.55
1:C:11:ALA:HA	1:C:92:THR:OG1	2.07	0.55
1:B:288[B]:GLU:HA	5:B:2544:HOH:O	2.07	0.55
1:B:15:THR:OG1	2:B:2402:LDO:HB1	2.07	0.55
1:A:10[B]:LEU:HD23	1:A:55:GLU:HB3	1.90	0.54
1:C:219:LYS:HE3	1:C:242:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:NZ	3:A:2501:1PE:H162	2.21	0.54
1:D:46[A]:VAL:HG23	1:D:139:VAL:HG11	1.90	0.54
1:B:304:ARG:O	1:B:308[B]:MET:HG3	2.08	0.53
1:D:110:LYS:HD2	5:D:1236:HOH:O	2.07	0.53
1:B:22:THR:HG22	1:B:23:GLY:N	2.23	0.53
1:D:43:VAL:O	1:D:43:VAL:HG13	2.09	0.53
1:B:45:GLU:O	1:B:48[B]:LYS:HE3	2.09	0.53
1:A:100[A]:GLU:OE1	1:A:301:ALA:HB1	2.09	0.53
1:D:43:VAL:HG11	1:D:135:LEU:HD23	1.90	0.53
1:D:46[A]:VAL:CG2	1:D:139:VAL:HG21	2.39	0.52
1:A:183:GLY:HA2	5:D:1209:HOH:O	2.09	0.52
1:A:208[B]:VAL:HG11	1:A:313:ARG:NH1	2.25	0.52
1:D:55:GLU:OE2	1:D:76[B]:ARG:HD3	2.10	0.52
1:C:264:ARG:HH21	1:C:264:ARG:HG3	1.74	0.52
1:D:71:LEU:O	1:D:75:GLN:HG3	2.10	0.51
1:A:264:ARG:HG3	1:A:264:ARG:NH2	2.25	0.51
1:A:299:ASN:OD1	1:A:302:HIS:HD2	1.92	0.51
1:A:293[B]:LEU:HD12	1:A:293[B]:LEU:N	2.24	0.51
1:D:121:MET:CE	1:D:172[A]:SER:HA	2.40	0.51
1:A:43[B]:VAL:CB	1:A:136[B]:LEU:HD11	2.34	0.51
1:B:60[A]:MET:HE3	1:B:65:MET:N	2.26	0.50
1:B:43:VAL:HG11	1:B:135:LEU:HD23	1.93	0.50
1:C:81:LEU:HD21	1:C:89[B]:VAL:HG23	1.93	0.50
1:C:289:GLU:O	1:C:289:GLU:HG3	2.11	0.50
1:D:304:ARG:O	1:D:308[A]:MET:HG3	2.12	0.50
1:D:110:LYS:HE3	1:D:207:SER:O	2.12	0.50
1:C:230:PRO:HG2	1:C:233:LEU:HD22	1.94	0.50
1:D:106:HIS:HA	1:D:152:VAL:HG23	1.94	0.50
1:D:140[B]:ARG:NH2	5:D:1110:HOH:O	2.44	0.49
1:A:148:ARG:HB3	1:A:148:ARG:NH2	2.27	0.49
1:D:4:LEU:N	5:D:1202:HOH:O	2.46	0.49
1:A:243:LYS:HZ2	3:A:2501:1PE:H162	1.78	0.48
1:A:208[B]:VAL:HG12	1:A:313:ARG:CZ	2.43	0.48
1:C:206[A]:ARG:HG3	1:C:206[A]:ARG:NH2	2.29	0.48
1:A:75:GLN:O	1:A:79:GLU:HG3	2.12	0.48
1:A:230:PRO:HB2	1:A:232:TYR:CD1	2.49	0.48
1:B:60[A]:MET:HE1	1:B:65:MET:CB	2.43	0.48
1:B:206[B]:ARG:HE	1:B:206[B]:ARG:CA	2.16	0.48
1:C:255[A]:VAL:HG21	1:C:260[A]:ILE:HD11	1.95	0.48
1:B:15:THR:OG1	2:B:2402:LDO:CB	2.62	0.48
1:B:230:PRO:HB2	1:B:232:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HD12	1:B:52:VAL:HG11	1.96	0.47
1:D:46[A]:VAL:HG23	1:D:139:VAL:HG21	1.95	0.47
1:C:269[B]:LYS:HA	1:C:269[B]:LYS:HE2	1.95	0.47
1:A:243:LYS:HZ1	3:A:2501:1PE:H142	1.78	0.47
1:D:6:ASN:HD22	1:D:51:ASN:HB2	1.79	0.47
1:D:145:LYS:H	1:D:145:LYS:CD	2.28	0.47
1:D:198:ARG:NH1	5:D:1142:HOH:O	2.48	0.47
1:A:34:LEU:N	1:A:34:LEU:CD1	2.77	0.47
1:B:34[B]:LEU:HD22	1:B:34[B]:LEU:N	2.30	0.47
1:B:183:GLY:HA2	5:C:2734:HOH:O	2.15	0.47
1:C:255[A]:VAL:CG2	1:C:260[A]:ILE:HD11	2.44	0.47
1:C:264:ARG:O	1:C:268:GLU:HG3	2.15	0.47
1:D:11:ALA:HA	1:D:92:THR:OG1	2.14	0.47
1:B:15:THR:OG1	2:B:2402:LDO:CE	2.53	0.46
5:B:2581:HOH:O	1:C:183:GLY:HA2	2.16	0.46
1:B:45:GLU:HB3	1:B:48[B]:LYS:HE3	1.98	0.46
1:D:137:GLU:OE1	1:D:158:ASP:OD1	2.34	0.46
1:C:137:GLU:OE1	1:C:158:ASP:OD1	2.34	0.45
1:C:140[B]:ARG:HH21	1:C:140[B]:ARG:HB2	1.82	0.45
1:A:128[A]:SER:OG	1:B:130:ASP:HA	2.16	0.45
1:B:265:LYS:N	1:B:265:LYS:HE3	2.32	0.45
1:A:81:LEU:HG	1:A:113:LYS:HB2	1.97	0.45
1:B:10[B]:LEU:HD23	1:B:55:GLU:HB3	1.98	0.45
1:D:199:ILE:HB	5:D:1222:HOH:O	2.16	0.45
2:B:2402:LDO:CE	5:B:2409:HOH:O	2.64	0.45
1:C:206[A]:ARG:HG3	1:C:206[A]:ARG:HH21	1.80	0.45
1:C:206[A]:ARG:HG2	5:C:2747:HOH:O	2.16	0.45
1:C:243:LYS:HB3	1:C:311:LEU:HD13	1.99	0.45
1:A:104:PHE:HE1	1:A:217:LEU:HD11	1.76	0.44
1:B:48[B]:LYS:HD2	1:B:49:LEU:HG	1.98	0.44
1:B:261:ALA:O	1:B:265:LYS:HD2	2.16	0.44
1:C:322:GLU:HA	1:C:322:GLU:OE1	2.17	0.44
1:B:318:LYS:HG2	5:B:2602:HOH:O	2.16	0.44
1:D:212:ARG:HG2	5:D:1230:HOH:O	2.17	0.44
1:D:230:PRO:HB2	1:D:232:TYR:CD1	2.51	0.44
1:A:19:SER:HB3	1:A:34:LEU:HD11	1.99	0.44
1:A:243:LYS:HZ3	3:A:2501:1PE:C13	2.16	0.43
1:D:210:ASP:HA	5:D:1215:HOH:O	2.18	0.43
1:D:145:LYS:N	1:D:145:LYS:HD3	2.34	0.43
1:A:145:LYS:H	1:A:145:LYS:CD	2.31	0.43
1:A:110:LYS:NZ	1:A:207:SER:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:NH2	5:A:2701:HOH:O	2.52	0.43
1:C:288:GLU:HG2	5:C:2830:HOH:O	2.18	0.43
1:B:121:MET:HB2	1:B:174:LEU:HD23	2.01	0.43
2:B:2402:LDO:HE2	5:B:2409:HOH:O	2.19	0.43
1:D:49:LEU:HD21	1:D:140[B]:ARG:NH1	2.33	0.43
1:A:299:ASN:OD1	1:A:302:HIS:CD2	2.71	0.43
1:C:85:ASP:N	4:C:2604:GOL:O1	2.49	0.43
1:A:137:GLU:OE1	1:A:158:ASP:OD1	2.37	0.42
1:C:127:ILE:HD13	1:D:136[B]:LEU:HD11	2.01	0.42
1:C:264:ARG:HE	1:C:291:PRO:HB3	1.85	0.42
1:D:185:LEU:HG	5:D:966:HOH:O	2.18	0.42
1:A:17:ALA:O	1:A:34:LEU:HD13	2.19	0.42
1:C:230:PRO:HB2	1:C:232:TYR:CE1	2.55	0.42
1:C:81:LEU:HD21	1:C:89[A]:VAL:HG13	2.00	0.42
1:D:66:THR:O	1:D:70:VAL:HG23	2.20	0.42
1:C:137:GLU:HB3	1:C:188:ILE:HD12	2.01	0.42
1:C:43:VAL:HG13	1:C:43:VAL:O	2.20	0.42
1:D:145:LYS:CD	1:D:145:LYS:N	2.83	0.42
1:A:11:ALA:HA	1:A:92:THR:OG1	2.20	0.42
1:D:43:VAL:O	1:D:46[A]:VAL:HG12	2.20	0.42
1:C:49:LEU:HD11	1:C:140[B]:ARG:NH2	2.35	0.41
1:A:43[B]:VAL:O	1:A:43[B]:VAL:HG23	2.19	0.41
1:A:243:LYS:NZ	3:A:2501:1PE:H142	2.36	0.41
1:B:22:THR:CG2	1:B:23:GLY:N	2.83	0.41
1:A:232:TYR:OH	1:C:237:ALA:HA	2.20	0.41
1:D:76[A]:ARG:NH2	1:D:79:GLU:OE2	2.53	0.41
1:A:148:ARG:HH21	1:A:148:ARG:CB	2.33	0.41
1:B:259:GLY:O	1:B:263:MET:HG3	2.20	0.41
1:C:140[B]:ARG:HB2	1:C:140[B]:ARG:NH2	2.36	0.41
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.92	0.41
1:B:144:ASP:OD1	1:B:146:GLN:HB2	2.20	0.41
1:C:137:GLU:HB3	1:C:188:ILE:CD1	2.51	0.41
1:C:259:GLY:O	1:C:263:MET:HG3	2.21	0.40
1:A:227:GLN:O	1:A:228:ASP:HB2	2.21	0.40
1:B:11:ALA:HA	1:B:92:THR:OG1	2.21	0.40
1:B:106:HIS:HA	1:B:152:VAL:HG23	2.04	0.40
1:B:313:ARG:HG2	1:B:313:ARG:HH21	1.87	0.40
4:C:2603:GOL:H11	5:C:2840:HOH:O	2.21	0.40
1:D:123:PRO:HG2	1:D:126:ALA:HB2	2.03	0.40
1:A:283:ILE:HD13	1:A:297:SER:HB3	2.04	0.40
1:B:288[A]:GLU:HG2	5:B:2576:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:GLU:HG2	1:D:24[A]:THR:HG23	2.04	0.40
1:A:5:PRO:HG2	1:A:50:ALA:HB2	2.03	0.40
1:C:4:LEU:HB2	1:C:51[A]:ASN:ND2	2.36	0.40
1:C:15:THR:OG1	1:C:29:TYR:CE2	2.73	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	335/327 (102%)	328 (98%)	6 (2%)	1 (0%)	41	24
1	B	337/327 (103%)	332 (98%)	4 (1%)	1 (0%)	41	24
1	C	333/327 (102%)	327 (98%)	5 (2%)	1 (0%)	41	24
1	D	336/327 (103%)	329 (98%)	6 (2%)	1 (0%)	41	24
All	All	1341/1308 (102%)	1316 (98%)	21 (2%)	4 (0%)	41	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	204	THR
1	D	204	THR
1	A	204	THR
1	B	204	THR

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	275/264 (104%)	272 (99%)	3 (1%)	73	63
1	B	277/264 (105%)	272 (98%)	5 (2%)	59	43
1	C	273/264 (103%)	271 (99%)	2 (1%)	84	77
1	D	276/264 (104%)	274 (99%)	2 (1%)	84	77
All	All	1101/1056 (104%)	1089 (99%)	12 (1%)	73	63

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	145	LYS
1	A	239	GLN
1	B	80	LEU
1	B	136	LEU
1	B	145	LYS
1	B	146	GLN
1	B	265	LYS
1	C	233	LEU
1	C	322	GLU
1	D	185	LEU
1	D	269	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	302	HIS
1	B	239	GLN
1	C	41	ASN
1	C	227	GLN
1	C	239	GLN
1	D	6	ASN
1	D	51	ASN
1	D	134	ASN
1	D	146	GLN
1	D	239	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	LDO	C	2403	1	8,9,9	0.75	0	9,10,10	0.71	0
2	LDO	A	2401	1	8,9,9	0.73	0	9,10,10	0.63	0
4	GOL	C	2604	-	5,5,5	0.27	0	5,5,5	2.05	1 (20%)
4	GOL	C	2603	-	5,5,5	0.33	0	5,5,5	2.09	1 (20%)
4	GOL	D	2602	-	5,5,5	0.27	0	5,5,5	2.12	1 (20%)
2	LDO	D	2404	1	8,9,9	0.77	0	9,10,10	0.68	0
4	GOL	C	2601	-	5,5,5	0.24	0	5,5,5	1.99	2 (40%)
3	1PE	A	2501	-	15,15,15	0.34	0	14,14,14	0.51	0
2	LDO	B	2402	1	8,9,9	0.73	0	9,10,10	0.73	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	LDO	C	2403	1	-	2/9/9/9	-
2	LDO	A	2401	1	-	1/9/9/9	-
4	GOL	C	2604	-	-	2/4/4/4	-
4	GOL	C	2603	-	-	3/4/4/4	-
4	GOL	D	2602	-	-	2/4/4/4	-
2	LDO	D	2404	1	-	1/9/9/9	-
4	GOL	C	2601	-	-	3/4/4/4	-
3	1PE	A	2501	-	-	4/13/13/13	-
2	LDO	B	2402	1	-	2/9/9/9	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2602	GOL	C3-C2-C1	4.19	127.98	111.70
4	C	2603	GOL	C3-C2-C1	4.06	127.48	111.70
4	C	2604	GOL	C3-C2-C1	3.90	126.85	111.70
4	C	2601	GOL	C3-C2-C1	3.58	125.62	111.70
4	C	2601	GOL	O2-C2-C3	2.02	118.02	109.12

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2604	GOL	C1-C2-C3-O3
4	D	2602	GOL	O1-C1-C2-O2
4	C	2603	GOL	O2-C2-C3-O3
3	A	2501	1PE	OH5-C14-C24-OH4
4	C	2603	GOL	C1-C2-C3-O3
4	C	2601	GOL	O1-C1-C2-O2
4	C	2603	GOL	O1-C1-C2-O2
4	C	2604	GOL	O1-C1-C2-O2
4	D	2602	GOL	O2-C2-C3-O3
3	A	2501	1PE	OH4-C13-C23-OH3
3	A	2501	1PE	C15-C25-OH5-C14
4	C	2601	GOL	O2-C2-C3-O3
2	B	2402	LDO	O-C-CA-N
2	C	2403	LDO	O-C-CA-N
3	A	2501	1PE	C16-C26-OH6-C15
2	B	2402	LDO	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	C	2403	LDO	OXT-C-CA-N
2	A	2401	LDO	OXT-C-CA-N
4	C	2601	GOL	C1-C2-C3-O3
2	D	2404	LDO	OXT-C-CA-N

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2403	LDO	2	0
2	A	2401	LDO	3	0
4	C	2604	GOL	1	0
4	C	2603	GOL	1	0
4	C	2601	GOL	1	0
3	A	2501	1PE	7	0
2	B	2402	LDO	7	0

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, 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(Å²)	Q<0.9
1	A	324/327 (99%)	-0.15	4 (1%)	79	82	6, 13, 24, 31	0
1	B	324/327 (99%)	-0.06	13 (4%)	38	42	7, 12, 25, 30	1 (0%)
1	C	324/327 (99%)	-0.19	0	100	100	7, 12, 24, 27	0
1	D	324/327 (99%)	-0.17	5 (1%)	73	77	7, 12, 24, 32	0
All	All	1296/1308 (99%)	-0.14	22 (1%)	70	74	6, 12, 24, 32	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	GLY	4.5
1	D	212	ARG	4.2
1	B	172[A]	SER	4.0
1	B	33	ALA	3.7
1	B	48[A]	LYS	3.3
1	B	21	ALA	3.1
1	B	30	LYS	3.0
1	B	288[A]	GLU	3.0
1	A	212	ARG	2.7
1	D	4	LEU	2.6
1	D	21	ALA	2.6
1	B	22	THR	2.5
1	B	4	LEU	2.5
1	A	315	SER	2.4
1	A	288[A]	GLU	2.3
1	B	215	THR	2.2
1	D	48	LYS	2.1
1	B	145	LYS	2.1
1	B	239	GLN	2.1
1	A	145	LYS	2.1
1	B	212	ARG	2.0
1	D	288	GLU	2.0

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 monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	C	2603	6/6	0.51	0.28	35,36,36,36	0
3	1PE	A	2501	16/16	0.78	0.17	24,26,32,34	0
4	GOL	C	2604	6/6	0.81	0.32	36,36,37,37	0
4	GOL	D	2602	6/6	0.88	0.15	18,22,22,23	0
2	LDO	C	2403	10/10	0.89	0.14	14,17,19,20	0
4	GOL	C	2601	6/6	0.91	0.11	14,15,15,15	0
2	LDO	A	2401	10/10	0.94	0.09	13,15,16,17	0
2	LDO	B	2402	10/10	0.95	0.10	13,14,18,18	0
2	LDO	D	2404	10/10	0.96	0.08	10,12,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.