



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:39 PM UTC

PDB ID : 5F52 / pdb_00005f52
Title : Erwinia chrysanthemi L-asparaginase + Aspartic acid
Authors : Nguyen, H.A.; Lavie, A.
Deposited on : 2015-12-04
Resolution : 1.63 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

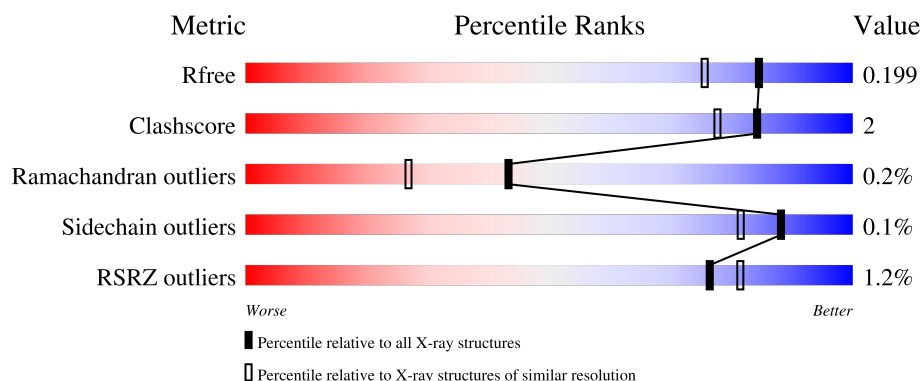
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	328	
1	B	328	
1	C	328	
1	D	328	

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	PEG	A	402	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11168 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.

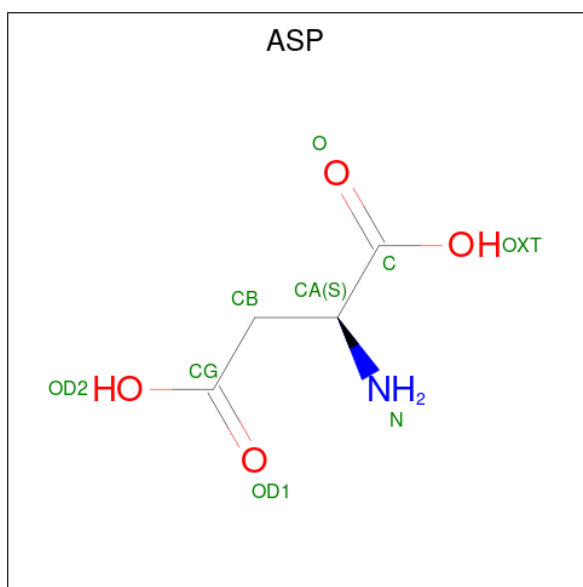
- Molecule 1 is a protein called L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	7	0
			2484	1562	436	477	9			
1	B	324	Total	C	N	O	S	4	7	0
			2488	1565	437	477	9			
1	C	324	Total	C	N	O	S	9	5	0
			2467	1551	432	475	9			
1	D	324	Total	C	N	O	S	14	7	0
			2483	1562	435	477	9			

There are 8 discrepancies between the modelled and reference sequences:

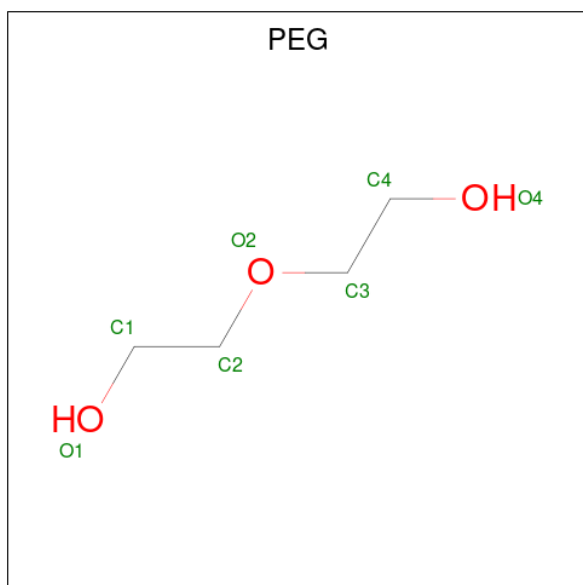
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P06608
A	1	MET	-	expression tag	UNP P06608
B	0	HIS	-	expression tag	UNP P06608
B	1	MET	-	expression tag	UNP P06608
C	0	HIS	-	expression tag	UNP P06608
C	1	MET	-	expression tag	UNP P06608
D	0	HIS	-	expression tag	UNP P06608
D	1	MET	-	expression tag	UNP P06608

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		
2	C	1	Total	C	N	O	0	0
			9	4	1	4		
2	D	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0

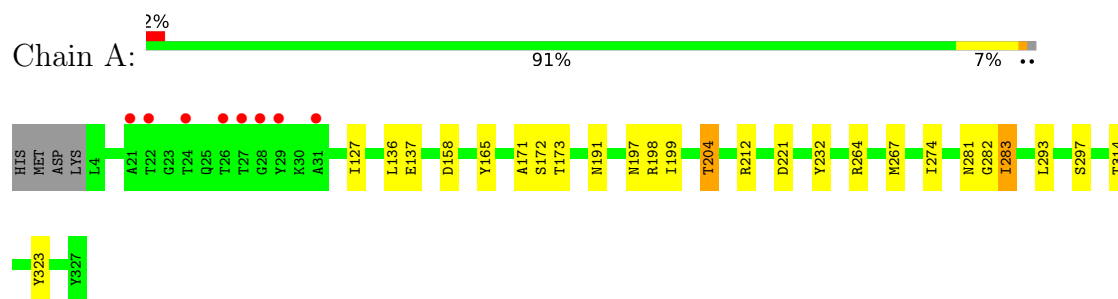
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	302	Total O 302 302	0	0
4	B	309	Total O 309 309	0	0
4	C	276	Total O 276 276	0	0
4	D	288	Total O 288 288	0	0

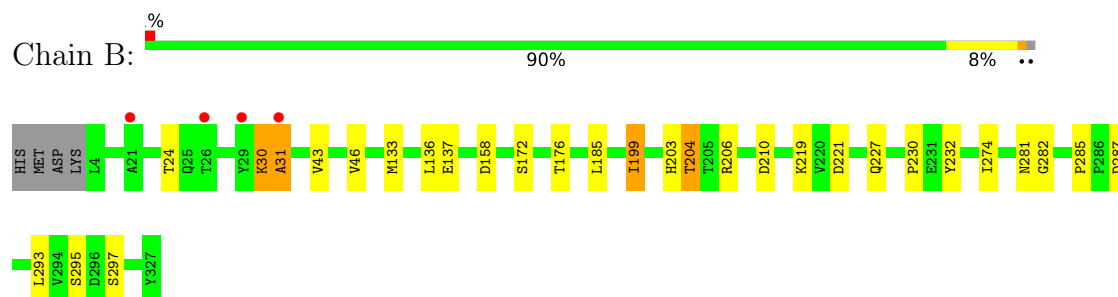
3 Residue-property plots [i](#)

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.

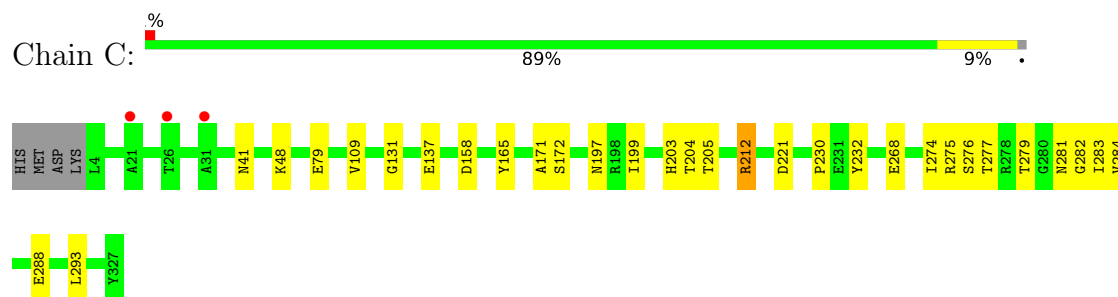
• Molecule 1: L-asparaginase



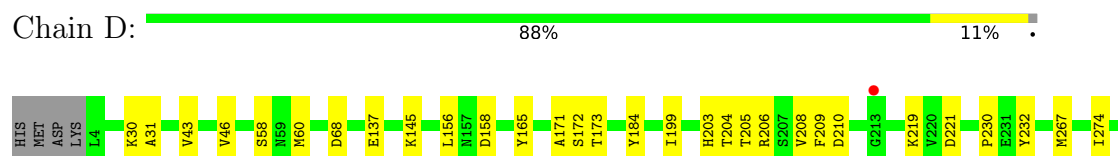
• Molecule 1: L-asparaginase



• Molecule 1: L-asparaginase



• Molecule 1: L-asparaginase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.96Å 88.22Å 176.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.04 – 1.63 88.04 – 1.63	Depositor EDS
% Data completeness (in resolution range)	98.3 (88.04-1.63) 98.5 (88.04-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.156 , 0.187 0.169 , 0.199	Depositor DCC
R_{free} test set	7466 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11168	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.31	9/2537 (0.4%)	1.03	4/3440 (0.1%)
1	B	1.30	12/2538 (0.5%)	1.03	3/3442 (0.1%)
1	C	1.32	15/2520 (0.6%)	1.05	11/3418 (0.3%)
1	D	1.34	19/2539 (0.7%)	1.07	7/3443 (0.2%)
All	All	1.32	55/10134 (0.5%)	1.05	25/13743 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	ASP	C-O	-8.40	1.15	1.23
1	C	283	ILE	C-O	-8.18	1.14	1.24
1	B	285	PRO	C-O	-8.08	1.15	1.24
1	A	197	ASN	C-O	-7.87	1.14	1.23
1	C	275	ARG	C-O	-7.50	1.14	1.24
1	C	281	ASN	C-O	-7.44	1.15	1.23
1	A	282	GLY	C-O	-7.41	1.16	1.24
1	D	203	HIS	C-O	-7.33	1.15	1.23
1	C	109	VAL	C-O	-7.21	1.16	1.24
1	C	282	GLY	C-O	-7.07	1.16	1.24
1	D	204	THR	C-O	-7.06	1.15	1.24
1	C	171	ALA	C-O	-7.03	1.15	1.24
1	C	203	HIS	C-O	-6.93	1.16	1.23
1	B	295	SER	C-O	-6.85	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	GLU	C-O	-6.85	1.16	1.24
1	D	209	PHE	C-O	-6.70	1.15	1.23
1	C	284	VAL	C-O	-6.70	1.16	1.24
1	D	281	ASN	C-O	-6.67	1.15	1.23
1	A	204	THR	C-O	-6.63	1.15	1.24
1	D	296	ASP	C-O	-6.56	1.18	1.24
1	D	58	SER	C-O	-6.54	1.16	1.23
1	A	283	ILE	C-O	-6.41	1.16	1.24
1	B	199	ILE	C-O	-6.34	1.16	1.24
1	D	206[A]	ARG	CA-C	6.27	1.61	1.52
1	D	206[B]	ARG	CA-C	6.27	1.61	1.52
1	C	172	SER	C-O	-6.21	1.16	1.24
1	D	171	ALA	C-O	-6.20	1.16	1.24
1	B	203	HIS	C-O	-6.20	1.17	1.23
1	C	277	THR	C-O	-6.16	1.16	1.23
1	A	198	ARG	C-O	-6.07	1.16	1.24
1	D	206[A]	ARG	N-CA	6.05	1.54	1.46
1	D	206[B]	ARG	N-CA	6.05	1.54	1.46
1	C	268	GLU	CB-CG	-6.04	1.34	1.52
1	D	208	VAL	C-O	-5.92	1.16	1.24
1	C	205	THR	C-O	-5.91	1.16	1.24
1	D	172	SER	C-O	-5.78	1.16	1.24
1	B	172	SER	C-O	-5.78	1.16	1.24
1	C	197	ASN	C-O	-5.78	1.16	1.23
1	D	60	MET	C-O	-5.75	1.16	1.23
1	D	156	LEU	C-O	-5.74	1.16	1.23
1	B	281	ASN	C-O	-5.67	1.17	1.23
1	A	171	ALA	C-O	-5.64	1.17	1.24
1	B	133	MET	N-CA	-5.56	1.39	1.46
1	B	297	SER	C-O	-5.55	1.16	1.24
1	D	210	ASP	C-O	-5.39	1.17	1.23
1	D	282	GLY	C-O	-5.38	1.17	1.23
1	C	276	SER	C-O	-5.38	1.16	1.24
1	A	281	ASN	C-O	-5.37	1.17	1.23
1	D	173	THR	C-O	-5.34	1.17	1.23
1	B	210	ASP	CA-C	-5.25	1.46	1.52
1	A	173	THR	C-O	-5.23	1.17	1.23
1	D	184	TYR	C-O	-5.23	1.17	1.23
1	B	204	THR	C-O	-5.08	1.17	1.24
1	B	227	GLN	C-O	-5.04	1.17	1.23
1	A	264	ARG	C-O	-5.03	1.18	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	GLY	O-C-N	7.92	123.92	121.07
1	D	206[A]	ARG	CA-C-O	7.24	127.82	119.35
1	D	206[B]	ARG	CA-C-O	7.24	127.82	119.35
1	A	172	SER	N-CA-C	6.73	124.52	114.09
1	A	314	THR	O-C-N	6.73	130.92	123.25
1	B	172	SER	N-CA-C	6.41	124.03	114.09
1	D	172	SER	N-CA-C	6.31	123.86	114.09
1	B	176	THR	N-CA-C	6.27	118.11	111.28
1	C	172	SER	N-CA-C	5.89	123.23	114.09
1	C	48	LYS	CG-CD-CE	5.88	124.83	111.30
1	C	212	ARG	CB-CA-C	5.85	119.02	109.90
1	C	283	ILE	N-CA-C	5.74	116.57	108.36
1	D	205	THR	CA-C-N	5.66	131.87	122.54
1	D	205	THR	C-N-CA	5.66	131.87	122.54
1	C	171	ALA	N-CA-C	5.66	117.44	111.28
1	C	279	THR	N-CA-C	5.64	117.43	111.28
1	C	268	GLU	CA-CB-CG	5.47	125.05	114.10
1	A	282	GLY	N-CA-C	5.47	119.83	112.17
1	A	212	ARG	CB-CA-C	5.43	118.38	109.90
1	B	282	GLY	N-CA-C	5.42	119.75	112.17
1	C	284	VAL	N-CA-C	-5.40	102.20	107.55
1	C	282	GLY	N-CA-C	5.32	119.61	112.17
1	C	283	ILE	CB-CA-C	-5.29	103.65	110.84
1	D	295	SER	N-CA-C	5.12	119.51	113.16
1	D	145	LYS	CB-CG-CD	5.01	122.83	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	30	LYS	Mainchain
1	B	31[A]	ALA	Mainchain
1	B	31[B]	ALA	Mainchain

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	2484	0	2525	16	0
1	B	2488	0	2528	16	0
1	C	2467	0	2500	8	0
1	D	2483	0	2525	13	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
2	C	9	0	3	0	0
2	D	9	0	3	0	0
3	A	14	0	20	8	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	7	0	10	0	0
4	A	302	0	0	3	0
4	B	309	0	0	2	1
4	C	276	0	0	2	1
4	D	288	0	0	2	0
All	All	11168	0	10140	46	2

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 2.

All (46) 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:B:30:LYS:HG2	1:B:31[B]:ALA:O	1.33	1.24
3:A:402:PEG:H22	1:B:24:THR:HG21	1.65	0.79
1:B:30:LYS:C	1:B:31[B]:ALA:O	2.36	0.66
1:B:221:ASP:OD2	1:D:232[B]:TYR:OH	2.16	0.64
1:A:136[B]:LEU:HD21	3:A:402:PEG:H22	1.78	0.64
1:B:232[B]:TYR:OH	1:D:221:ASP:OD2	2.17	0.62
1:B:206[B]:ARG:NH1	4:B:501:HOH:O	2.33	0.61
1:A:191:ASN:OD1	3:A:402:PEG:H32	2.02	0.60
1:A:267:MET:HE1	4:A:716:HOH:O	2.02	0.58
1:D:30:LYS:HG2	1:D:31[B]:ALA:O	2.04	0.58
1:D:68:ASP:OD1	4:D:501:HOH:O	2.17	0.57
1:A:232[B]:TYR:OH	1:C:221:ASP:OD2	2.21	0.57
1:B:206[B]:ARG:CZ	4:B:501:HOH:O	2.53	0.56
1:C:41:ASN:ND2	4:C:501:HOH:O	2.24	0.55
1:A:221:ASP:OD2	1:C:232[B]:TYR:OH	2.23	0.54
1:B:185:LEU:HD21	1:B:199:ILE:HG23	1.92	0.52
1:D:137:GLU:OE2	1:D:158:ASP:OD1	2.28	0.52
3:A:402:PEG:H12	4:A:682:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLU:OE2	1:B:158:ASP:OD1	2.29	0.50
1:C:137:GLU:OE2	1:C:158:ASP:OD1	2.30	0.50
1:D:43:VAL:O	1:D:46[A]:VAL:HG22	2.12	0.49
1:B:43:VAL:O	1:B:46[A]:VAL:HG22	2.12	0.49
1:D:267:MET:HE1	4:D:665:HOH:O	2.11	0.49
1:A:127:ILE:HD13	1:B:136[B]:LEU:HD11	1.95	0.49
1:A:127:ILE:HD13	1:B:136[B]:LEU:CD1	2.42	0.49
1:A:137:GLU:OE2	1:A:158:ASP:OD1	2.30	0.48
1:A:136[B]:LEU:HG	3:A:402:PEG:C4	2.43	0.47
1:C:212:ARG:NH1	4:C:504:HOH:O	2.44	0.47
1:B:219:LYS:HE3	1:D:232[B]:TYR:OH	2.16	0.45
1:B:274:ILE:HD13	1:B:293:LEU:HB2	1.97	0.45
1:A:136[B]:LEU:HD21	3:A:402:PEG:C2	2.46	0.45
1:A:136[B]:LEU:CD2	3:A:402:PEG:H31	2.47	0.44
1:A:274:ILE:HD13	1:A:293:LEU:HB2	1.98	0.43
1:B:230:PRO:HB2	1:B:232[A]:TYR:CD2	2.54	0.43
1:C:274:ILE:HD13	1:C:293:LEU:HB2	2.00	0.43
1:A:165:TYR:CE2	1:A:199:ILE:HG13	2.54	0.43
1:A:323:TYR:CE1	4:A:501:HOH:O	2.69	0.42
1:A:136[B]:LEU:HD21	3:A:402:PEG:H31	2.01	0.42
1:C:230:PRO:HB2	1:C:232[A]:TYR:CD2	2.55	0.42
1:A:283:ILE:HD13	1:A:297:SER:HB3	2.01	0.41
1:D:199:ILE:HD13	1:D:199:ILE:HG21	1.79	0.41
1:B:232[B]:TYR:OH	1:D:219:LYS:HE3	2.19	0.41
1:D:274:ILE:HD13	1:D:293:LEU:HB2	2.02	0.41
1:D:230:PRO:HB2	1:D:232[A]:TYR:CD2	2.56	0.41
1:C:165:TYR:CE2	1:C:199:ILE:HG13	2.55	0.41
1:D:165:TYR:CE2	1:D:199:ILE:HG13	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:717:HOH:O	4:B:767:HOH:O[4_545]	2.01	0.19
4:C:745:HOH:O	4:C:756:HOH:O[4_455]	2.13	0.07

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	329/328 (100%)	321 (98%)	7 (2%)	1 (0%)	36	20
1	B	329/328 (100%)	321 (98%)	7 (2%)	1 (0%)	36	20
1	C	327/328 (100%)	320 (98%)	6 (2%)	1 (0%)	36	20
1	D	329/328 (100%)	322 (98%)	7 (2%)	0	100	100
All	All	1314/1312 (100%)	1284 (98%)	27 (2%)	3 (0%)	43	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	THR
1	B	204	THR
1	C	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	268/266 (101%)	268 (100%)	0	100	100
1	B	268/266 (101%)	268 (100%)	0	100	100
1	C	266/266 (100%)	265 (100%)	1 (0%)	84	76
1	D	268/266 (101%)	268 (100%)	0	100	100
All	All	1070/1064 (101%)	1069 (100%)	1 (0%)	88	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	281	ASN
1	B	180	ASN
1	B	191	ASN
1	B	281	ASN
1	C	180	ASN
1	C	281	ASN
1	D	180	ASN
1	D	191	ASN
1	D	281	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](#)

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
3	PEG	A	403	-	6,6,6	0.58	0	5,5,5	0.41	0
2	ASP	C	401	-	7,8,8	0.96	1 (14%)	6,10,10	1.41	1 (16%)
3	PEG	B	402	-	6,6,6	0.64	0	5,5,5	0.91	0
2	ASP	A	401	-	7,8,8	1.34	1 (14%)	6,10,10	1.94	2 (33%)
3	PEG	A	402	-	6,6,6	1.08	0	5,5,5	1.60	1 (20%)
3	PEG	D	402	-	6,6,6	0.56	0	5,5,5	1.15	0
2	ASP	D	401	-	7,8,8	1.51	2 (28%)	6,10,10	1.78	3 (50%)
3	PEG	C	402	-	6,6,6	0.48	0	5,5,5	0.82	0
2	ASP	B	401	-	7,8,8	1.57	2 (28%)	6,10,10	0.99	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	PEG	A	403	-	-	3/4/4/4	-
2	ASP	C	401	-	-	3/8/8/8	-
3	PEG	B	402	-	-	2/4/4/4	-
2	ASP	A	401	-	-	4/8/8/8	-
3	PEG	A	402	-	-	3/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-
2	ASP	D	401	-	-	2/8/8/8	-
3	PEG	C	402	-	-	1/4/4/4	-
2	ASP	B	401	-	-	4/8/8/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ASP	O-C	2.69	1.30	1.22
2	A	401	ASP	OD1-CG	2.52	1.30	1.22
2	D	401	ASP	CB-CG	2.45	1.57	1.51
2	B	401	ASP	CB-CG	2.19	1.56	1.51
2	C	401	ASP	OD1-CG	2.17	1.29	1.22
2	D	401	ASP	OD1-CG	2.10	1.29	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ASP	OD1-CG-CB	-3.41	112.37	122.84
3	A	402	PEG	O2-C2-C1	3.37	124.95	110.11
2	D	401	ASP	OD1-CG-CB	-2.62	114.79	122.84
2	C	401	ASP	OXT-C-O	-2.49	118.44	124.08
2	D	401	ASP	OXT-C-O	-2.46	118.50	124.08
2	D	401	ASP	OD2-CG-CB	2.18	120.78	114.00
2	A	401	ASP	OD2-CG-OD1	2.07	128.67	123.33

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	ASP	O-C-CA-N
2	C	401	ASP	O-C-CA-N
2	D	401	ASP	O-C-CA-N
2	A	401	ASP	OXT-C-CA-N
2	B	401	ASP	OXT-C-CA-N
2	D	401	ASP	OXT-C-CA-N
2	C	401	ASP	OXT-C-CA-N
3	B	402	PEG	O2-C3-C4-O4
3	D	402	PEG	C1-C2-O2-C3
3	A	403	PEG	O1-C1-C2-O2
3	D	402	PEG	C4-C3-O2-C2
2	A	401	ASP	O-C-CA-N
3	C	402	PEG	O2-C3-C4-O4
3	A	403	PEG	O2-C3-C4-O4
2	A	401	ASP	OXT-C-CA-CB
3	A	402	PEG	O2-C3-C4-O4
2	B	401	ASP	OXT-C-CA-CB
3	A	402	PEG	O1-C1-C2-O2
3	A	403	PEG	C4-C3-O2-C2
2	A	401	ASP	O-C-CA-CB
3	D	402	PEG	O1-C1-C2-O2
2	B	401	ASP	O-C-CA-CB
3	A	402	PEG	C4-C3-O2-C2
2	C	401	ASP	O-C-CA-CB
3	B	402	PEG	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	PEG	8	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 ⓘ

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(Å ²)	Q<0.9
1	A	324/328 (98%)	-0.46	8 (2%) 58 64	6, 14, 30, 50	7 (2%)
1	B	324/328 (98%)	-0.42	4 (1%) 76 81	6, 15, 32, 53	7 (2%)
1	C	324/328 (98%)	-0.41	3 (0%) 81 85	8, 15, 33, 46	8 (2%)
1	D	324/328 (98%)	-0.46	1 (0%) 90 91	7, 14, 29, 43	13 (4%)
All	All	1296/1312 (98%)	-0.44	16 (1%) 76 81	6, 14, 32, 53	35 (2%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ALA	4.1
1	D	213	GLY	3.7
1	A	28	GLY	3.3
1	A	26	THR	2.9
1	A	31[A]	ALA	2.7
1	C	31[A]	ALA	2.6
1	A	24	THR	2.5
1	B	26	THR	2.4
1	A	22	THR	2.3
1	B	31[A]	ALA	2.3
1	A	27	THR	2.3
1	C	26	THR	2.3
1	B	29	TYR	2.3
1	B	21	ALA	2.1
1	C	21	ALA	2.0
1	A	29	TYR	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 [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
3	PEG	A	402	7/7	0.79	0.18	31,41,55,56	0
3	PEG	B	402	7/7	0.80	0.17	38,40,54,57	0
3	PEG	D	402	7/7	0.80	0.16	43,54,56,58	0
3	PEG	C	402	7/7	0.81	0.14	40,49,58,65	0
3	PEG	A	403	7/7	0.82	0.14	41,45,59,63	0
2	ASP	D	401	9/9	0.97	0.05	14,17,19,21	0
2	ASP	A	401	9/9	0.97	0.06	12,15,17,18	0
2	ASP	B	401	9/9	0.97	0.05	14,17,20,23	0
2	ASP	C	401	9/9	0.98	0.04	13,16,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.