



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1ASN
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI ASPARTATE AMINO-TRANSFERASE IN TWO CONFORMATIONS: COMPARISON OF AN UNLIGANDED OPEN AND TWO LIGANDED CLOSED FORMS
Authors : Jaeger, J.; Jansonius, J.N.
Deposited on : 1993-09-16
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

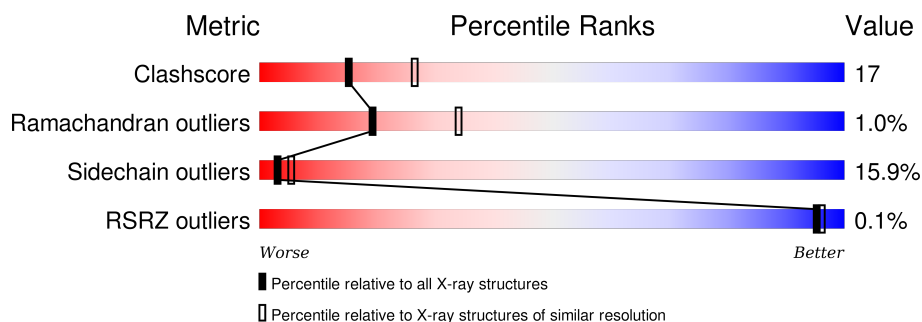
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	

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	SO4	A	410	-	-	X	X
2	SO4	B	410	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLP	A	411	-	-	-	X
3	PLP	B	411	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6406 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 ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			
1	B	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

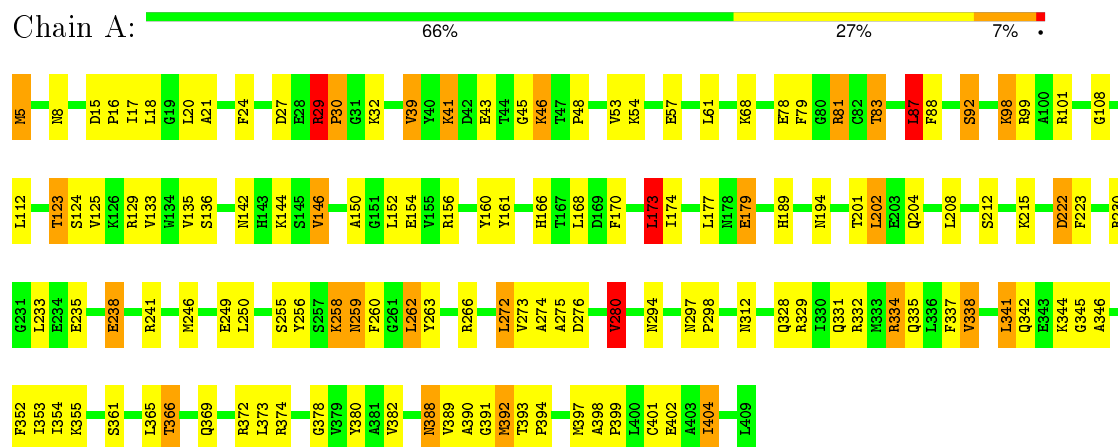
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	111	Total	O	0	0
			111	111		

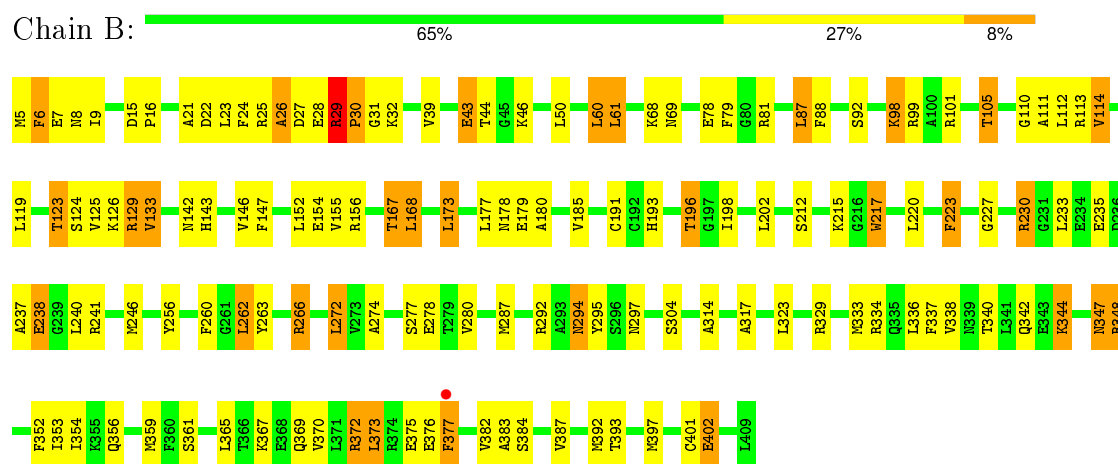
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.60 Å 79.80 Å 89.60 Å 90.00° 119.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 15.03 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 88.5 (15.03-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.51 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , (Not available) 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 37.2	EDS
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.469 for h,-k,-h-l 0.000 for -h-l,-k,l 0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 33324 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6406	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, PLP

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	0.85	0/3130	1.03	13/4240 (0.3%)
1	B	0.88	0/3130	1.02	7/4240 (0.2%)
All	All	0.86	0/6260	1.03	20/8480 (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	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	B	81	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	B	377	PHE	N-CA-C	6.93	129.72	111.00
1	A	272	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	250	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	348	ARG	NE-CZ-NH2	6.65	123.62	120.30
1	A	173	LEU	CA-CB-CG	6.61	130.51	115.30
1	B	217	TRP	CA-CB-CG	6.59	126.23	113.70
1	A	20	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	258	LYS	CB-CA-C	6.01	122.42	110.40
1	A	334	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	87	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	287	MET	CG-SD-CE	5.81	109.49	100.20
1	B	359	MET	CG-SD-CE	5.74	109.39	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	MET	CG-SD-CE	5.60	109.16	100.20
1	B	272	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	280	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	222	ASP	N-CA-C	-5.40	96.42	111.00
1	A	5	MET	CG-SD-CE	5.24	108.58	100.20
1	A	392	MET	CG-SD-CE	5.16	108.45	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	295	TYR	Sidechain

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	3069	0	3016	100	0
1	B	3069	0	3016	121	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	6	0	0
4	A	117	0	0	5	0
4	B	111	0	0	1	0
All	All	6406	0	6045	213	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 17.

All (213) 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:29:ARG:HB3	1:B:30:PRO:HD2	1.34	1.06
1:B:191:CYS:HG	1:B:223:PHE:HE1	1.07	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HH11	1:B:129:ARG:HB3	1.27	0.99
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.11	0.94
1:A:41:LYS:HB3	1:A:41:LYS:NZ	1.81	0.93
1:B:196:THR:HG22	1:B:198:ILE:H	1.31	0.93
1:B:129:ARG:NH1	1:B:129:ARG:HB3	1.84	0.92
1:B:98:LYS:HA	1:B:98:LYS:HE2	1.50	0.91
1:A:201:THR:H	1:A:204:GLN:HE21	1.21	0.88
1:B:260:PHE:HB3	1:B:262:LEU:HD22	1.58	0.85
1:A:366:THR:HG22	1:A:369:GLN:H	1.41	0.85
1:A:17:ILE:HD13	2:A:410:SO4:O4	1.77	0.83
1:B:29:ARG:HG2	1:B:377:PHE:HE2	1.44	0.81
1:A:352:PHE:HA	1:A:355:LYS:HD3	1.62	0.81
1:B:196:THR:CG2	1:B:198:ILE:H	1.94	0.80
1:A:29:ARG:HG3	1:A:30:PRO:HD2	1.63	0.79
1:A:297:ASN:O	1:B:266:ARG:HD3	1.81	0.79
1:B:167:THR:HG22	1:B:168:LEU:H	1.48	0.79
1:A:29:ARG:HG3	1:A:30:PRO:CD	2.12	0.79
1:B:29:ARG:CB	1:B:30:PRO:HD2	2.14	0.78
1:A:123:THR:HG22	1:A:125:VAL:H	1.48	0.78
1:B:99:ARG:HG2	1:B:274:ALA:O	1.85	0.76
1:B:105:THR:HG21	1:B:111:ALA:HB2	1.66	0.76
1:B:123:THR:CG2	1:B:125:VAL:HG23	2.17	0.75
1:B:123:THR:HG22	1:B:125:VAL:H	1.51	0.75
1:B:333:MET:HE2	1:B:393:THR:HA	1.68	0.74
1:A:41:LYS:NZ	1:A:45:GLY:HA2	2.03	0.74
1:A:41:LYS:HB3	1:A:41:LYS:HZ2	1.52	0.72
1:A:123:THR:CG2	1:A:125:VAL:HG23	2.19	0.72
1:A:99:ARG:HG2	1:A:274:ALA:O	1.89	0.71
1:B:333:MET:HE2	1:B:393:THR:CA	2.20	0.70
1:A:328:GLN:O	1:A:332:ARG:HD3	1.91	0.69
1:B:110:GLY:O	1:B:114:VAL:HG13	1.93	0.68
1:B:98:LYS:HA	1:B:98:LYS:CE	2.19	0.68
1:B:29:ARG:HG2	1:B:377:PHE:CE2	2.29	0.67
1:B:29:ARG:HB3	1:B:30:PRO:CD	2.15	0.66
1:B:375:GLU:C	1:B:377:PHE:H	1.99	0.66
1:A:366:THR:HG22	1:A:369:GLN:N	2.10	0.66
1:A:341:LEU:HD11	1:A:404:ILE:HG12	1.76	0.66
1:B:230:ARG:NH1	1:B:235:GLU:HB3	2.09	0.66
1:A:39:VAL:HG22	1:A:263:TYR:CE1	2.30	0.66
1:A:79:PHE:O	1:A:83:THR:HG23	1.96	0.65
1:A:123:THR:CG2	1:A:125:VAL:H	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:O	1:A:238:GLU:HG3	1.97	0.64
1:B:196:THR:CG2	1:B:198:ILE:HB	2.28	0.64
1:A:21:ALA:O	1:A:24:PHE:HB3	1.98	0.63
1:A:98:LYS:HE3	1:A:101:ARG:HD3	1.79	0.63
1:B:348:ARG:HH11	1:B:348:ARG:CG	2.13	0.62
1:A:39:VAL:HG21	1:B:69:ASN:ND2	2.15	0.62
1:A:337:PHE:HD1	1:A:397:MET:HE2	1.64	0.62
1:A:98:LYS:HE2	1:A:98:LYS:O	1.99	0.61
1:B:123:THR:CG2	1:B:125:VAL:H	2.13	0.61
1:A:68:LYS:O	1:B:263:TYR:HB2	2.01	0.61
1:B:29:ARG:CG	1:B:377:PHE:HE2	2.13	0.61
1:B:143:HIS:O	1:B:147:PHE:HD2	1.84	0.61
1:A:24:PHE:O	1:A:27:ASP:HB3	2.01	0.61
1:A:266:ARG:HD2	1:B:297:ASN:O	2.00	0.61
1:A:388:ASN:HD22	1:A:388:ASN:C	2.04	0.60
1:A:388:ASN:ND2	1:A:390:ALA:H	2.01	0.59
1:B:129:ARG:CB	1:B:129:ARG:NH1	2.64	0.59
1:A:27:ASP:OD1	1:A:29:ARG:HB2	2.03	0.58
1:A:201:THR:H	1:A:204:GLN:NE2	1.96	0.58
1:B:129:ARG:NH2	1:B:156:ARG:HG2	2.19	0.58
1:A:123:THR:HG21	1:A:125:VAL:HG23	1.84	0.57
1:B:123:THR:HG21	1:B:125:VAL:HG23	1.85	0.57
1:B:202:LEU:HD13	1:B:238:GLU:CG	2.35	0.56
1:B:193:HIS:ND1	1:B:196:THR:HB	2.19	0.56
1:B:60:LEU:HD21	1:B:304:SER:HB3	1.87	0.56
1:B:334:ARG:O	1:B:338:VAL:HG13	2.05	0.56
1:B:344:LYS:HD3	1:B:402:GLU:HG3	1.87	0.56
1:B:196:THR:HG23	1:B:198:ILE:CG1	2.36	0.55
1:B:143:HIS:O	1:B:147:PHE:CD2	2.58	0.55
1:B:27:ASP:OD1	1:B:29:ARG:HB2	2.07	0.55
1:A:334:ARG:O	1:A:338:VAL:HG13	2.07	0.55
1:A:338:VAL:HG11	1:A:354:ILE:HG13	1.88	0.55
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.89	0.55
1:B:39:VAL:HG22	1:B:263:TYR:CE1	2.42	0.55
1:B:375:GLU:C	1:B:377:PHE:N	2.60	0.55
1:B:6:PHE:HA	1:B:9:ILE:HD12	1.88	0.54
1:A:41:LYS:HZ2	1:A:45:GLY:HA2	1.72	0.54
1:A:41:LYS:HB3	1:A:41:LYS:HZ1	1.72	0.54
1:B:370:VAL:HG21	1:B:383:ALA:HA	1.89	0.54
1:A:378:GLY:O	1:A:380:TYR:HD1	1.91	0.54
1:B:202:LEU:HD13	1:B:238:GLU:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:SER:HA	1:B:217:TRP:CD1	2.44	0.53
1:B:142:ASN:O	1:B:146:VAL:HG13	2.09	0.53
1:B:129:ARG:CZ	1:B:156:ARG:HG3	2.39	0.52
1:A:388:ASN:HD22	1:A:390:ALA:H	1.57	0.52
1:B:397:MET:HE2	1:B:401:CYS:SG	2.49	0.52
1:B:24:PHE:O	1:B:32:LYS:NZ	2.43	0.52
1:A:24:PHE:O	1:A:32:LYS:NZ	2.39	0.51
1:B:230:ARG:HH11	1:B:235:GLU:HB3	1.73	0.51
1:A:382:VAL:HG13	4:A:484:HOH:O	2.11	0.51
1:A:27:ASP:HB2	1:A:380:TYR:OH	2.10	0.51
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.76	0.51
1:A:161:TYR:OH	1:A:166:HIS:HD2	1.93	0.51
1:B:79:PHE:CZ	1:B:256:TYR:CE2	2.98	0.51
1:B:6:PHE:N	1:B:6:PHE:CD1	2.79	0.51
1:B:21:ALA:O	1:B:25:ARG:HG2	2.11	0.51
1:B:277:SER:HA	1:B:280:VAL:HG12	1.93	0.50
1:A:334:ARG:HG2	1:A:389:VAL:HG11	1.92	0.50
1:B:294:ASN:ND2	4:B:511:HOH:O	2.45	0.50
1:B:196:THR:CG2	1:B:198:ILE:N	2.72	0.50
1:A:108:GLY:HA3	1:A:255:SER:HB2	1.93	0.49
1:A:29:ARG:NE	4:A:442:HOH:O	2.45	0.49
1:A:41:LYS:HE3	1:A:391:GLY:HA2	1.94	0.49
1:A:24:PHE:CE1	1:A:32:LYS:HD2	2.48	0.48
1:B:21:ALA:O	1:B:24:PHE:HB3	2.13	0.48
1:A:179:GLU:HG3	1:A:179:GLU:O	2.13	0.48
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.96	0.48
1:B:266:ARG:NE	1:B:266:ARG:HA	2.28	0.48
1:A:150:ALA:HA	4:A:510:HOH:O	2.14	0.48
1:B:196:THR:HG23	1:B:198:ILE:CB	2.43	0.48
1:B:129:ARG:NH2	1:B:154:GLU:HG3	2.29	0.48
1:B:344:LYS:HA	1:B:344:LYS:HE2	1.96	0.47
1:B:338:VAL:HG11	1:B:354:ILE:HG13	1.97	0.47
1:A:142:ASN:O	1:A:146:VAL:HG13	2.15	0.47
1:B:333:MET:CE	1:B:392:MET:C	2.83	0.47
1:B:101:ARG:HG2	1:B:280:VAL:HG22	1.96	0.47
1:A:17:ILE:CD1	2:A:410:SO4:O4	2.56	0.47
1:A:39:VAL:HG22	1:A:263:TYR:CZ	2.50	0.47
1:A:249:GLU:OE2	1:B:5:MET:O	2.32	0.47
1:B:129:ARG:CZ	1:B:156:ARG:CG	2.92	0.47
1:A:87:LEU:O	1:A:241:ARG:HD2	2.15	0.47
1:B:352:PHE:CE2	1:B:353:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:HD1	1:A:397:MET:CE	2.27	0.46
1:A:88:PHE:O	1:A:92:SER:HB2	2.14	0.46
1:A:46:LYS:O	1:A:48:PRO:HD3	2.15	0.46
1:B:29:ARG:CB	1:B:377:PHE:HE2	2.28	0.46
1:B:87:LEU:O	1:B:241:ARG:HD2	2.16	0.46
1:A:123:THR:HG23	1:A:125:VAL:HG23	1.98	0.46
1:B:173:LEU:C	1:B:173:LEU:HD12	2.36	0.46
1:A:345:GLY:O	1:A:346:ALA:C	2.54	0.46
1:B:43:GLU:CD	1:B:43:GLU:H	2.19	0.46
1:B:180:ALA:O	1:B:217:TRP:HZ3	1.99	0.46
1:A:202:LEU:HD22	1:A:202:LEU:O	2.16	0.45
1:A:29:ARG:HH11	1:A:29:ARG:HA	1.82	0.45
1:A:208:LEU:O	1:A:212:SER:HB2	2.17	0.45
1:A:276:ASP:O	1:A:280:VAL:HG22	2.16	0.45
1:B:344:LYS:CD	1:B:402:GLU:HG3	2.47	0.45
1:B:340:THR:O	1:B:344:LYS:HB2	2.16	0.45
1:B:372:ARG:O	1:B:376:GLU:HB2	2.17	0.45
1:A:341:LEU:HD11	1:A:404:ILE:CG1	2.43	0.45
1:A:144:LYS:HB2	1:A:144:LYS:HE3	1.71	0.45
1:B:126:LYS:HE2	1:B:126:LYS:HB3	1.48	0.45
1:B:29:ARG:CB	1:B:30:PRO:CD	2.86	0.44
1:A:393:THR:HB	1:A:394:PRO:HD2	1.98	0.44
1:B:25:ARG:HA	1:B:28:GLU:OE1	2.17	0.44
1:A:344:LYS:HG3	1:A:402:GLU:HG2	1.99	0.44
1:A:397:MET:HA	1:A:397:MET:HE3	1.99	0.44
1:B:237:ALA:O	1:B:241:ARG:HD3	2.17	0.44
1:B:27:ASP:O	1:B:29:ARG:HD3	2.18	0.44
1:A:123:THR:HG21	1:A:125:VAL:CG2	2.45	0.44
1:B:60:LEU:HD21	1:B:304:SER:CB	2.46	0.44
1:A:222:ASP:OD2	3:A:411:PLP:N1	2.50	0.44
1:A:398:ALA:HB3	1:A:399:PRO:CD	2.47	0.44
1:B:129:ARG:CZ	1:B:154:GLU:HG3	2.48	0.44
1:A:123:THR:CG2	1:A:124:SER:N	2.81	0.44
1:A:341:LEU:HD13	1:A:401:CYS:SG	2.58	0.44
1:B:196:THR:HG21	1:B:198:ILE:HB	2.00	0.44
1:A:388:ASN:HD22	1:A:389:VAL:N	2.14	0.44
1:A:123:THR:HG23	1:A:124:SER:N	2.33	0.43
1:A:329:ARG:NH2	1:A:392:MET:O	2.51	0.43
1:B:333:MET:HE3	1:B:392:MET:C	2.38	0.43
1:B:347:ASN:HD22	1:B:348:ARG:N	2.17	0.43
1:A:331:GLN:HB2	4:A:447:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:O	1:A:83:THR:CG2	2.65	0.43
1:A:388:ASN:ND2	1:A:388:ASN:C	2.72	0.43
1:A:344:LYS:CG	1:A:402:GLU:HG2	2.49	0.43
1:B:123:THR:CG2	1:B:124:SER:N	2.82	0.43
1:B:337:PHE:HD1	1:B:397:MET:CE	2.32	0.43
1:B:5:MET:C	1:B:7:GLU:H	2.23	0.43
1:B:382:VAL:HG12	1:B:384:SER:H	1.84	0.43
1:B:44:THR:O	1:B:44:THR:HG22	2.19	0.43
1:A:98:LYS:CE	1:A:101:ARG:HD3	2.46	0.42
1:A:53:VAL:O	1:A:57:GLU:HG3	2.19	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.64	0.42
1:B:375:GLU:O	1:B:377:PHE:CD1	2.72	0.42
1:A:29:ARG:CG	1:A:30:PRO:CD	2.90	0.42
1:A:99:ARG:CG	1:A:274:ALA:O	2.64	0.42
1:B:344:LYS:CA	1:B:344:LYS:HE2	2.49	0.42
1:B:22:ASP:O	1:B:26:ALA:HB2	2.19	0.42
1:A:39:VAL:HG21	1:B:69:ASN:HD21	1.82	0.42
4:A:513:HOH:O	1:B:46:LYS:HE3	2.20	0.42
1:B:196:THR:CG2	1:B:198:ILE:CB	2.96	0.42
1:B:30:PRO:HB2	1:B:31:GLY:H	1.63	0.42
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.88	0.42
1:B:314:ALA:O	1:B:317:ALA:HB3	2.20	0.42
1:A:135:VAL:HG23	1:A:136:SER:O	2.19	0.41
1:B:88:PHE:O	1:B:92:SER:HB2	2.20	0.41
1:A:329:ARG:NH2	1:A:393:THR:HG22	2.35	0.41
1:B:356:GLN:NE2	1:B:361:SER:OG	2.53	0.41
1:B:99:ARG:CG	1:B:274:ALA:O	2.64	0.41
1:B:180:ALA:HB3	1:B:217:TRP:CH2	2.55	0.41
1:B:369:GLN:O	1:B:373:LEU:HB2	2.20	0.41
1:A:170:PHE:O	1:A:173:LEU:HB3	2.20	0.41
1:B:133:VAL:HB	1:B:185:VAL:HB	2.03	0.41
1:A:99:ARG:HD2	1:A:275:ALA:O	2.21	0.41
1:B:262:LEU:HA	1:B:262:LEU:HD12	1.88	0.41
1:B:123:THR:HG23	1:B:124:SER:N	2.35	0.41
1:B:15:ASP:HA	1:B:16:PRO:HD2	1.91	0.41
1:A:189:HIS:CD2	1:A:194:ASN:H	2.39	0.41
1:B:333:MET:CE	1:B:393:THR:CA	2.95	0.41
1:A:263:TYR:HB2	1:B:68:LYS:O	2.21	0.41
1:B:227:GLY:HA3	1:B:323:LEU:HD21	2.03	0.41
1:B:196:THR:HG23	1:B:198:ILE:HD12	2.02	0.40
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HG	1:B:397:MET:HG2	2.04	0.40
1:A:78:GLU:CD	1:A:78:GLU:H	2.24	0.40
1:B:348:ARG:HH11	1:B:348:ARG:HG3	1.84	0.40
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.81	0.40
1:B:180:ALA:HB3	1:B:217:TRP:CZ3	2.57	0.40
1:A:123:THR:CG2	1:A:125:VAL:CG2	2.96	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	394/396 (100%)	377 (96%)	12 (3%)	5 (1%)	15	26
1	B	394/396 (100%)	373 (95%)	18 (5%)	3 (1%)	24	41
All	All	788/792 (100%)	750 (95%)	30 (4%)	8 (1%)	19	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	30	PRO
1	B	30	PRO
1	B	26	ALA
1	A	92	SER
1	A	160	TYR
1	B	29	ARG
1	A	16	PRO

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	320/320 (100%)	269 (84%)	51 (16%)	3	5
1	B	320/320 (100%)	269 (84%)	51 (16%)	3	5
All	All	640/640 (100%)	538 (84%)	102 (16%)	3	5

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	8	ASN
1	A	29	ARG
1	A	39	VAL
1	A	41	LYS
1	A	43	GLU
1	A	46	LYS
1	A	54	LYS
1	A	61	LEU
1	A	81	ARG
1	A	83	THR
1	A	87	LEU
1	A	98	LYS
1	A	112	LEU
1	A	123	THR
1	A	129	ARG
1	A	133	VAL
1	A	146	VAL
1	A	152	LEU
1	A	154	GLU
1	A	156	ARG
1	A	168	LEU
1	A	173	LEU
1	A	174	ILE
1	A	179	GLU
1	A	202	LEU
1	A	215	LYS

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Mol	Chain	Res	Type
1	A	223	PHE
1	A	230	ARG
1	A	233	LEU
1	A	238	GLU
1	A	258	LYS
1	A	259	ASN
1	A	262	LEU
1	A	272	LEU
1	A	273	VAL
1	A	280	VAL
1	A	298	PRO
1	A	312	ASN
1	A	335	GLN
1	A	338	VAL
1	A	341	LEU
1	A	342	GLN
1	A	353	ILE
1	A	361	SER
1	A	365	LEU
1	A	366	THR
1	A	372	ARG
1	A	374	ARG
1	A	388	ASN
1	A	404	ILE
1	B	6	PHE
1	B	8	ASN
1	B	23	LEU
1	B	29	ARG
1	B	43	GLU
1	B	50	LEU
1	B	60	LEU
1	B	61	LEU
1	B	78	GLU
1	B	87	LEU
1	B	98	LYS
1	B	105	THR
1	B	112	LEU
1	B	113	ARG
1	B	114	VAL
1	B	119	LEU
1	B	123	THR
1	B	129	ARG

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Mol	Chain	Res	Type
1	B	133	VAL
1	B	152	LEU
1	B	155	VAL
1	B	167	THR
1	B	168	LEU
1	B	173	LEU
1	B	178	ASN
1	B	179	GLU
1	B	196	THR
1	B	215	LYS
1	B	220	LEU
1	B	223	PHE
1	B	230	ARG
1	B	233	LEU
1	B	238	GLU
1	B	240	LEU
1	B	246	MET
1	B	262	LEU
1	B	266	ARG
1	B	272	LEU
1	B	278	GLU
1	B	292	ARG
1	B	294	ASN
1	B	329	ARG
1	B	342	GLN
1	B	344	LYS
1	B	347	ASN
1	B	365	LEU
1	B	367	LYS
1	B	372	ARG
1	B	373	LEU
1	B	387	VAL
1	B	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	166	HIS
1	A	178	ASN
1	A	189	HIS
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	206	GLN
1	A	226	GLN
1	A	259	ASN
1	A	312	ASN
1	A	328	GLN
1	A	335	GLN
1	A	339	ASN
1	A	342	GLN
1	A	388	ASN
1	B	69	ASN
1	B	148	ASN
1	B	178	ASN
1	B	206	GLN
1	B	226	GLN
1	B	247	HIS
1	B	294	ASN
1	B	328	GLN
1	B	335	GLN
1	B	347	ASN
1	B	356	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	SO4	A	410	-	4,4,4	1.90	2 (50%)	6,6,6	0.96	0
3	PLP	A	411	1	15,15,16	2.13	2 (13%)	21,22,23	2.35	3 (14%)
2	SO4	B	410	-	4,4,4	1.67	1 (25%)	6,6,6	0.70	0
3	PLP	B	411	1	15,15,16	2.03	2 (13%)	21,22,23	1.84	2 (9%)

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	SO4	A	410	-	-	0/0/0/0	0/0/0/0
3	PLP	A	411	1	-	0/6/6/8	0/1/1/1
2	SO4	B	410	-	-	0/0/0/0	0/0/0/0
3	PLP	B	411	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	411	PLP	C3-C2	-6.81	1.36	1.40
3	B	411	PLP	C3-C2	-6.48	1.36	1.40
3	A	411	PLP	C5-C4	-2.30	1.37	1.40
3	B	411	PLP	P-O2P	-2.16	1.47	1.54
2	A	410	SO4	O2-S	2.60	1.56	1.47
2	B	410	SO4	O2-S	2.64	1.56	1.47
2	A	410	SO4	O4-S	2.75	1.57	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	411	PLP	C5-C6-N1	-2.29	119.89	123.86
3	B	411	PLP	C5-C6-N1	-2.07	120.27	123.86
3	A	411	PLP	O4P-P-O1P	2.22	112.79	107.14
3	B	411	PLP	O4P-C5A-C5	7.59	121.55	108.99
3	A	411	PLP	O4P-C5A-C5	9.54	124.77	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	410	SO4	2	0
3	A	411	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/396 (100%)	-0.83	0 100 100	8, 27, 72, 109	0
1	B	396/396 (100%)	-0.81	1 (0%) 94 95	9, 27, 74, 124	0
All	All	792/792 (100%)	-0.82	1 (0%) 95 96	8, 27, 73, 124	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	PHE	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	410	5/5	0.95	0.53	16.40	10,12,16,16	0
2	SO4	B	410	5/5	0.83	0.52	7.08	8,11,13,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PLP	A	411	15/16	0.95	0.13	3.95	12,25,29,32	0
3	PLP	B	411	15/16	0.97	0.13	2.72	8,21,28,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.