



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:34 PM UTC

PDB ID : 2X5D / pdb_00002x5d
Title : Crystal Structure of a probable aminotransferase from *Pseudomonas aeruginosa*
Authors : Oke, M.; Carter, L.G.; Johnson, K.A.; Liu, H.; McMahon, S.A.; White, M.F.; Naismith, J.H.
Deposited on : 2010-02-08
Resolution : 2.25 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

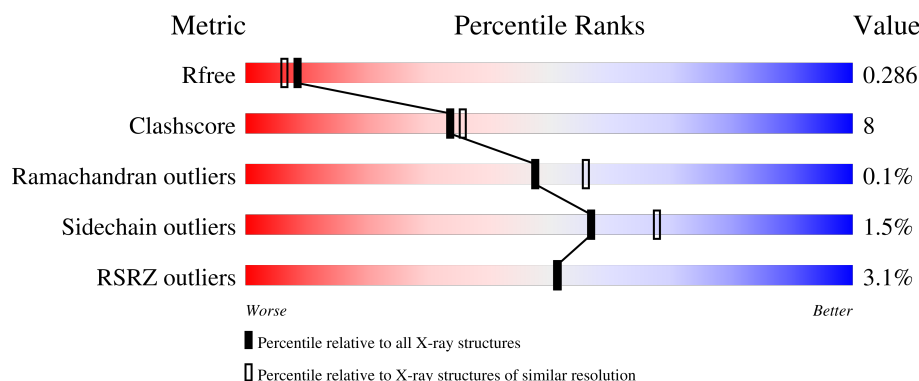
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	412	2% 74% 15% • 10%
1	B	412	3% 75% 14% • 11%
1	C	412	3% 74% 15% • 10%
1	D	412	2% 80% 12% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12078 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 PROBABLE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2914	1862	513	524	15			
1	B	367	Total	C	N	O	S	0	0	0
			2887	1844	510	518	15			
1	C	371	Total	C	N	O	S	0	0	0
			2920	1864	517	524	15			
1	D	380	Total	C	N	O	S	0	0	0
			2986	1904	528	539	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q9HV83
B	0	GLY	-	expression tag	UNP Q9HV83
C	0	GLY	-	expression tag	UNP Q9HV83
D	0	GLY	-	expression tag	UNP Q9HV83

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

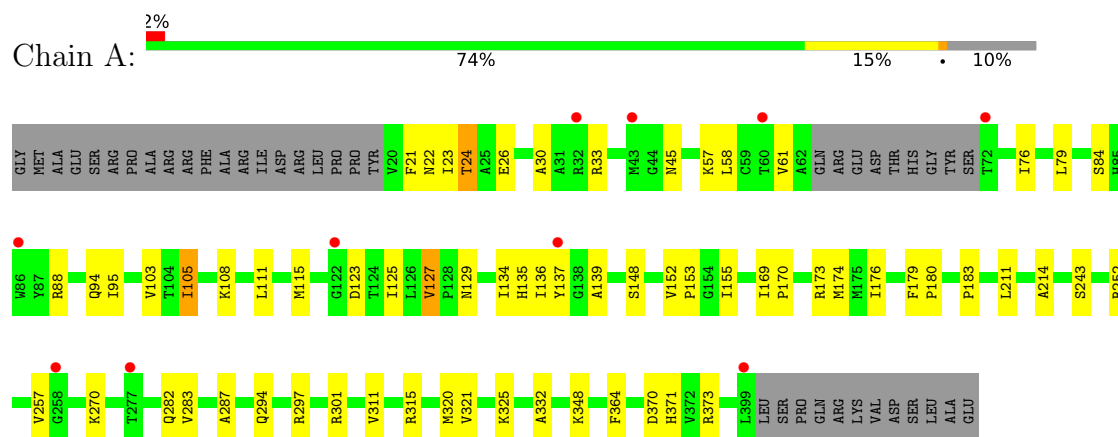
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total	O	0	0
			84	84		
4	B	57	Total	O	0	0
			57	57		
4	C	48	Total	O	0	0
			48	48		
4	D	96	Total	O	0	0
			96	96		

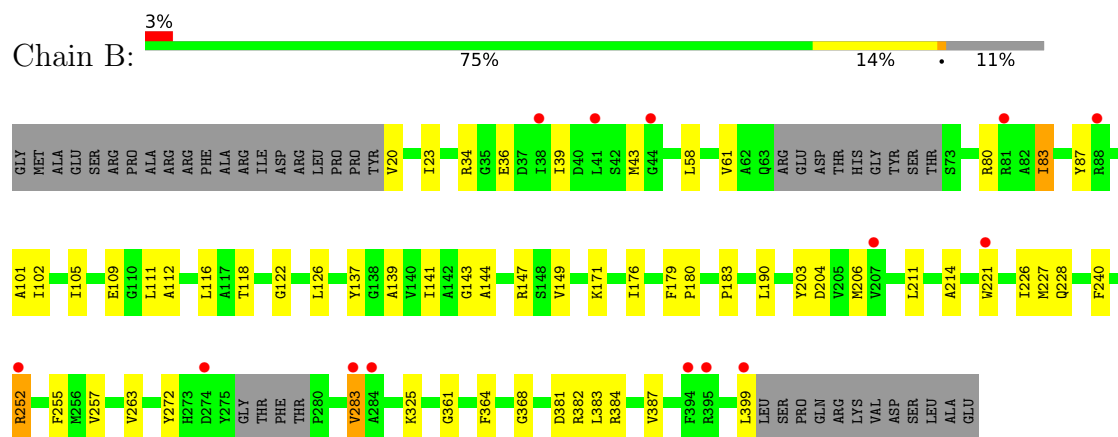
3 Residue-property plots [i](#)

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.

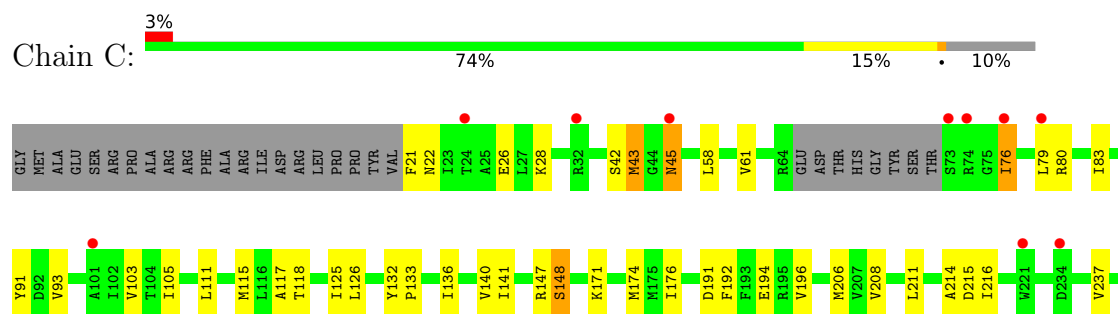
• Molecule 1: PROBABLE AMINOTRANSFERASE



• Molecule 1: PROBABLE AMINOTRANSFERASE

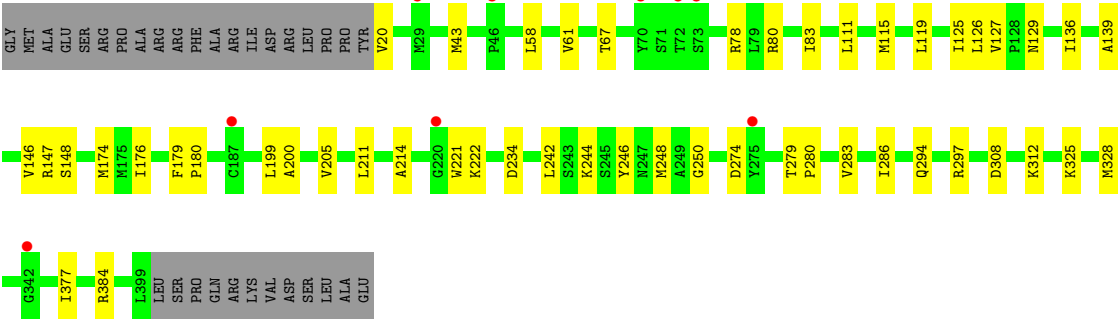
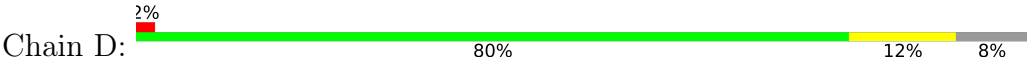


• Molecule 1: PROBABLE AMINOTRANSFERASE





● Molecule 1: PROBABLE AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.86Å 173.81Å 76.97Å 90.00° 114.51° 90.00°	Depositor
Resolution (Å)	28.89 – 2.25 28.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.4 (28.89-2.25) 50.2 (28.89-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.216 , 0.244 0.261 , 0.286	Depositor DCC
R_{free} test set	1853 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.953 for H, K, L 0.047 for -H, -K, H+L	Depositor
Outliers	0 of 36793 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12078	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.92% 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: PLP, SO4

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	0.79	0/2982	0.93	3/4044 (0.1%)
1	B	0.66	0/2953	0.84	1/4001 (0.0%)
1	C	0.68	0/2988	0.87	1/4050 (0.0%)
1	D	0.80	0/3057	0.91	0/4147
All	All	0.73	0/11980	0.89	5/16242 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	MET	N-CA-C	-7.75	100.34	110.33
1	B	149	VAL	N-CA-C	6.58	114.64	107.60
1	A	137	TYR	N-CA-C	5.84	117.32	111.07
1	A	311	VAL	CB-CA-C	-5.38	105.09	111.97
1	A	243	SER	N-CA-C	5.17	117.31	111.11

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	2914	0	2919	48	0
1	B	2887	0	2896	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2920	0	2926	52	0
1	D	2986	0	2980	44	0
2	A	15	0	6	1	0
2	D	16	0	8	2	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	20	0	0	1	0
3	D	15	0	0	1	0
4	A	84	0	0	1	0
4	B	57	0	0	0	0
4	C	48	0	0	2	0
4	D	96	0	0	3	0
All	All	12078	0	11735	180	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 (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:HG22	1:A:252:ARG:HG2	1.35	1.08
1:B:83:ILE:CD1	1:B:101:ALA:HB1	1.93	0.98
1:B:34:ARG:NH1	1:B:36:GLU:OE1	2.00	0.94
1:C:111:LEU:HG	1:C:115:MET:HE3	1.50	0.94
1:A:103:VAL:O	1:A:270:LYS:NZ	2.03	0.90
1:A:115:MET:HE1	1:A:176:ILE:HD11	1.52	0.90
1:B:118:THR:HG21	1:B:206:MET:HE1	1.57	0.84
1:B:83:ILE:HD11	1:B:101:ALA:HB1	1.59	0.82
1:A:115:MET:HE1	1:A:176:ILE:CD1	2.10	0.81
1:B:118:THR:HG21	1:B:206:MET:CE	2.10	0.80
1:B:111:LEU:HD21	1:B:176:ILE:HD13	1.68	0.76
1:D:221:TRP:CZ3	1:D:325:LYS:NZ	2.54	0.76
1:A:105:ILE:HG22	1:A:252:ARG:CG	2.13	0.75
1:A:58:LEU:HD21	1:D:58:LEU:CD2	2.18	0.73
1:B:83:ILE:CD1	1:B:101:ALA:CB	2.67	0.72
1:B:83:ILE:HD11	1:B:101:ALA:CB	2.21	0.71
1:B:211:LEU:HG	1:B:214:ALA:HB2	1.71	0.70
1:B:221:TRP:CZ3	1:B:325:LYS:HD2	2.26	0.70
1:C:117:ALA:HB1	1:C:265:ALA:HB1	1.73	0.70
1:A:23:ILE:HG21	1:A:348:LYS:HZ1	1.56	0.69
1:C:105:ILE:HG22	1:C:105:ILE:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HD23	1:C:103:VAL:HG21	1.76	0.68
1:D:80:ARG:HA	1:D:83:ILE:HD12	1.78	0.66
1:A:115:MET:HE3	1:A:139:ALA:HB2	1.79	0.65
1:A:94:GLN:HA	1:A:94:GLN:OE1	1.97	0.64
1:D:43:MET:O	1:D:377:ILE:HD13	1.97	0.64
1:C:147:ARG:NH1	1:C:148:SER:O	2.30	0.64
1:D:211:LEU:HG	1:D:214:ALA:HB2	1.79	0.64
1:B:118:THR:CG2	1:B:206:MET:HE1	2.27	0.63
1:B:240:PHE:HB3	1:B:255:PHE:CE2	2.34	0.63
1:A:21:PHE:HA	1:A:24:THR:HG23	1.80	0.62
1:B:83:ILE:HG22	1:B:255:PHE:CE1	2.34	0.62
1:D:115:MET:SD	1:D:174:MET:HE1	2.40	0.62
1:B:111:LEU:HD21	1:B:176:ILE:CD1	2.30	0.62
1:B:226:ILE:HG23	1:B:227:MET:HE2	1.81	0.62
1:D:200:ALA:HB1	1:D:205:VAL:O	2.00	0.61
1:A:294:GLN:OE1	1:A:297:ARG:NH2	2.33	0.61
1:A:45:ASN:OD1	2:A:1400:PLP:N1	2.34	0.60
1:D:242:LEU:HD23	1:D:248:MET:CE	2.31	0.60
1:A:58:LEU:HD21	1:D:58:LEU:HD21	1.83	0.60
1:C:216:ILE:HD12	1:C:303:TYR:CD2	2.37	0.59
1:C:384:ARG:O	1:C:388:ARG:HG3	2.02	0.59
1:D:244:LYS:HZ1	2:D:1400:PLP:C4A	2.15	0.59
1:C:58:LEU:HD12	1:C:251:TRP:CZ3	2.37	0.59
1:A:315:ARG:O	1:A:320:MET:HE1	2.03	0.59
1:B:80:ARG:O	1:B:83:ILE:HG13	2.04	0.58
1:B:83:ILE:HG22	1:B:255:PHE:CZ	2.39	0.58
1:C:42:SER:OG	1:C:43:MET:N	2.32	0.57
1:A:123:ASP:CG	1:A:173:ARG:HD3	2.30	0.57
1:A:61:VAL:HG21	1:A:283:VAL:HG11	1.85	0.57
1:C:58:LEU:C	1:C:58:LEU:HD23	2.30	0.57
1:C:91:TYR:O	1:C:93:VAL:HG23	2.05	0.57
1:D:221:TRP:HZ3	1:D:325:LYS:HZ1	1.40	0.57
1:D:179:PHE:HA	1:D:180:PRO:C	2.30	0.56
1:A:108:LYS:HG3	1:A:134:ILE:HG21	1.87	0.56
1:C:171:LYS:HG3	4:C:2019:HOH:O	2.04	0.56
1:D:174:MET:HE3	1:D:176:ILE:HD11	1.87	0.56
1:A:211:LEU:HG	1:A:214:ALA:HB2	1.87	0.56
1:B:83:ILE:CG2	1:B:255:PHE:CE1	2.88	0.56
1:A:179:PHE:HA	1:A:180:PRO:C	2.31	0.55
1:B:171:LYS:HD2	1:B:203:TYR:O	2.06	0.55
1:D:78:ARG:NH1	4:D:2016:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:VAL:HG21	1:C:380:ARG:HG2	1.89	0.54
1:C:118:THR:HG21	1:C:206:MET:HE1	1.90	0.54
1:D:129:ASN:HB2	1:D:148:SER:HB2	1.90	0.53
1:B:116:LEU:HD22	1:C:141:ILE:HD13	1.89	0.53
1:C:216:ILE:HD12	1:C:303:TYR:HD2	1.74	0.53
1:C:126:LEU:HD23	1:C:147:ARG:HB3	1.90	0.53
1:C:58:LEU:HD23	1:C:58:LEU:O	2.09	0.53
1:B:102:ILE:HB	1:B:263:VAL:HG13	1.90	0.53
1:C:191:ASP:HA	1:C:194:GLU:HG2	1.91	0.53
1:A:127:VAL:O	1:A:148:SER:HA	2.09	0.53
1:C:206:MET:HE2	1:C:262:LEU:HD21	1.90	0.52
1:C:259:ASN:O	1:C:263:VAL:HG23	2.09	0.52
1:C:42:SER:C	1:C:43:MET:O	2.49	0.52
1:B:118:THR:HG21	1:B:206:MET:HE3	1.90	0.52
1:C:43:MET:HG3	1:C:45:ASN:OD1	2.09	0.52
1:B:116:LEU:CD2	1:C:141:ILE:HD13	2.40	0.52
1:D:78:ARG:HG2	1:D:286:ILE:HD13	1.92	0.52
1:A:301:ARG:NH2	4:A:2059:HOH:O	2.42	0.51
1:C:248:MET:HE3	1:C:251:TRP:CE3	2.44	0.51
1:A:23:ILE:HG21	1:A:348:LYS:NZ	2.26	0.51
1:D:115:MET:HE3	1:D:139:ALA:HB2	1.92	0.51
1:C:211:LEU:HG	1:C:214:ALA:HB2	1.93	0.51
1:B:58:LEU:HD21	1:C:58:LEU:HD21	1.93	0.50
1:B:179:PHE:HA	1:B:180:PRO:C	2.36	0.50
1:B:83:ILE:HG21	1:B:255:PHE:CD1	2.46	0.50
1:C:215:ASP:HB2	1:C:245:SER:OG	2.12	0.50
1:C:21:PHE:N	4:C:2001:HOH:O	2.44	0.49
1:C:61:VAL:HG21	1:C:283:VAL:HG11	1.93	0.49
1:C:76:ILE:HG22	1:C:79:LEU:H	1.76	0.49
1:B:381:ASP:OD1	1:B:384:ARG:NH2	2.45	0.49
1:D:221:TRP:CD1	1:D:222:LYS:O	2.66	0.49
1:A:125:ILE:CD1	1:A:176:ILE:HD12	2.43	0.49
1:A:125:ILE:HD12	1:A:176:ILE:HD12	1.95	0.49
1:A:88:ARG:NE	1:A:94:GLN:HE22	2.11	0.48
1:A:111:LEU:O	1:A:115:MET:HG2	2.13	0.48
1:C:111:LEU:HD21	1:C:176:ILE:HD13	1.94	0.48
1:B:87:TYR:CZ	1:B:257:VAL:HG21	2.48	0.48
1:D:119:LEU:HD11	1:D:174:MET:CE	2.43	0.48
1:D:246:TYR:HB2	1:D:248:MET:HE2	1.94	0.48
1:D:242:LEU:HD23	1:D:248:MET:HE3	1.95	0.48
1:A:129:ASN:HB2	1:A:148:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:O	1:A:26:GLU:HG2	2.14	0.47
1:A:58:LEU:HD21	1:D:58:LEU:HD22	1.94	0.47
1:D:58:LEU:C	1:D:58:LEU:HD23	2.40	0.47
1:A:30:ALA:HA	1:A:33:ARG:HD3	1.97	0.47
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.96	0.47
1:C:384:ARG:O	1:C:388:ARG:CG	2.63	0.47
1:D:221:TRP:CD1	1:D:222:LYS:N	2.83	0.47
1:D:250:GLY:N	4:D:2067:HOH:O	2.47	0.47
1:C:80:ARG:HA	1:C:83:ILE:HD12	1.97	0.47
1:C:133:PRO:HB2	1:C:136:ILE:HD12	1.97	0.47
1:D:308:ASP:O	1:D:312:LYS:HG2	2.15	0.47
1:C:111:LEU:CG	1:C:115:MET:HE3	2.34	0.46
1:D:279:THR:HB	1:D:280:PRO:HD3	1.96	0.46
1:D:125:ILE:CG2	1:D:174:MET:HE2	2.44	0.46
1:C:42:SER:HB3	1:C:357:SER:OG	2.16	0.46
1:D:136:ILE:HG23	1:D:146:VAL:HG21	1.98	0.46
1:B:126:LEU:HD23	1:B:147:ARG:HB2	1.97	0.45
1:C:28:LYS:NZ	1:C:43:MET:HE2	2.31	0.45
1:A:169:ILE:HA	1:A:170:PRO:C	2.41	0.45
1:B:83:ILE:CG2	1:B:255:PHE:CD1	3.00	0.45
1:B:139:ALA:HA	1:B:144:ALA:HB3	1.98	0.45
1:B:87:TYR:CE1	1:B:257:VAL:HG21	2.52	0.45
1:C:313:GLY:HA3	1:C:387:VAL:HG11	1.98	0.45
1:A:23:ILE:CG2	1:A:348:LYS:NZ	2.81	0.44
1:A:76:ILE:HD12	1:A:282:GLN:CB	2.48	0.44
1:A:152:VAL:HG12	1:A:153:PRO:O	2.18	0.44
1:C:105:ILE:O	1:C:105:ILE:CG2	2.64	0.44
1:B:183:PRO:HG3	1:B:364:PHE:CG	2.53	0.44
1:A:88:ARG:CZ	1:A:94:GLN:HE22	2.31	0.44
1:B:190:LEU:HD11	1:B:228:GLN:HB2	2.00	0.44
1:B:272:TYR:CD1	1:C:140:VAL:HG21	2.53	0.44
1:A:108:LYS:NZ	1:D:274:ASP:O	2.50	0.43
1:D:119:LEU:HD11	1:D:174:MET:HE1	2.00	0.43
1:D:126:LEU:HD23	1:D:147:ARG:HB3	2.00	0.43
1:D:20:VAL:N	4:D:2002:HOH:O	2.50	0.43
1:C:125:ILE:HG22	1:C:174:MET:HG2	2.00	0.43
1:D:294:GLN:OE1	1:D:297:ARG:NH2	2.48	0.43
1:A:58:LEU:CD2	1:D:58:LEU:CD2	2.95	0.43
1:A:79:LEU:HD23	1:A:103:VAL:HG21	2.01	0.43
1:D:61:VAL:HG21	1:D:283:VAL:HG11	2.00	0.43
1:D:127:VAL:O	1:D:148:SER:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LYS:NZ	2:D:1400:PLP:C4A	2.81	0.43
1:B:109:GLU:O	1:B:112:ALA:HB3	2.18	0.43
1:D:119:LEU:HD11	1:D:125:ILE:HG21	2.00	0.43
1:D:125:ILE:HG21	1:D:174:MET:HE2	2.00	0.43
1:D:384:ARG:NH1	3:D:1403:SO4:O1	2.52	0.43
1:A:135:HIS:O	1:A:136:ILE:C	2.62	0.43
1:A:183:PRO:HG3	1:A:364:PHE:CG	2.54	0.42
1:B:122:GLY:HA2	1:B:143:GLY:O	2.18	0.42
1:C:241:THR:O	1:C:241:THR:HG23	2.19	0.42
1:A:57:LYS:HG3	1:A:287:ALA:HB2	2.00	0.42
1:A:76:ILE:HD12	1:A:282:GLN:HB3	2.00	0.42
1:B:361:GLY:HA3	1:B:368:GLY:O	2.19	0.42
1:B:383:LEU:O	1:B:387:VAL:HG23	2.19	0.42
1:A:84:SER:OG	1:A:95:ILE:O	2.29	0.42
1:C:22:ASN:O	1:C:26:GLU:HG2	2.20	0.42
1:D:221:TRP:HZ3	1:D:325:LYS:NZ	2.08	0.42
1:B:61:VAL:HG21	1:B:283:VAL:HB	2.00	0.42
1:A:152:VAL:O	1:A:153:PRO:C	2.62	0.42
1:B:20:VAL:O	1:B:23:ILE:HB	2.19	0.42
1:B:399:LEU:N	1:B:399:LEU:HD12	2.35	0.42
1:C:208:VAL:HG22	1:C:237:VAL:CG2	2.50	0.41
1:B:39:ILE:HD13	1:B:382:ARG:O	2.20	0.41
1:C:76:ILE:HD11	1:C:279:THR:HG23	2.02	0.41
1:C:311:VAL:HG21	1:C:323:ASN:OD1	2.20	0.41
1:C:388:ARG:CD	3:C:1400:SO4:O3	2.69	0.41
1:A:321:VAL:HG12	1:A:332:ALA:HB1	2.02	0.41
1:C:192:PHE:O	1:C:196:VAL:HG23	2.21	0.41
1:C:105:ILE:HD11	1:C:277:THR:HG23	2.03	0.41
1:C:279:THR:HB	1:C:280:PRO:HD3	2.02	0.41
1:D:242:LEU:CD2	1:D:248:MET:HE3	2.51	0.41
1:B:105:ILE:O	1:B:252:ARG:HB3	2.21	0.40
1:C:132:TYR:CD2	1:C:133:PRO:HD2	2.56	0.40
1:D:111:LEU:O	1:D:115:MET:HG2	2.20	0.40
1:A:183:PRO:HB3	1:A:373:ARG:HD3	2.02	0.40
1:B:137:TYR:CE2	1:B:141:ILE:HD11	2.56	0.40
1:A:370:ASP:OD2	1:A:371:HIS:ND1	2.49	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	367/412 (89%)	355 (97%)	11 (3%)	1 (0%)	36	40
1	B	361/412 (88%)	351 (97%)	9 (2%)	1 (0%)	36	40
1	C	367/412 (89%)	354 (96%)	13 (4%)	0	100	100
1	D	378/412 (92%)	371 (98%)	7 (2%)	0	100	100
All	All	1473/1648 (89%)	1431 (97%)	40 (3%)	2 (0%)	48	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	ARG
1	A	105	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/341 (90%)	300 (98%)	6 (2%)	48	59
1	B	303/341 (89%)	299 (99%)	4 (1%)	61	72
1	C	306/341 (90%)	301 (98%)	5 (2%)	55	66
1	D	313/341 (92%)	309 (99%)	4 (1%)	61	72
All	All	1228/1364 (90%)	1209 (98%)	19 (2%)	57	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	127	VAL
1	A	155	ILE
1	A	174	MET
1	A	257	VAL
1	A	325	LYS
1	B	43	MET
1	B	83	ILE
1	B	204	ASP
1	B	283	VAL
1	C	45	ASN
1	C	76	ILE
1	C	148	SER
1	C	297	ARG
1	C	388	ARG
1	D	67	THR
1	D	199	LEU
1	D	234	ASP
1	D	328	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	159	ASN
1	A	302	GLN
1	A	340	HIS
1	B	293	GLN
1	C	94	GLN
1	C	294	GLN
1	C	304	GLN
1	D	45	ASN
1	D	85	HIS
1	D	273	HIS
1	D	323	ASN

5.3.3 RNA ⓘ

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](#)

13 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	SO4	C	1402	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	D	1402	-	4,4,4	0.21	0	6,6,6	0.34	0
3	SO4	D	1401	-	4,4,4	0.26	0	6,6,6	0.28	0
3	SO4	B	1401	-	4,4,4	0.21	0	6,6,6	0.15	0
3	SO4	C	1403	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	D	1403	-	4,4,4	0.25	0	6,6,6	0.25	0
3	SO4	B	1400	-	4,4,4	0.26	0	6,6,6	0.30	0
2	PLP	A	1400	1	15,15,16	2.17	5 (33%)	21,22,23	1.63	5 (23%)
2	PLP	D	1400	-	16,16,16	1.24	1 (6%)	20,23,23	1.08	2 (10%)
3	SO4	A	1402	-	4,4,4	0.23	0	6,6,6	0.30	0
3	SO4	C	1400	-	4,4,4	0.35	0	6,6,6	0.57	0
3	SO4	C	1401	-	4,4,4	0.29	0	6,6,6	0.42	0
3	SO4	A	1401	-	4,4,4	0.31	0	6,6,6	0.50	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	PLP	A	1400	1	-	3/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	D	1400	-	-	5/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1400	PLP	O3-C3	-5.05	1.25	1.36
2	A	1400	PLP	C3-C2	-3.69	1.37	1.41
2	A	1400	PLP	C2-N1	3.57	1.40	1.33
2	D	1400	PLP	C2-N1	2.77	1.38	1.33
2	A	1400	PLP	C6-N1	2.55	1.39	1.34
2	A	1400	PLP	P-O3P	-2.07	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1400	PLP	O4P-C5A-C5	4.10	117.03	109.36
2	A	1400	PLP	C2A-C2-C3	-2.76	117.57	120.80
2	A	1400	PLP	C2A-C2-N1	2.55	122.45	117.64
2	A	1400	PLP	C5-C6-N1	-2.42	119.90	123.83
2	D	1400	PLP	O4A-C4A-C4	-2.24	119.50	124.80
2	D	1400	PLP	C5-C6-N1	-2.22	120.22	123.83
2	A	1400	PLP	O3P-P-O4P	-2.01	101.43	106.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1400	PLP	C5A-O4P-P-O1P
2	A	1400	PLP	C5A-O4P-P-O3P
2	D	1400	PLP	C5A-O4P-P-O2P
2	D	1400	PLP	C5A-O4P-P-O3P
2	D	1400	PLP	C3-C4-C4A-O4A
2	D	1400	PLP	C5A-O4P-P-O1P
2	D	1400	PLP	C5-C4-C4A-O4A
2	A	1400	PLP	C5A-O4P-P-O2P

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1403	SO4	1	0
2	A	1400	PLP	1	0
2	D	1400	PLP	2	0
3	C	1400	SO4	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

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	371/412 (90%)	0.41	10 (2%) 56 57	2, 46, 68, 120	0
1	B	367/412 (89%)	0.56	14 (3%) 44 44	39, 56, 83, 96	0
1	C	371/412 (90%)	0.55	13 (3%) 47 47	36, 55, 83, 136	0
1	D	380/412 (92%)	0.49	9 (2%) 59 61	28, 47, 67, 79	0
All	All	1489/1648 (90%)	0.50	46 (3%) 51 51	2, 51, 78, 136	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	ILE	4.3
1	C	73	SER	3.7
1	C	74	ARG	3.3
1	B	399	LEU	3.2
1	B	88	ARG	3.2
1	C	24	THR	3.1
1	B	274	ASP	3.0
1	A	72	THR	2.9
1	D	70	TYR	2.8
1	C	221	TRP	2.7
1	A	60	THR	2.6
1	B	41	LEU	2.6
1	C	234	ASP	2.5
1	D	342	GLY	2.5
1	A	277	THR	2.5
1	B	283	VAL	2.5
1	B	207	VAL	2.5
1	A	43	MET	2.5
1	D	187	CYS	2.4
1	A	32	ARG	2.4
1	B	284	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	289	LEU	2.4
1	C	45	ASN	2.3
1	A	86	TRP	2.3
1	B	221	TRP	2.3
1	B	252	ARG	2.3
1	C	288	ALA	2.3
1	A	399	LEU	2.3
1	A	137	TYR	2.2
1	D	72	THR	2.2
1	A	258	GLY	2.2
1	B	44	GLY	2.2
1	C	79	LEU	2.2
1	C	76	ILE	2.2
1	D	29	MET	2.2
1	D	73	SER	2.2
1	B	81	ARG	2.1
1	B	394	PHE	2.1
1	A	122	GLY	2.1
1	C	339	ALA	2.1
1	D	220	GLY	2.1
1	D	275	TYR	2.0
1	C	32	ARG	2.0
1	C	101	ALA	2.0
1	B	395	ARG	2.0
1	D	46	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	B	1401	5/5	0.68	0.28	67,67,68,68	5
3	SO4	D	1403	5/5	0.84	0.11	69,69,70,71	0
2	PLP	D	1400	16/16	0.89	0.13	60,74,82,85	0
3	SO4	C	1403	5/5	0.89	0.07	67,69,69,69	0
3	SO4	D	1402	5/5	0.89	0.14	65,66,67,67	0
3	SO4	B	1400	5/5	0.89	0.07	61,62,62,66	0
3	SO4	C	1401	5/5	0.91	0.08	66,66,67,68	0
3	SO4	D	1401	5/5	0.91	0.12	64,65,66,66	0
3	SO4	A	1402	5/5	0.93	0.10	52,52,54,55	0
2	PLP	A	1400	15/16	0.93	0.20	2,3,5,11	0
3	SO4	C	1402	5/5	0.94	0.09	61,62,62,63	0
3	SO4	A	1401	5/5	0.96	0.08	41,41,43,44	0
3	SO4	C	1400	5/5	0.96	0.08	46,48,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.