



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:08 AM UTC

PDB ID : 1WYD / pdb_00001wyd
Title : Crystal Structure of Aspartyl-tRNA synthetase from *Sulfolobus tokodaii*
Authors : Maeda, Y.; Hossain, M.T.; Ubukata, S.; Suzuki, K.; Sekiguchi, T.; Takenaka, A.
Deposited on : 2005-02-12
Resolution : 2.30 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

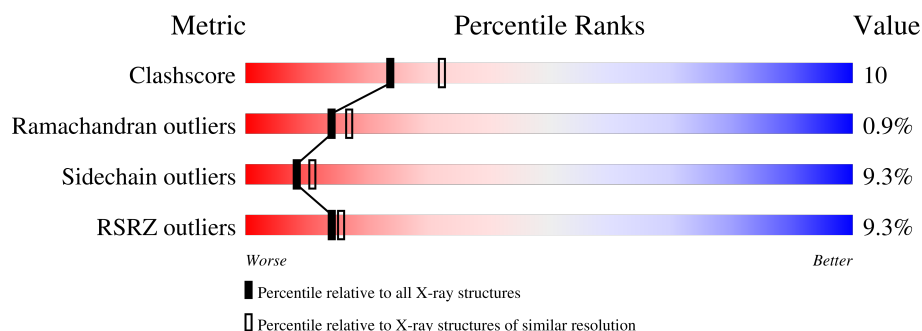
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	429	12% 69% 27% .
1	B	429	7% 71% 26% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7093 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.

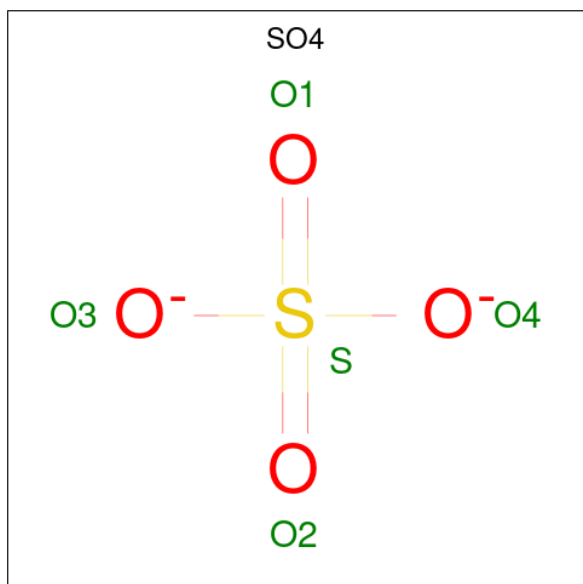
- Molecule 1 is a protein called hypothetical aspartyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3386	2196	561	619	10			
1	B	429	Total	C	N	O	S	0	0	0
			3395	2200	565	620	10			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

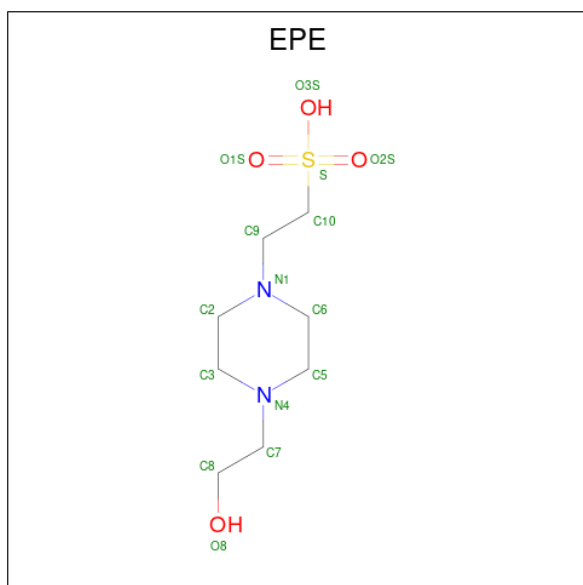
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

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



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 2 3 1	0	0
4	B	1	Total C N O S 12 6 2 3 1	0	0

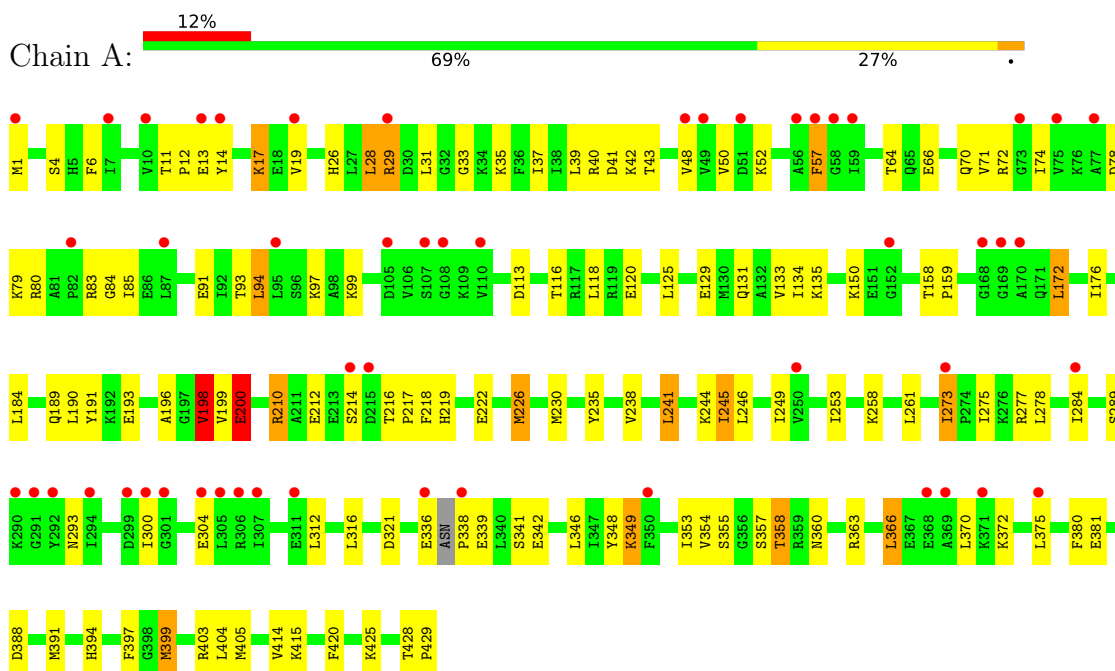
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	117	Total O 117 117	0	0
5	B	159	Total O 159 159	0	0

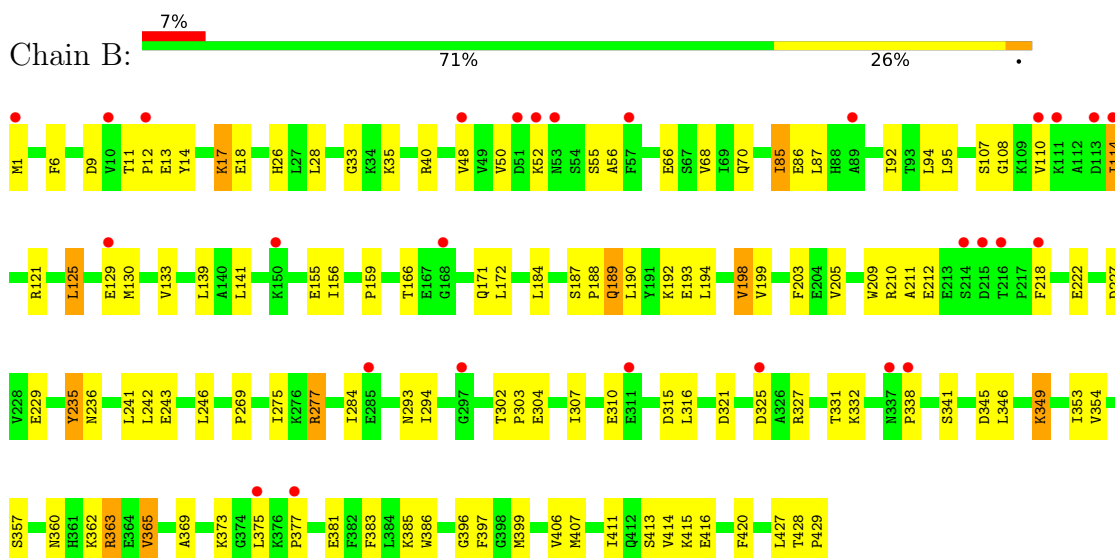
3 Residue-property plots [i](#)

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: hypothetical aspartyl-tRNA synthetase



• Molecule 1: hypothetical aspartyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.30Å 139.25Å 75.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.30) 98.8 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.54 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.279 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	1.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7093	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: SO4, EPE, CL

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	0.92	8/3460 (0.2%)	1.07	6/4676 (0.1%)
1	B	0.88	1/3468 (0.0%)	1.05	8/4687 (0.2%)
All	All	0.90	9/6928 (0.1%)	1.06	14/9363 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	MET	SD-CE	11.03	2.07	1.79
1	A	391	MET	SD-CE	-6.74	1.62	1.79
1	A	133	VAL	CA-CB	6.67	1.62	1.54
1	A	399	MET	SD-CE	6.67	1.96	1.79
1	A	1	MET	SD-CE	5.92	1.94	1.79
1	B	130	MET	SD-CE	5.75	1.94	1.79
1	A	176	ILE	CA-CB	5.65	1.60	1.53
1	A	230	MET	SD-CE	5.63	1.93	1.79
1	A	198	VAL	CA-CB	5.60	1.61	1.55

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	PRO	N-CA-CB	7.35	110.83	103.48
1	B	377	PRO	N-CA-CB	6.89	110.60	103.23
1	B	427	LEU	N-CA-C	-6.38	106.71	114.75
1	A	4	SER	N-CA-C	-6.14	106.39	114.31
1	A	273	ILE	N-CA-C	6.01	113.03	107.56
1	A	339	GLU	N-CA-C	-5.71	105.58	112.54
1	B	211	ALA	N-CA-C	5.53	119.02	112.72
1	B	357	SER	N-CA-C	5.42	115.53	107.88
1	B	156	ILE	N-CA-C	5.40	116.68	108.80
1	A	200	GLU	N-CA-C	5.22	121.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ILE	N-CA-C	5.21	116.20	108.65
1	A	405	MET	CG-SD-CE	-5.12	89.63	100.90
1	A	57	PHE	N-CA-C	5.08	117.20	111.11
1	B	108	GLY	N-CA-C	5.05	121.94	115.32

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	3386	0	3389	72	0
1	B	3395	0	3401	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	12	0	12	2	0
4	B	12	0	12	0	0
5	A	117	0	0	5	0
5	B	159	0	0	1	0
All	All	7093	0	6814	137	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 10.

All (137) 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:226:MET:CE	1:A:226:MET:SD	2.07	1.43
1:B:413:SER:HB3	1:B:416:GLU:HG3	1.49	0.95
1:B:17:LYS:HE3	1:B:18:GLU:H	1.36	0.88
1:A:342:GLU:OE2	1:A:358:THR:HG21	1.77	0.84
1:B:236:ASN:ND2	1:B:277:ARG:HH12	1.79	0.79
1:B:316:LEU:HD13	1:B:407:MET:HE3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HD2	1:A:212:GLU:OE1	1.91	0.71
1:B:184:LEU:HD13	1:B:209:TRP:CD2	2.27	0.70
1:A:363:ARG:NH2	1:A:381:GLU:OE1	2.25	0.69
1:A:26:HIS:HD2	1:A:40:ARG:HH21	1.41	0.68
1:B:11:THR:H	1:B:14:TYR:HD1	1.42	0.65
1:A:131:GLN:HE21	1:B:199:VAL:HG12	1.61	0.64
1:A:275:ILE:O	1:A:277:ARG:NH1	2.31	0.63
1:A:342:GLU:OE2	1:A:358:THR:CG2	2.47	0.61
1:B:209:TRP:NE1	1:B:222:GLU:HG3	2.16	0.61
1:B:302:THR:N	1:B:303:PRO:HD2	2.15	0.60
1:A:125:LEU:HD22	1:A:134:ILE:HD11	1.84	0.59
1:A:198:VAL:HG22	1:A:199:VAL:HG13	1.83	0.59
1:B:218:PHE:CZ	1:B:406:VAL:CG2	2.86	0.59
1:A:135:LYS:HE2	5:A:1102:HOH:O	2.03	0.59
1:B:362:LYS:HB2	1:B:365:VAL:HG12	1.84	0.58
1:B:218:PHE:CZ	1:B:406:VAL:HG21	2.39	0.57
1:B:385:LYS:HG3	1:B:386:TRP:N	2.17	0.57
1:B:114:ILE:HG13	1:B:415:LYS:HE2	1.87	0.57
1:A:420:PHE:HB2	1:B:159:PRO:HG3	1.87	0.57
1:A:278:LEU:HD22	1:A:312:LEU:HD11	1.87	0.56
1:B:236:ASN:HD22	1:B:277:ARG:HH12	1.48	0.56
1:B:243:GLU:HG2	1:B:275:ILE:HD12	1.88	0.56
1:A:52:LYS:HG2	1:A:57:PHE:CZ	2.41	0.56
1:A:94:LEU:HD11	1:A:97:LYS:HB2	1.87	0.56
1:A:113:ASP:HB3	1:A:116:THR:OG1	2.06	0.56
1:B:315:ASP:OD1	1:B:349:LYS:HE2	2.06	0.56
1:B:26:HIS:NE2	1:B:107:SER:HB3	2.21	0.55
1:B:428:THR:HA	1:B:429:PRO:C	2.31	0.55
1:A:226:MET:CE	1:A:226:MET:CG	2.85	0.55
1:A:12:PRO:C	1:A:14:TYR:H	2.14	0.55
1:A:218:PHE:CD2	1:A:414:VAL:HB	2.41	0.54
1:A:342:GLU:O	1:A:357:SER:HB2	2.07	0.54
1:A:428:THR:HA	1:A:429:PRO:C	2.32	0.54
1:B:332:LYS:HA	1:B:360:ASN:HD21	1.71	0.54
1:B:332:LYS:HA	1:B:360:ASN:ND2	2.23	0.54
1:A:11:THR:O	1:A:14:TYR:HB2	2.06	0.54
1:A:370:LEU:HD22	1:A:380:PHE:CD1	2.43	0.54
1:B:192:LYS:NZ	1:B:227:ASP:OD1	2.40	0.53
1:A:241:LEU:O	1:A:245:ILE:HG13	2.09	0.53
1:B:171:GLN:NE2	1:B:212:GLU:HG3	2.24	0.53
1:B:56:ALA:HB1	1:B:92:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLY:O	1:A:52:LYS:HG3	2.09	0.52
1:B:210:ARG:HD2	1:B:212:GLU:OE1	2.09	0.52
1:B:316:LEU:HD13	1:B:407:MET:CE	2.39	0.52
1:A:348:TYR:O	1:A:349:LYS:HB2	2.09	0.52
1:B:354:VAL:HG22	1:B:399:MET:HB2	1.91	0.52
1:B:218:PHE:CD2	1:B:414:VAL:HB	2.45	0.52
1:A:342:GLU:HB2	1:A:358:THR:HG23	1.92	0.52
1:A:246:LEU:HD11	1:A:346:LEU:CD2	2.40	0.52
1:B:141:LEU:HD22	1:B:205:VAL:HG11	1.92	0.52
1:A:222:GLU:OE2	1:B:159:PRO:HA	2.10	0.52
1:A:253:ILE:HG22	1:A:261:LEU:HD11	1.91	0.51
1:A:216:THR:HB	1:A:217:PRO:HD2	1.91	0.51
1:A:249:ILE:O	1:A:253:ILE:HG12	2.10	0.51
1:A:72:ARG:NH2	1:A:91:GLU:HB2	2.26	0.51
1:B:411:ILE:HG22	1:B:413:SER:H	1.76	0.51
1:B:121:ARG:HG3	1:B:125:LEU:HD22	1.93	0.50
1:B:192:LYS:HE3	1:B:229:GLU:OE2	2.12	0.50
5:A:1090:HOH:O	1:B:1:MET:HE3	2.11	0.49
1:A:253:ILE:CG2	1:A:261:LEU:HD11	2.42	0.49
1:B:40:ARG:NH2	1:B:66:GLU:OE1	2.41	0.49
1:A:336:GLU:O	1:A:338:PRO:HD3	2.13	0.49
1:B:209:TRP:CD1	1:B:222:GLU:HG3	2.48	0.49
1:A:6:PHE:HB3	1:A:43:THR:HG21	1.95	0.49
1:A:78:ASP:C	1:A:80:ARG:H	2.21	0.49
1:A:28:LEU:O	1:A:29:ARG:HG2	2.13	0.48
1:A:40:ARG:HG2	1:A:41:ASP:N	2.28	0.48
1:A:238:VAL:CG1	1:A:397:PHE:HD1	2.27	0.48
1:A:14:TYR:O	1:A:17:LYS:HB2	2.13	0.48
1:A:28:LEU:CD1	1:A:37:ILE:HG12	2.43	0.48
1:A:64:THR:HB	5:A:1075:HOH:O	2.13	0.48
1:A:363:ARG:HH22	1:A:381:GLU:CD	2.21	0.48
1:A:196:ALA:O	1:A:200:GLU:HA	2.14	0.47
1:B:198:VAL:CG2	1:B:199:VAL:N	2.76	0.47
1:B:12:PRO:C	1:B:14:TYR:H	2.22	0.47
1:B:17:LYS:HD2	1:B:17:LYS:HA	1.75	0.47
1:A:360:ASN:HB2	1:A:366:LEU:HD13	1.96	0.47
1:A:363:ARG:HD2	1:A:388:ASP:OD2	2.15	0.47
1:B:11:THR:O	1:B:14:TYR:HB2	2.14	0.47
1:B:189:GLN:O	1:B:193:GLU:HG3	2.16	0.46
1:A:420:PHE:HB2	1:B:159:PRO:CG	2.45	0.46
1:B:155:GLU:HB2	1:B:203:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:THR:HB	1:A:159:PRO:CD	2.47	0.45
1:A:83:ARG:HD2	5:A:1112:HOH:O	2.14	0.45
1:B:129:GLU:O	1:B:133:VAL:HG23	2.16	0.45
1:A:85:ILE:HD11	5:A:1112:HOH:O	2.16	0.45
1:B:363:ARG:NH2	1:B:381:GLU:OE1	2.50	0.45
1:A:193:GLU:HG2	1:A:394:HIS:CD2	2.52	0.44
1:B:293:ASN:C	1:B:293:ASN:HD22	2.24	0.44
1:A:40:ARG:NH2	1:A:66:GLU:OE1	2.48	0.44
1:A:79:LYS:HA	1:A:84:GLY:HA2	2.00	0.44
1:B:68:VAL:HG12	1:B:95:LEU:HD12	2.00	0.44
1:B:229:GLU:OE2	1:B:396:GLY:HA3	2.18	0.44
1:B:190:LEU:HD13	1:B:383:PHE:CD1	2.52	0.44
1:A:219:HIS:HA	4:A:1003:EPE:H92	2.00	0.43
1:B:188:PRO:HG2	1:B:192:LYS:HD3	2.00	0.43
1:B:33:GLY:O	1:B:52:LYS:HG2	2.18	0.43
1:A:120:GLU:HA	1:A:120:GLU:OE1	2.18	0.43
1:B:40:ARG:HH22	1:B:66:GLU:CD	2.27	0.43
1:A:131:GLN:NE2	1:B:199:VAL:HG12	2.31	0.43
1:B:35:LYS:HB2	1:B:35:LYS:HE2	1.80	0.43
1:B:235:TYR:OH	1:B:321:ASP:OD2	2.30	0.43
1:A:219:HIS:CD2	4:A:1003:EPE:H61	2.53	0.43
1:A:403:ARG:O	1:A:404:LEU:C	2.61	0.43
1:B:194:LEU:O	1:B:198:VAL:HG13	2.19	0.42
1:A:159:PRO:HG3	1:B:420:PHE:HB2	2.00	0.42
1:B:205:VAL:HB	5:B:1021:HOH:O	2.18	0.42
1:B:327:ARG:HH22	1:B:345:ASP:CG	2.25	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.94	0.42
1:A:158:THR:HB	1:A:159:PRO:HD2	2.01	0.42
1:A:28:LEU:HD12	1:A:37:ILE:HG12	1.99	0.42
1:A:172:LEU:HG	1:A:184:LEU:O	2.20	0.42
1:B:284:ILE:HD12	1:B:294:ILE:HG12	2.01	0.42
1:B:269:PRO:HG2	1:B:407:MET:HE2	2.01	0.42
1:A:321:ASP:HA	1:A:341:SER:O	2.21	0.41
1:B:321:ASP:HA	1:B:341:SER:O	2.20	0.41
1:A:354:VAL:HG22	1:A:399:MET:HB2	2.01	0.41
1:A:11:THR:H	1:A:14:TYR:HD1	1.66	0.41
1:A:70:GLN:HB3	1:A:93:THR:HB	2.02	0.41
1:A:300:ILE:HG23	1:A:304:GLU:HB3	2.03	0.41
1:B:198:VAL:HG23	1:B:199:VAL:HG13	2.02	0.41
1:B:284:ILE:HD13	1:B:284:ILE:HA	1.86	0.41
1:B:397:PHE:CD2	1:B:397:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG12	1:A:355:SER:N	2.35	0.41
1:B:6:PHE:O	1:B:9:ASP:HB2	2.21	0.41
1:B:304:GLU:HA	1:B:307:ILE:HD12	2.03	0.41
1:A:158:THR:CG2	1:A:191:TYR:HB3	2.51	0.41
1:B:246:LEU:HD11	1:B:346:LEU:CD2	2.51	0.41
1:B:369:ALA:O	1:B:373:LYS:HG3	2.20	0.41
1:B:411:ILE:HG21	1:B:416:GLU:HB2	2.02	0.41
1:A:342:GLU:CB	1:A:358:THR:HG23	2.50	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	424/429 (99%)	403 (95%)	17 (4%)	4 (1%)	14	17
1	B	427/429 (100%)	401 (94%)	22 (5%)	4 (1%)	14	17
All	All	851/858 (99%)	804 (94%)	39 (5%)	8 (1%)	14	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	B	13	GLU
1	A	13	GLU
1	A	349	LYS
1	B	189	GLN
1	B	349	LYS
1	A	200	GLU
1	B	110	VAL

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	354/374 (95%)	316 (89%)	38 (11%)	6	8
1	B	355/374 (95%)	327 (92%)	28 (8%)	11	15
All	All	709/748 (95%)	643 (91%)	66 (9%)	8	11

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	19	VAL
1	A	28	LEU
1	A	29	ARG
1	A	31	LEU
1	A	35	LYS
1	A	39	LEU
1	A	42	LYS
1	A	48	VAL
1	A	50	VAL
1	A	71	VAL
1	A	74	ILE
1	A	94	LEU
1	A	99	LYS
1	A	118	LEU
1	A	129	GLU
1	A	150	LYS
1	A	172	LEU
1	A	190	LEU
1	A	198	VAL
1	A	210	ARG
1	A	214	SER
1	A	235	TYR
1	A	241	LEU
1	A	244	LYS
1	A	245	ILE
1	A	258	LYS

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Mol	Chain	Res	Type
1	A	273	ILE
1	A	284	ILE
1	A	289	SER
1	A	293	ASN
1	A	353	ILE
1	A	358	THR
1	A	366	LEU
1	A	372	LYS
1	A	375	LEU
1	A	415	LYS
1	A	425	LYS
1	B	17	LYS
1	B	28	LEU
1	B	48	VAL
1	B	50	VAL
1	B	55	SER
1	B	70	GLN
1	B	85	ILE
1	B	86	GLU
1	B	87	LEU
1	B	94	LEU
1	B	114	ILE
1	B	125	LEU
1	B	139	LEU
1	B	166	THR
1	B	172	LEU
1	B	187	SER
1	B	198	VAL
1	B	235	TYR
1	B	241	LEU
1	B	242	LEU
1	B	277	ARG
1	B	310	GLU
1	B	325	ASP
1	B	331	THR
1	B	353	ILE
1	B	363	ARG
1	B	365	VAL
1	B	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	65	GLN
1	A	131	GLN
1	A	137	GLN
1	A	236	ASN
1	A	361	HIS
1	B	47	GLN
1	B	131	GLN
1	B	171	GLN
1	B	236	ASN
1	B	293	ASN
1	B	337	ASN
1	B	360	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
4	EPE	A	1003	-	12,12,15	0.82	1 (8%)	15,16,20	2.03	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPE	B	1004	-	12,12,15	1.01	1 (8%)	15,16,20	2.18	6 (40%)
3	SO4	A	1001	-	4,4,4	0.31	0	6,6,6	0.40	0
3	SO4	B	1002	-	4,4,4	0.33	0	6,6,6	0.19	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
4	EPE	A	1003	-	-	0/6/14/19	0/1/1/1
4	EPE	B	1004	-	-	2/6/14/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1004	EPE	C10-S	2.98	1.81	1.77
4	A	1003	EPE	C10-S	2.12	1.80	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	EPE	O2S-S-C10	4.63	113.73	106.73
4	A	1003	EPE	O3S-S-C10	4.42	114.65	106.00
4	A	1003	EPE	O3S-S-O1S	-3.79	101.91	111.40
4	B	1004	EPE	O3S-S-C10	3.39	112.63	106.00
4	A	1003	EPE	C5-N4-C3	3.08	119.11	110.40
4	B	1004	EPE	O1S-S-C10	-2.89	102.36	106.73
4	B	1004	EPE	C5-N4-C3	2.82	118.37	110.40
4	A	1003	EPE	O1S-S-C10	2.64	110.72	106.73
4	B	1004	EPE	C5-C6-N1	2.54	116.19	111.14
4	B	1004	EPE	C6-N1-C2	2.34	113.89	108.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1004	EPE	C10-C9-N1-C2
4	B	1004	EPE	C10-C9-N1-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	EPE	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	428/429 (99%)	0.93	52 (12%) 8 9	32, 52, 81, 98	0
1	B	429/429 (100%)	0.78	28 (6%) 25 27	32, 51, 72, 78	0
All	All	857/858 (99%)	0.85	80 (9%) 14 16	32, 51, 77, 98	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	VAL	5.7
1	A	57	PHE	5.0
1	A	1	MET	4.4
1	A	75	VAL	4.2
1	A	338	PRO	4.1
1	A	292	TYR	3.8
1	A	56	ALA	3.6
1	B	53	ASN	3.4
1	A	49	VAL	3.3
1	B	111	LYS	3.3
1	A	7	ILE	3.2
1	A	368	GLU	3.2
1	B	338	PRO	3.1
1	A	108	GLY	3.1
1	A	307	ILE	3.1
1	B	214	SER	3.0
1	B	89	ALA	3.0
1	A	350	PHE	3.0
1	A	371	LYS	3.0
1	A	273	ILE	2.9
1	A	19	VAL	2.9
1	B	218	PHE	2.8
1	B	215	ASP	2.7
1	A	168	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	51	ASP	2.7
1	B	113	ASP	2.7
1	B	337	ASN	2.7
1	B	377	PRO	2.7
1	A	336	GLU	2.7
1	A	284	ILE	2.7
1	B	375	LEU	2.7
1	A	291	GLY	2.6
1	A	305	LEU	2.6
1	A	294	ILE	2.6
1	A	13	GLU	2.6
1	A	311	GLU	2.6
1	A	369	ALA	2.6
1	A	48	VAL	2.6
1	A	300	ILE	2.6
1	A	77	ALA	2.5
1	B	52	LYS	2.5
1	A	29	ARG	2.4
1	B	297	GLY	2.4
1	A	82	PRO	2.4
1	A	250	VAL	2.4
1	A	95	LEU	2.4
1	A	10	VAL	2.4
1	B	10	VAL	2.4
1	A	59	ILE	2.3
1	A	105	ASP	2.3
1	B	325	ASP	2.3
1	B	216	THR	2.3
1	B	12	PRO	2.3
1	B	150	LYS	2.3
1	A	152	GLY	2.3
1	A	301	GLY	2.3
1	B	285	GLU	2.3
1	A	169	GLY	2.2
1	B	114	ILE	2.2
1	A	87	LEU	2.2
1	B	48	VAL	2.2
1	A	215	ASP	2.2
1	A	58	GLY	2.2
1	A	290	LYS	2.2
1	A	107	SER	2.2
1	A	73	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	311	GLU	2.1
1	A	170	ALA	2.1
1	A	14	TYR	2.1
1	B	57	PHE	2.1
1	B	168	GLY	2.1
1	A	51	ASP	2.1
1	B	110	VAL	2.1
1	A	306	ARG	2.1
1	B	1	MET	2.0
1	A	304	GLU	2.0
1	A	299	ASP	2.0
1	A	375	LEU	2.0
1	A	214	SER	2.0
1	B	129	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EPE	B	1004	12/15	0.83	0.21	60,68,75,76	0
3	SO4	B	1002	5/5	0.84	0.16	78,79,80,80	0
2	CL	A	431	1/1	0.86	0.13	73,73,73,73	0
3	SO4	A	1001	5/5	0.91	0.12	65,67,68,69	0
4	EPE	A	1003	12/15	0.92	0.14	48,55,59,59	0
2	CL	B	430	1/1	0.95	0.12	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.