Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:10 AM EDT

PDB ID	:	1WYD
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:

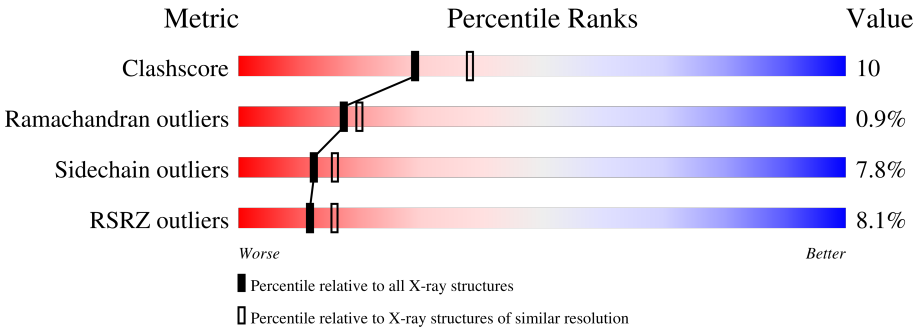
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	10% 70% 26% ·
1	B	429	6% 73% 24% ·

2 Entry composition

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.

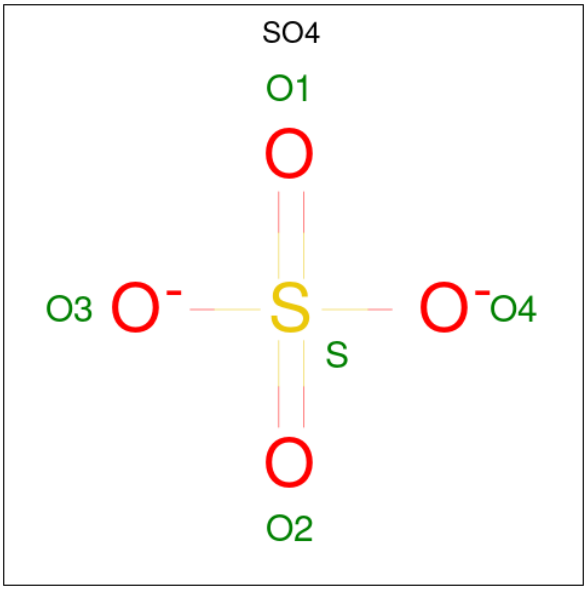
- Molecule 1 is a protein called hypothetical aspartyl-tRNA synthetase.

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 (three-letter code: CL) (formula: Cl).

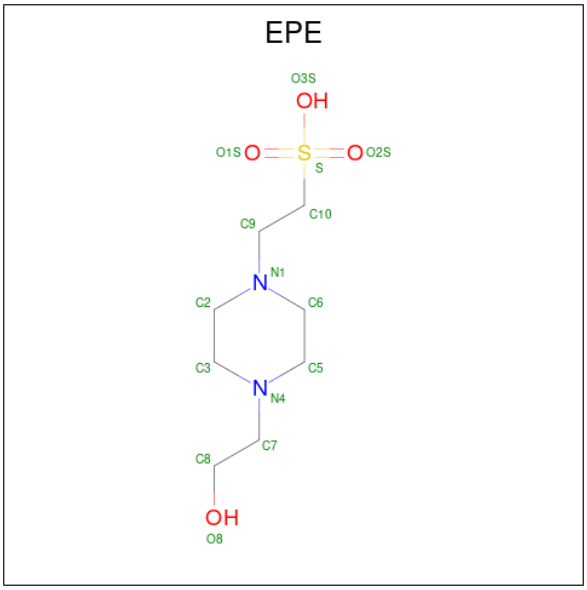
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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 (three-letter code: 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.

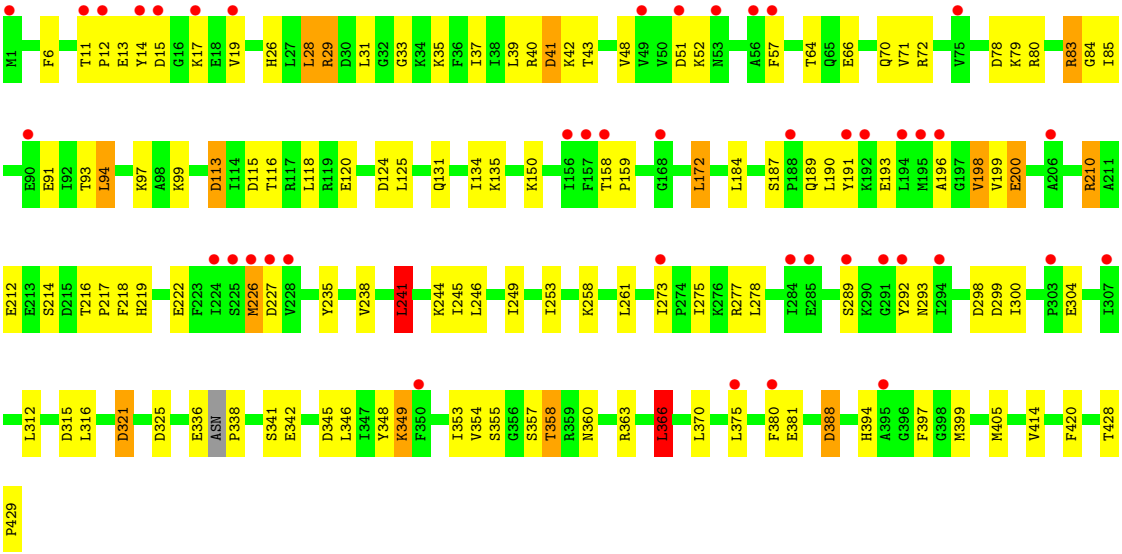
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	117	Total O 117 117	0	0
5	B	159	Total O 159 159	0	0

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.

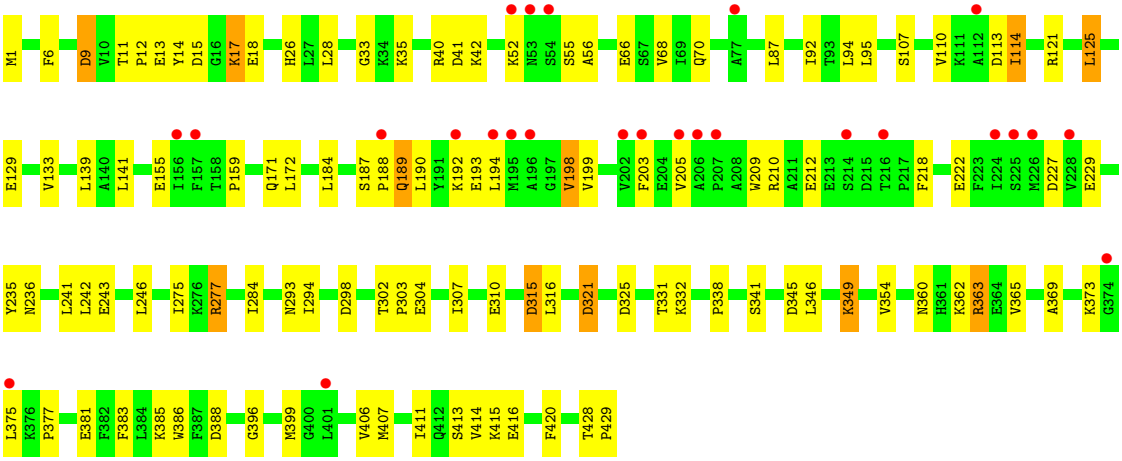
• Molecule 1: hypothetical aspartyl-tRNA synthetase

Chain A:



• Molecule 1: hypothetical aspartyl-tRNA synthetase

Chain B:



4 Data and refinement statistics (i)

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 37.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.30) 98.9 (37.65-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.33 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.74	1/3460 (0.0%)	0.89	17/4676 (0.4%)
1	B	0.71	0/3468	0.86	11/4687 (0.2%)
All	All	0.73	1/6928 (0.0%)	0.88	28/9363 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	MET	SD-CE	5.23	2.07	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ASP	CB-CG-OD2	8.65	126.08	118.30
1	B	41	ASP	CB-CG-OD2	8.37	125.83	118.30
1	B	388	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	241	LEU	CA-CB-CG	6.68	130.67	115.30
1	B	345	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	41	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	405	MET	CG-SD-CE	-6.61	89.63	100.20
1	B	9	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	388	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	338	PRO	N-CA-CB	6.27	110.83	103.30
1	A	321	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	377	PRO	N-CA-CB	6.09	110.60	103.30
1	B	113	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	321	ASP	CB-CG-OD2	5.93	123.63	118.30
1	B	315	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	298	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	345	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	113	ASP	CB-CG-OD2	5.45	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	315	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	325	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	51	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	298	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	15	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	15	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	366	LEU	CA-CB-CG	5.03	126.88	115.30
1	A	115	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	299	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	71	0
1	B	3395	0	3401	66	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	131	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 (131) 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: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:385:LYS:HG3	1:B:386:TRP:N	2.17	0.58
1:B:316:LEU:HD13	1:B:407:MET:HE3	1.86	0.58
1:B:218:PHE:CZ	1:B:406:VAL:HG21	2.39	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:A:226:MET:CE	1:A:226:MET:CG	2.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:428:THR:HA	1:B:429:PRO:C	2.31	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:A:12:PRO:C	1:A:14:TYR:H	2.14	0.50
1:B:121:ARG:HG3	1:B:125:LEU:HD22	1.93	0.50
1:A:428:THR:HA	1:A:429:PRO:C	2.32	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:78:ASP:C	1:A:80:ARG:H	2.21	0.44
1:B:316:LEU:CD1	1:B:407:MET:HE1	2.48	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:A:363:ARG:HH22	1:A:381:GLU:CD	2.21	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: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:A:219:HIS:CD2	4:A:1003:EPE:H61	2.53	0.43
1:B:12:PRO:C	1:B:14:TYR:H	2.22	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: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: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:HG12	1:A:355:SER:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	424/429 (99%)	403 (95%)	17 (4%)	4 (1%)	17	20
1	B	427/429 (100%)	401 (94%)	22 (5%)	4 (1%)	17	20
All	All	851/858 (99%)	804 (94%)	39 (5%)	8 (1%)	17	20

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 (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	354/374 (95%)	322 (91%)	32 (9%)	9 11
1	B	355/374 (95%)	332 (94%)	23 (6%)	17 23
All	All	709/748 (95%)	654 (92%)	55 (8%)	12 16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	71	VAL
1	A	83	ARG
1	A	94	LEU
1	A	99	LYS
1	A	118	LEU
1	A	150	LYS
1	A	172	LEU
1	A	187	SER
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	258	LYS
1	A	273	ILE
1	A	289	SER
1	A	292	TYR

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Mol	Chain	Res	Type
1	A	293	ASN
1	A	353	ILE
1	A	358	THR
1	A	366	LEU
1	A	375	LEU
1	B	17	LYS
1	B	28	LEU
1	B	42	LYS
1	B	55	SER
1	B	70	GLN
1	B	87	LEU
1	B	94	LEU
1	B	114	ILE
1	B	125	LEU
1	B	139	LEU
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	293	ASN
1	B	310	GLU
1	B	325	ASP
1	B	331	THR
1	B	363	ARG
1	B	375	LEU

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	26	HIS
1	A	131	GLN
1	A	236	ASN
1	A	360	ASN
1	B	70	GLN
1	B	131	GLN
1	B	171	GLN
1	B	236	ASN
1	B	293	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 monosaccharides 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	$\#\|Z\| > 2$
3	SO4	A	1001	-	4,4,4	0.31	0	6,6,6	0.40	0
4	EPE	A	1003	-	12,12,15	0.82	1 (8%)	15,16,20	2.03	4 (26%)
4	EPE	B	1004	-	12,12,15	1.01	1 (8%)	15,16,20	2.18	6 (40%)
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(^{o})	Ideal(^{o})
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, 95^{th} 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%)	0.54	43 (10%)	7	10	32, 52, 81, 98	0
1	B	429/429 (100%)	0.31	26 (6%)	21	27	32, 51, 72, 78	0
All	All	857/858 (99%)	0.42	69 (8%)	12	16	32, 51, 77, 98	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	VAL	4.4
1	A	57	PHE	4.2
1	A	292	TYR	3.9
1	A	294	ILE	3.7
1	B	156	ILE	3.7
1	A	375	LEU	3.7
1	A	156	ILE	3.7
1	A	289	SER	3.6
1	A	157	PHE	3.6
1	B	205	VAL	3.4
1	B	225	SER	3.4
1	B	224	ILE	3.3
1	A	14	TYR	3.3
1	B	228	VAL	3.3
1	A	291	GLY	3.2
1	B	206	ALA	3.2
1	A	224	ILE	3.1
1	A	307	ILE	3.0
1	B	188	PRO	2.9
1	B	214	SER	2.9
1	A	1	MET	2.9
1	A	395	ALA	2.9
1	A	273	ILE	2.9
1	B	195	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	49	VAL	2.7
1	A	12	PRO	2.7
1	B	202	VAL	2.7
1	A	228	VAL	2.7
1	A	56	ALA	2.7
1	B	53	ASN	2.7
1	B	112	ALA	2.7
1	A	51	ASP	2.6
1	A	158	THR	2.6
1	B	52	LYS	2.6
1	A	226	MET	2.6
1	A	188	PRO	2.5
1	A	17	LYS	2.5
1	A	15	ASP	2.5
1	B	196	ALA	2.5
1	A	192	LYS	2.5
1	A	284	ILE	2.5
1	B	192	LYS	2.4
1	B	157	PHE	2.4
1	A	350	PHE	2.4
1	A	303	PRO	2.4
1	A	225	SER	2.3
1	B	207	PRO	2.3
1	A	196	ALA	2.3
1	B	194	LEU	2.3
1	B	77	ALA	2.3
1	B	226	MET	2.3
1	B	54	SER	2.3
1	B	374	GLY	2.2
1	A	53	ASN	2.2
1	A	11	THR	2.2
1	A	206	ALA	2.2
1	A	191	TYR	2.2
1	A	90	GLU	2.2
1	A	285	GLU	2.2
1	B	203	PHE	2.1
1	B	216	THR	2.1
1	A	168	GLY	2.1
1	B	401	LEU	2.1
1	A	75	VAL	2.1
1	A	195	MET	2.1
1	A	194	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	PHE	2.1
1	B	375	LEU	2.0
1	A	227	ASP	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EPE	B	1004	12/15	0.88	0.24	60,68,75,76	0
3	SO4	B	1002	5/5	0.92	0.12	78,79,80,80	0
2	CL	A	431	1/1	0.92	0.08	73,73,73,73	0
4	EPE	A	1003	12/15	0.96	0.12	48,55,59,59	0
3	SO4	A	1001	5/5	0.96	0.10	65,67,68,69	0
2	CL	B	430	1/1	0.97	0.11	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.