



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:56 PM UTC

PDB ID : 2DOU / pdb_00002dou
Title : probable N-succinyldiaminopimelate aminotransferase (TTHA0342) from
Thermus thermophilus HB8
Authors : Omi, R.; Goto, M.; Miyahara, I.; Hirotsu, K.; RIKEN Structural Ge-
nomics/Proteomics Initiative (RSGI)
Deposited on : 2006-05-03
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

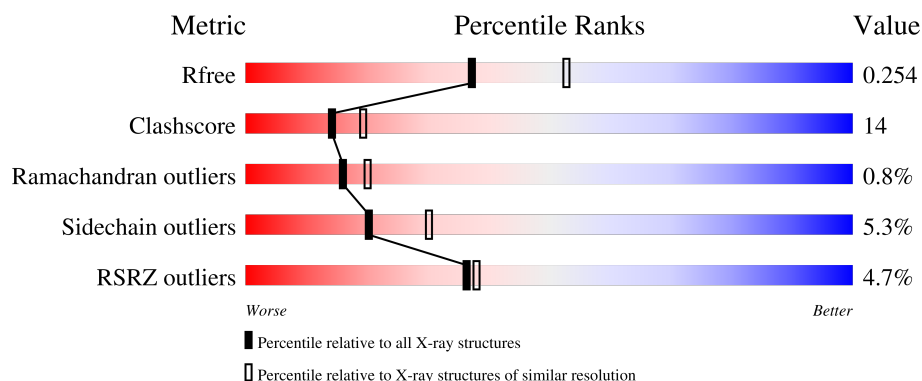
1 Overall quality at a glance

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))
R_{free}	180053	6319 (2.30-2.30)
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	376	3% 71% 25% ..
1	B	376	6% 66% 26% 5% ..

2 Entry composition [i](#)

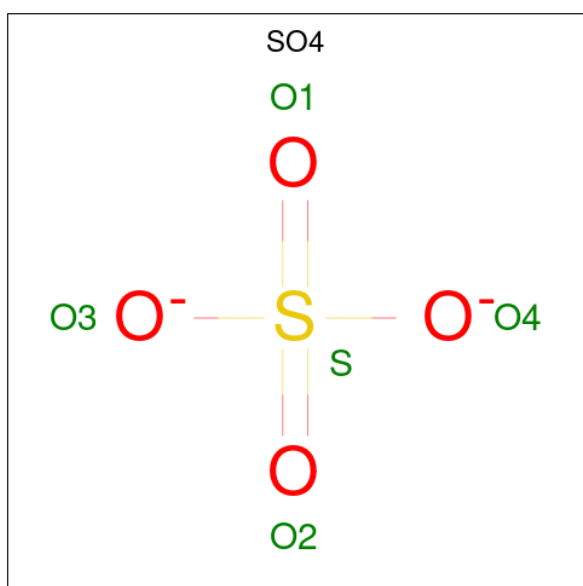
There are 4 unique types of molecules in this entry. The entry contains 5821 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-succinyldiaminopimelate aminotransferase.

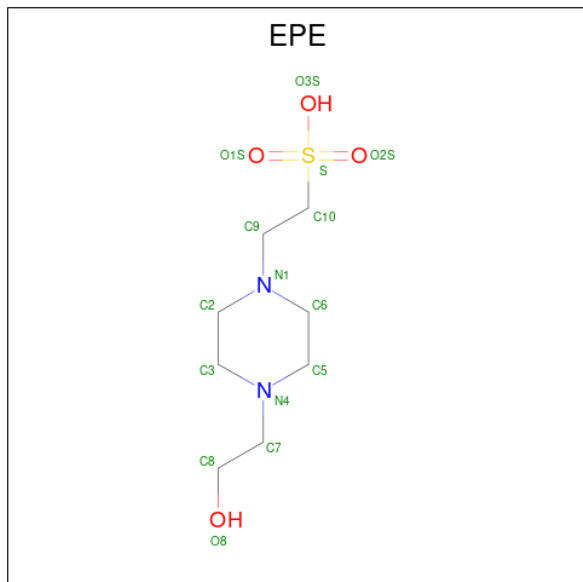
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2829	1828	489	507	5			
1	B	368	Total	C	N	O	S	0	0	0
			2753	1778	475	495	5			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

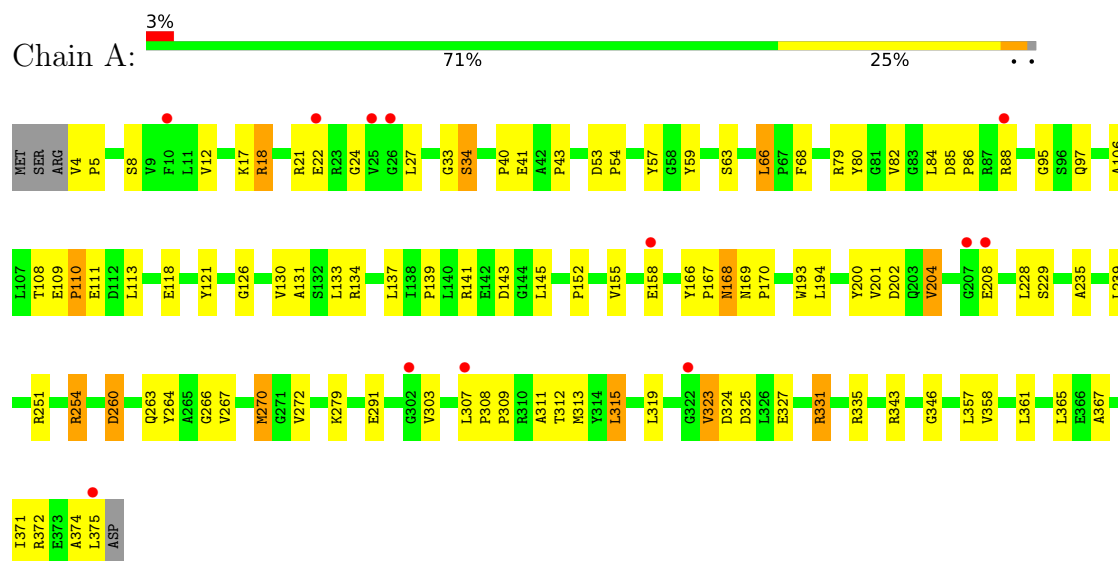
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	106	Total	O	0	0
			106	106		

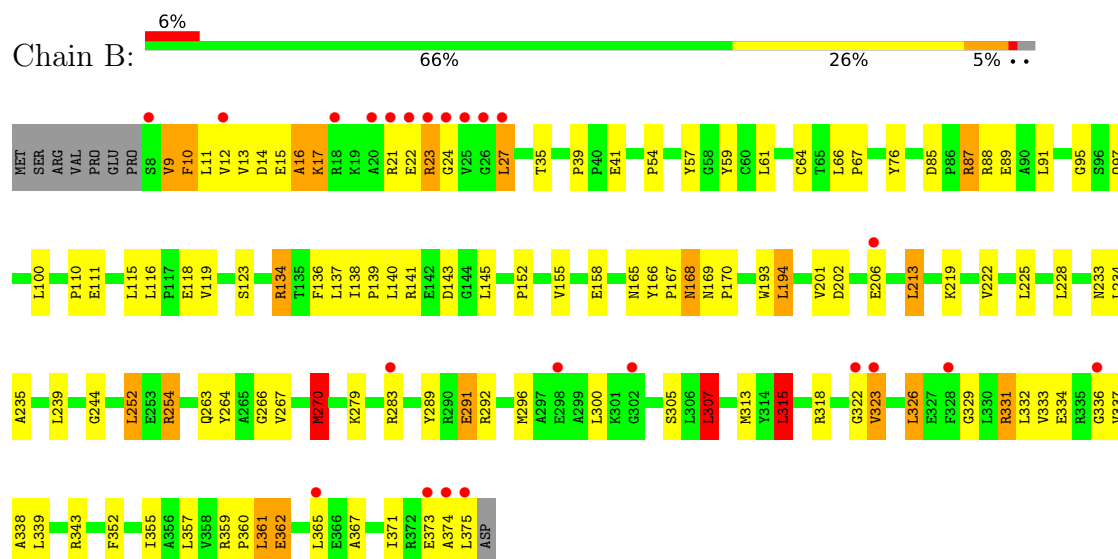
3 Residue-property plots

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 N-succinyldiaminopimelate aminotransferase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.49Å 121.49Å 172.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-2.30) 99.7 (19.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.254 0.222 , 0.254	Depositor DCC
R_{free} test set	5791 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5821	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: EPE, 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	0.59	2/2895 (0.1%)	1.00	20/3941 (0.5%)
1	B	0.46	0/2817	1.04	16/3842 (0.4%)
All	All	0.53	2/5712 (0.0%)	1.02	36/7783 (0.5%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	SER	C-N	17.30	1.57	1.33
1	A	33	GLY	C-N	8.30	1.44	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	VAL	N-CA-C	-12.80	101.55	113.71
1	A	168	ASN	N-CA-C	7.88	122.69	109.76
1	A	33	GLY	CA-C-N	-7.79	112.02	123.00
1	A	33	GLY	C-N-CA	-7.79	112.02	123.00
1	A	95	GLY	N-CA-C	-7.53	103.37	112.48
1	B	95	GLY	N-CA-C	-7.22	102.50	112.18
1	B	168	ASN	N-CA-C	7.11	121.62	110.17
1	B	11	LEU	N-CA-C	-6.53	103.85	110.97
1	A	169	ASN	N-CA-C	-6.41	99.63	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	THR	N-CA-C	6.40	117.88	108.86
1	A	34	SER	O-C-N	6.33	130.61	123.27
1	A	53	ASP	CA-C-N	6.30	126.21	119.28
1	A	53	ASP	C-N-CA	6.30	126.21	119.28
1	B	134	ARG	N-CA-C	-6.29	102.06	110.55
1	B	10	PHE	N-CA-C	-6.24	105.15	112.89
1	B	307	LEU	N-CA-C	-6.18	101.12	110.39
1	B	193	TRP	N-CA-C	-5.98	100.81	110.32
1	B	222	VAL	N-CA-C	5.85	116.36	108.17
1	A	41	GLU	N-CA-C	5.82	117.70	111.36
1	B	169	ASN	N-CA-C	-5.76	100.18	109.40
1	A	229	SER	N-CA-C	5.63	117.10	110.97
1	B	244	GLY	N-CA-C	5.60	118.78	110.60
1	A	346	GLY	CA-C-N	5.57	125.67	119.32
1	A	346	GLY	C-N-CA	5.57	125.67	119.32
1	A	358	VAL	N-CA-C	5.51	117.50	111.77
1	A	270	MET	N-CA-C	-5.44	105.35	111.28
1	B	41	GLU	N-CA-C	5.40	117.25	111.36
1	A	193	TRP	N-CA-C	-5.38	101.76	110.32
1	A	307	LEU	N-CA-C	-5.37	102.39	110.24
1	B	270	MET	N-CA-C	-5.24	105.74	111.82
1	B	17	LYS	N-CA-C	-5.17	107.04	113.55
1	A	260	ASP	N-CA-C	5.17	115.11	108.34
1	B	315	LEU	N-CA-C	-5.14	101.02	109.40
1	A	204	VAL	N-CA-C	-5.12	103.00	109.80
1	A	313	MET	N-CA-C	-5.12	107.20	112.93
1	B	27	LEU	N-CA-C	5.09	116.71	108.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	SER	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2829	0	2847	73	0
1	B	2753	0	2722	88	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	15	0	18	5	0
4	A	98	0	0	1	0
4	B	106	0	0	0	0
All	All	5821	0	5587	159	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 14.

All (159) 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:307:LEU:HD12	1:B:307:LEU:H	1.06	1.11
1:B:254:ARG:HH11	1:B:254:ARG:HG3	1.14	1.09
1:A:254:ARG:HH11	1:A:254:ARG:HG3	1.31	0.95
1:B:307:LEU:HD12	1:B:307:LEU:N	1.91	0.86
1:B:87:ARG:HH11	1:B:87:ARG:HB3	1.38	0.85
1:A:331:ARG:NH2	1:A:335:ARG:HH21	1.78	0.82
1:B:254:ARG:HG3	1:B:254:ARG:NH1	1.86	0.82
1:B:296:MET:HE2	1:B:300:LEU:HD11	1.63	0.80
1:B:85:ASP:OD2	1:B:88:ARG:HD3	1.83	0.79
1:B:166:TYR:HA	1:B:167:PRO:C	2.08	0.77
1:A:97:GLN:HE22	1:A:121:TYR:HE2	1.30	0.76
1:A:254:ARG:HG3	1:A:254:ARG:NH1	1.99	0.76
1:B:307:LEU:H	1:B:307:LEU:CD1	1.88	0.76
1:B:291:GLU:HG2	1:B:292:ARG:N	2.02	0.75
1:B:17:LYS:HD3	1:B:21:ARG:HH12	1.53	0.72
1:B:17:LYS:HD3	1:B:21:ARG:NH1	2.04	0.72
1:A:200:TYR:OH	3:A:501:EPE:H82	1.91	0.71
1:B:141:ARG:NH2	1:B:145:LEU:HD12	2.05	0.71
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.56	0.71
1:B:9:VAL:HG11	1:B:343:ARG:HD2	1.76	0.68
1:A:166:TYR:HA	1:A:167:PRO:C	2.19	0.67
1:B:315:LEU:HD22	1:B:357:LEU:HD21	1.78	0.66
1:B:296:MET:HE1	1:B:355:ILE:HG21	1.77	0.64
1:B:362:GLU:N	1:B:362:GLU:OE1	2.30	0.64
1:A:200:TYR:OH	3:A:501:EPE:H32	1.98	0.62
1:B:296:MET:HE1	1:B:355:ILE:HD13	1.82	0.62
1:B:91:LEU:HD23	1:B:252:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:O	1:A:134:ARG:HD3	2.00	0.61
1:A:22:GLU:C	1:A:24:GLY:H	2.08	0.61
1:A:121:TYR:CZ	3:A:501:EPE:H51	2.35	0.61
1:A:63:SER:HA	1:A:66:LEU:HD23	1.84	0.60
1:B:10:PHE:O	1:B:14:ASP:HB2	2.01	0.60
1:B:289:TYR:OH	1:B:313:MET:HE3	2.02	0.60
1:B:279:LYS:O	1:B:283:ARG:HG2	2.01	0.60
1:B:100:LEU:C	1:B:100:LEU:HD13	2.27	0.59
1:B:87:ARG:HB3	1:B:87:ARG:NH1	2.15	0.58
1:B:152:PRO:HG2	1:B:155:VAL:HG23	1.84	0.58
1:A:200:TYR:OH	3:A:501:EPE:C8	2.51	0.58
1:A:367:ALA:O	1:A:371:ILE:HG13	2.04	0.57
1:B:16:ALA:O	1:B:333:VAL:HG11	2.04	0.57
1:B:66:LEU:HB2	1:B:67:PRO:HD3	1.87	0.57
1:A:319:LEU:HB3	1:A:323:VAL:HG22	1.86	0.57
1:B:331:ARG:HH11	1:B:331:ARG:HG2	1.70	0.57
1:A:85:ASP:OD2	1:A:88:ARG:HD3	2.06	0.56
1:B:264:TYR:CE2	1:B:266:GLY:HA3	2.41	0.56
1:B:35:THR:HB	1:B:313:MET:HE1	1.86	0.56
1:A:228:LEU:HD11	1:A:239:LEU:HD23	1.87	0.56
1:A:84:LEU:O	1:A:86:PRO:HD3	2.05	0.55
1:A:59:TYR:CE2	1:B:235:ALA:HB1	2.42	0.55
1:A:264:TYR:CE2	1:A:266:GLY:HA3	2.42	0.54
1:A:152:PRO:HG2	1:A:155:VAL:CG2	2.38	0.54
1:A:315:LEU:HD22	1:A:357:LEU:HD21	1.90	0.54
1:A:40:PRO:O	1:A:43:PRO:HD2	2.08	0.54
1:B:305:SER:HB3	1:B:318:ARG:HB3	1.89	0.54
1:A:118:GLU:CD	1:A:139:PRO:HA	2.33	0.53
1:B:87:ARG:HH11	1:B:87:ARG:CB	2.18	0.53
1:B:110:PRO:O	1:B:111:GLU:HB2	2.08	0.53
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.73	0.53
1:B:115:LEU:HD23	1:B:136:PHE:HB3	1.90	0.53
1:A:85:ASP:OD2	1:A:88:ARG:NH1	2.41	0.53
1:A:22:GLU:C	1:A:24:GLY:N	2.67	0.53
1:A:80:TYR:O	1:A:82:VAL:HG23	2.08	0.53
1:B:367:ALA:O	1:B:371:ILE:HG13	2.08	0.53
1:A:235:ALA:HB1	1:B:59:TYR:CE2	2.44	0.52
1:B:76:TYR:OH	1:B:213:LEU:HB3	2.09	0.52
1:B:263:GLN:HG3	1:B:264:TYR:N	2.24	0.52
1:A:152:PRO:HG2	1:A:155:VAL:HG23	1.91	0.52
1:B:337:VAL:HG12	1:B:339:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:C	1:B:27:LEU:HD23	2.35	0.52
1:B:254:ARG:NH1	1:B:254:ARG:CG	2.62	0.51
1:B:22:GLU:C	1:B:24:GLY:H	2.18	0.51
3:A:501:EPE:H61	1:B:59:TYR:OH	2.11	0.50
1:B:23:ARG:NH2	1:B:334:GLU:OE1	2.45	0.50
1:A:21:ARG:HG3	1:A:21:ARG:NH1	2.26	0.50
1:A:79:ARG:HD2	1:A:208:GLU:OE1	2.12	0.50
1:A:254:ARG:HD2	1:A:254:ARG:O	2.12	0.50
1:A:145:LEU:HD13	1:A:166:TYR:CE2	2.47	0.49
1:A:8:SER:O	1:A:12:VAL:HG23	2.13	0.49
1:B:228:LEU:HD12	1:B:239:LEU:HB3	1.94	0.49
1:A:331:ARG:HH21	1:A:335:ARG:HH21	1.55	0.49
1:B:359:ARG:HD3	1:B:360:PRO:CD	2.42	0.49
1:B:296:MET:CE	1:B:355:ILE:HD13	2.42	0.48
1:A:263:GLN:HG3	1:A:264:TYR:N	2.29	0.48
1:B:213:LEU:HD22	1:B:213:LEU:O	2.14	0.48
1:B:329:GLY:O	1:B:333:VAL:HG23	2.14	0.48
1:B:152:PRO:HG2	1:B:155:VAL:CG2	2.43	0.48
1:A:204:VAL:HA	1:A:311:ALA:HB2	1.96	0.48
1:A:201:VAL:HG13	1:A:202:ASP:N	2.29	0.48
1:B:118:GLU:CD	1:B:139:PRO:HA	2.39	0.48
1:B:332:LEU:CD2	1:B:339:LEU:HD22	2.44	0.48
1:A:141:ARG:NH2	1:A:143:ASP:OD2	2.47	0.48
1:B:115:LEU:HD21	1:B:155:VAL:CG1	2.44	0.47
1:B:35:THR:HB	1:B:313:MET:CE	2.45	0.47
1:B:239:LEU:HD22	1:B:267:VAL:HG12	1.96	0.47
1:B:111:GLU:O	1:B:134:ARG:HD3	2.14	0.47
1:A:113:LEU:HD23	1:A:158:GLU:HG3	1.97	0.46
1:B:296:MET:O	1:B:300:LEU:HG	2.15	0.46
1:A:324:ASP:OD1	1:A:327:GLU:HG3	2.14	0.46
1:A:361:LEU:O	1:A:365:LEU:HG	2.14	0.46
1:A:17:LYS:O	1:A:21:ARG:HG2	2.15	0.46
1:B:166:TYR:CD2	1:B:168:ASN:HB2	2.51	0.46
1:B:228:LEU:HD11	1:B:239:LEU:HD23	1.98	0.46
1:A:109:GLU:HA	1:A:109:GLU:OE1	2.16	0.45
1:A:331:ARG:NH2	1:A:335:ARG:NH2	2.56	0.45
1:B:15:GLU:C	1:B:17:LYS:H	2.24	0.45
1:A:303:VAL:CG1	1:A:375:LEU:HD12	2.46	0.45
1:B:27:LEU:CD1	1:B:333:VAL:HG13	2.46	0.45
1:B:362:GLU:H	1:B:362:GLU:CD	2.22	0.45
1:B:27:LEU:HA	1:B:336:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLY:O	1:A:130:VAL:HG23	2.16	0.44
1:A:110:PRO:O	1:A:111:GLU:HB2	2.17	0.44
1:A:311:ALA:C	1:A:312:THR:HG23	2.43	0.44
1:A:131:ALA:HB3	1:A:133:LEU:HG	1.98	0.44
1:A:267:VAL:O	1:A:270:MET:HB3	2.18	0.44
1:B:322:GLY:O	1:B:323:VAL:C	2.59	0.44
1:B:118:GLU:HG3	1:B:140:LEU:HD13	1.99	0.44
1:A:325:ASP:OD2	1:A:343:ARG:HB2	2.18	0.44
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.82	0.43
1:B:61:LEU:O	1:B:64:CYS:HB3	2.17	0.43
1:B:254:ARG:HH11	1:B:254:ARG:CG	2.01	0.43
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.93	0.43
1:B:318:ARG:HB2	1:B:352:PHE:CE2	2.53	0.43
1:B:141:ARG:HB2	1:B:143:ASP:OD1	2.17	0.43
1:A:324:ASP:OD2	1:A:343:ARG:NH2	2.51	0.43
1:B:194:LEU:CD2	1:B:194:LEU:C	2.92	0.43
1:A:113:LEU:CD2	1:A:158:GLU:HG3	2.48	0.43
1:A:303:VAL:HG22	1:A:372:ARG:HG3	2.00	0.43
1:B:116:LEU:O	1:B:137:LEU:HA	2.19	0.43
1:B:359:ARG:HD3	1:B:360:PRO:HD2	2.01	0.43
1:A:335:ARG:CD	1:A:374:ALA:HB2	2.48	0.42
1:A:4:VAL:HA	1:A:5:PRO:HD3	1.92	0.42
1:B:119:VAL:HB	1:B:140:LEU:HD21	2.01	0.42
1:A:54:PRO:HA	1:A:57:TYR:CE1	2.54	0.42
1:A:118:GLU:HA	1:A:137:LEU:HB3	2.01	0.42
1:B:373:GLU:C	1:B:375:LEU:H	2.27	0.42
1:A:22:GLU:O	1:A:24:GLY:N	2.53	0.42
1:A:166:TYR:CD2	1:A:168:ASN:HB2	2.55	0.42
1:A:319:LEU:HB3	1:A:323:VAL:CG2	2.49	0.41
1:B:201:VAL:HG13	1:B:202:ASP:N	2.35	0.41
1:A:17:LYS:HG2	1:A:27:LEU:HD21	2.03	0.41
1:A:68:PHE:HA	1:A:272:VAL:HG22	2.02	0.41
1:B:234:LEU:HD22	1:B:270:MET:HE2	2.02	0.41
1:A:66:LEU:HD13	1:A:66:LEU:HA	1.83	0.41
1:A:260:ASP:HB2	4:A:506:HOH:O	2.19	0.41
1:B:89:GLU:OE1	1:B:219:LYS:HD3	2.21	0.41
1:A:204:VAL:HA	1:A:311:ALA:CB	2.51	0.41
1:A:254:ARG:NH1	1:A:254:ARG:CG	2.73	0.41
1:B:21:ARG:O	1:B:22:GLU:C	2.64	0.41
1:B:27:LEU:HD21	1:B:338:ALA:HB2	2.02	0.41
1:B:118:GLU:HG2	1:B:138:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.79	0.41
1:A:18:ARG:HH11	1:A:18:ARG:HG3	1.86	0.41
1:A:331:ARG:HG2	1:A:331:ARG:HH11	1.85	0.40
1:B:97:GLN:NE2	1:B:123:SER:OG	2.54	0.40
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.82	0.40
1:A:106:ALA:HB1	1:A:251:ARG:HB3	2.02	0.40
1:B:39:PRO:HB3	1:B:233:ASN:O	2.21	0.40
1:B:361:LEU:HD22	1:B:365:LEU:HG	2.02	0.40
1:B:54:PRO:HA	1:B:57:TYR:CE1	2.56	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	370/376 (98%)	356 (96%)	14 (4%)	0	100	100
1	B	366/376 (97%)	336 (92%)	24 (7%)	6 (2%)	7	7
All	All	736/752 (98%)	692 (94%)	38 (5%)	6 (1%)	16	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	VAL
1	B	23	ARG
1	B	374	ALA
1	B	16	ALA
1	B	323	VAL
1	B	13	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	280/296 (95%)	269 (96%)	11 (4%)	28	43
1	B	265/296 (90%)	247 (93%)	18 (7%)	14	20
All	All	545/592 (92%)	516 (95%)	29 (5%)	20	30

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	66	LEU
1	A	110	PRO
1	A	170	PRO
1	A	194	LEU
1	A	254	ARG
1	A	279	LYS
1	A	291	GLU
1	A	315	LEU
1	A	323	VAL
1	A	331	ARG
1	B	87	ARG
1	B	158	GLU
1	B	165	ASN
1	B	170	PRO
1	B	194	LEU
1	B	206	GLU
1	B	213	LEU
1	B	225	LEU
1	B	252	LEU
1	B	254	ARG
1	B	270	MET
1	B	291	GLU
1	B	307	LEU
1	B	315	LEU
1	B	326	LEU
1	B	331	ARG

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Mol	Chain	Res	Type
1	B	361	LEU
1	B	362	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	203	GLN
1	A	262	ASN
1	B	52	ASN
1	B	190	HIS

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](#)

5 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	502	-	4,4,4	0.49	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	A	501	-	15,15,15	2.09	2 (13%)	19,20,20	1.64	3 (15%)
2	SO4	B	505	-	4,4,4	0.53	0	6,6,6	0.11	0
2	SO4	B	504	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	A	503	-	4,4,4	0.37	0	6,6,6	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	501	-	-	5/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	EPE	C9-N1	-5.49	1.34	1.47
3	A	501	EPE	C10-S	4.49	1.83	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	EPE	O1S-S-C10	4.99	114.28	106.73
3	A	501	EPE	O3S-S-O2S	-2.37	105.48	111.40
3	A	501	EPE	C3-C2-N1	2.29	115.27	110.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	EPE	C8-C7-N4-C3
3	A	501	EPE	C9-C10-S-O1S
3	A	501	EPE	C9-C10-S-O3S
3	A	501	EPE	C9-C10-S-O2S
3	A	501	EPE	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	EPE	5	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	372/376 (98%)	0.13	12 (3%) 50 52	24, 34, 50, 65	0
1	B	368/376 (97%)	0.29	23 (6%) 26 28	23, 34, 61, 81	0
All	All	740/752 (98%)	0.21	35 (4%) 36 38	23, 34, 57, 81	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	VAL	4.7
1	A	25	VAL	4.3
1	B	375	LEU	3.7
1	A	22	GLU	3.4
1	B	22	GLU	3.4
1	B	328	PHE	3.3
1	B	24	GLY	3.3
1	A	307	LEU	3.3
1	A	26	GLY	3.1
1	B	21	ARG	3.0
1	B	18	ARG	2.8
1	A	207	GLY	2.7
1	B	26	GLY	2.7
1	B	336	GLY	2.6
1	B	12	VAL	2.6
1	A	10	PHE	2.6
1	A	302	GLY	2.5
1	B	374	ALA	2.5
1	B	20	ALA	2.5
1	B	8	SER	2.4
1	A	375	LEU	2.4
1	A	322	GLY	2.3
1	A	88	ARG	2.3
1	B	373	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	283	ARG	2.3
1	B	298	GLU	2.3
1	B	27	LEU	2.3
1	A	158	GLU	2.2
1	B	302	GLY	2.2
1	A	208	GLU	2.1
1	B	23	ARG	2.1
1	B	323	VAL	2.1
1	B	322	GLY	2.1
1	B	206	GLU	2.0
1	B	365	LEU	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(Å ²)	Q<0.9
3	EPE	A	501	15/15	0.83	0.22	47,59,63,64	0
2	SO4	B	505	5/5	0.89	0.13	68,69,70,71	0
2	SO4	A	502	5/5	0.94	0.13	46,48,51,51	0
2	SO4	A	503	5/5	0.98	0.06	31,32,34,34	0
2	SO4	B	504	5/5	0.99	0.04	33,33,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.