



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:23 AM UTC

PDB ID : 3IJQ / pdb_00003ijq
Title : Structure of dipeptide epimerase from *Bacteroides thetaiotaomicron* complexed with L-Ala-D-Glu; productive substrate binding.
Authors : Fedorov, A.A.; Fedorov, E.V.; Lukk, T.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2009-08-04
Resolution : 2.00 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

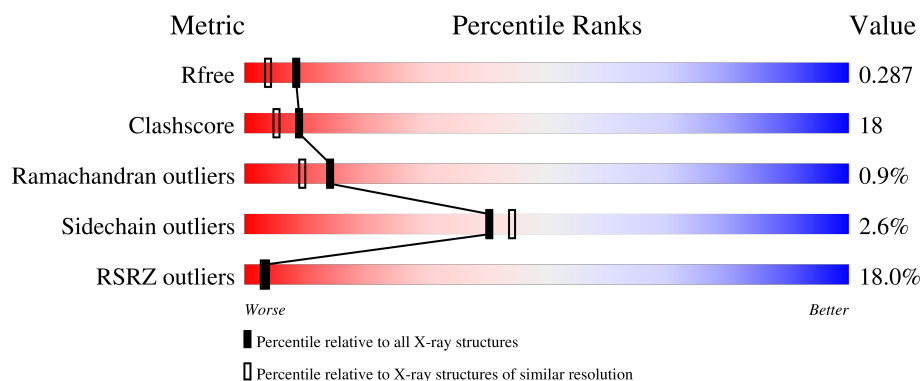
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	338	19% 68% 29% .
1	B	338	17% 64% 31% .

2 Entry composition [i](#)

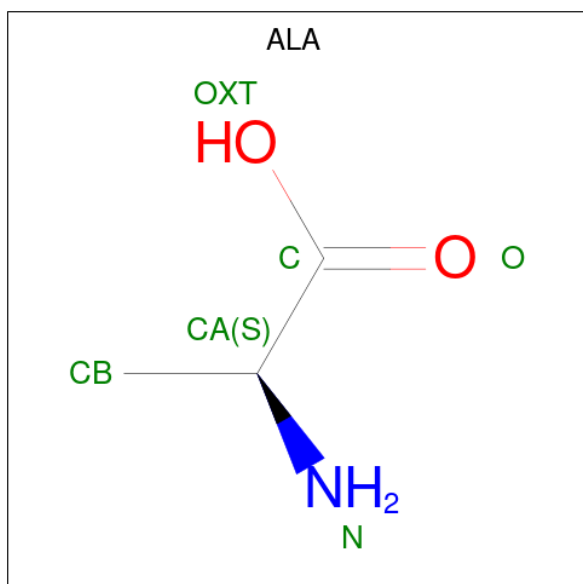
There are 6 unique types of molecules in this entry. The entry contains 5465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Muconate cycloisomerase.

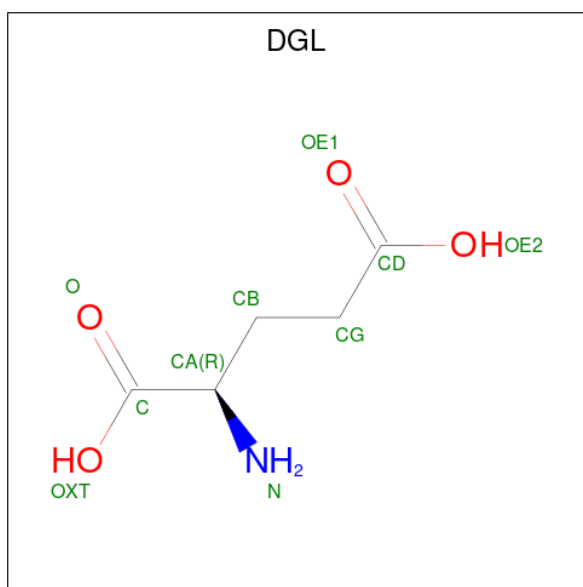
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2620	1677	429	495	19			
1	B	337	Total	C	N	O	S	0	0	0
			2620	1677	429	495	19			

- Molecule 2 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



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

- Molecule 3 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$).

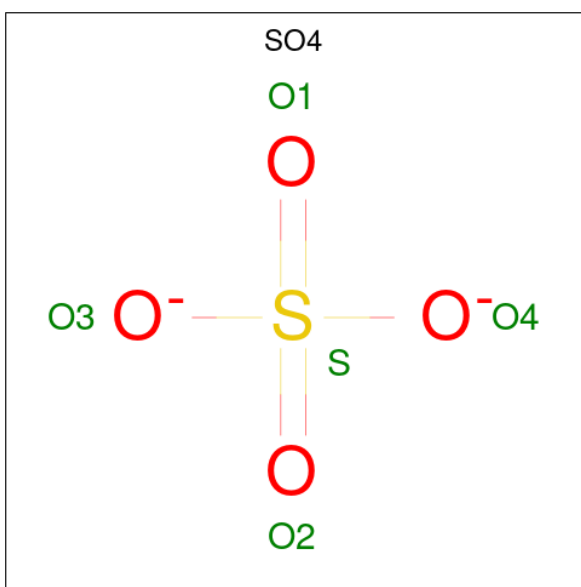


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		
6	B	103	Total	O	0	0
			103	103		

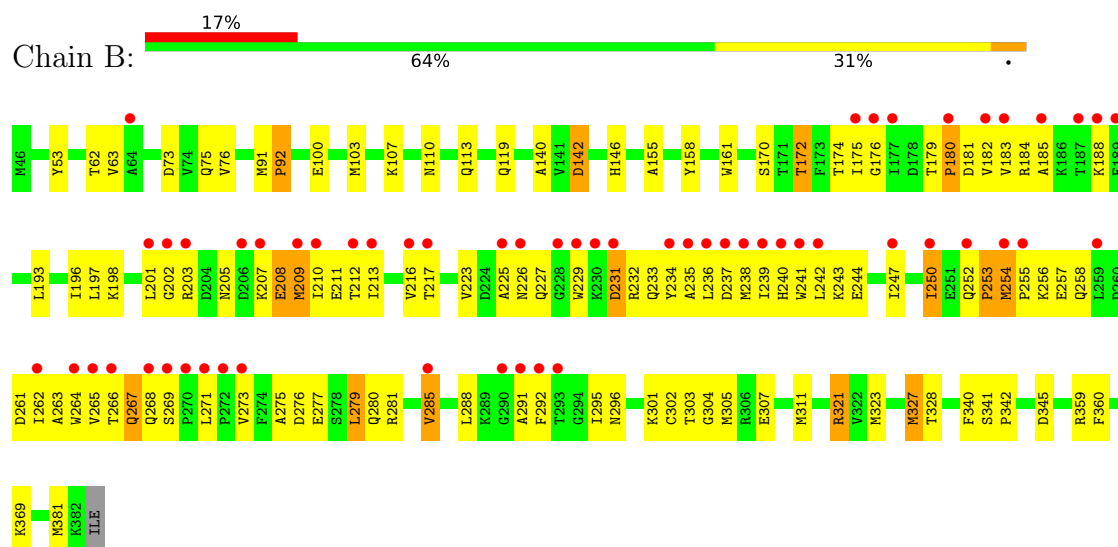
3 Residue-property plots

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: Muconate cycloisomerase



• Molecule 1: Muconate cycloisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.71Å 99.86Å 60.85Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	24.93 – 2.00 24.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (24.93-2.00) 96.1 (24.93-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.82Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.287 0.247 , 0.287	Depositor DCC
R_{free} test set	3197 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5465	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: DGL, MG, 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	0.38	0/2672	0.92	11/3621 (0.3%)
1	B	0.42	0/2672	0.94	9/3621 (0.2%)
All	All	0.40	0/5344	0.93	20/7242 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	THR	N-CA-C	-7.21	98.99	109.59
1	A	370	ILE	N-CA-C	-6.81	100.79	109.30
1	B	328	THR	N-CA-C	-6.78	99.62	109.59
1	B	327	MET	N-CA-C	-6.73	99.33	109.96
1	A	304	GLY	N-CA-C	6.68	119.87	111.85
1	A	327	MET	N-CA-C	-6.63	100.40	109.95
1	B	285	VAL	N-CA-C	6.61	117.23	110.82
1	B	304	GLY	N-CA-C	6.38	119.87	111.70
1	B	266	THR	N-CA-C	6.12	118.03	111.36
1	A	285	VAL	N-CA-C	6.06	116.18	110.30
1	B	174	THR	N-CA-C	6.05	119.38	109.76
1	B	305	MET	N-CA-C	5.95	117.77	111.28
1	B	92	PRO	N-CA-C	-5.89	103.51	110.70
1	A	305	MET	N-CA-C	5.66	117.13	111.07
1	A	92	PRO	N-CA-C	-5.63	103.83	110.70
1	A	96	GLY	N-CA-C	5.48	122.40	114.67
1	A	170	SER	N-CA-C	-5.37	101.71	110.20
1	A	116	ASP	CA-C-N	5.35	125.16	119.28
1	A	116	ASP	C-N-CA	5.35	125.16	119.28
1	B	155	ALA	N-CA-C	5.17	114.78	108.11

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	2620	0	2652	80	0
1	B	2620	0	2652	117	0
2	A	5	0	4	0	0
2	B	5	0	4	0	0
3	A	10	0	5	1	0
3	B	10	0	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	5	0	0	0	0
6	A	85	0	0	2	0
6	B	103	0	0	6	0
All	All	5465	0	5322	195	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 18.

All (195) 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:243:LYS:HD3	1:B:271:LEU:HD11	1.33	1.07
1:B:254:MET:HE3	1:B:261:ASP:HB3	1.35	1.05
1:B:175:ILE:HD11	1:B:197:LEU:HD13	1.42	1.00
1:B:227:GLN:NE2	1:B:256:LYS:H	1.60	0.98
1:B:232:ARG:HA	1:B:254:MET:HE1	1.46	0.97
1:B:75:GLN:HE21	1:B:359:ARG:HH11	1.10	0.92
1:B:227:GLN:HE21	1:B:256:LYS:H	1.05	0.90
1:A:231:ASP:HB3	1:A:234:TYR:HB3	1.53	0.90
1:B:227:GLN:HE21	1:B:256:LYS:N	1.71	0.88
1:A:180:PRO:HB3	1:A:184:ARG:HH12	1.40	0.87
1:A:75:GLN:HE21	1:A:359:ARG:HH11	1.19	0.87
1:B:183:VAL:HG21	1:B:209:MET:HE1	1.58	0.84
1:B:237:ASP:HA	1:B:240:HIS:HD2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:MET:HA	1:A:238:MET:HE2	1.61	0.83
1:B:209:MET:HE2	1:B:209:MET:HA	1.59	0.81
1:B:267:GLN:NE2	1:B:267:GLN:H	1.79	0.80
1:B:261:ASP:O	1:B:265:VAL:HG23	1.81	0.79
1:A:298:LYS:HE3	1:A:327:MET:HE1	1.68	0.75
1:B:75:GLN:HE21	1:B:359:ARG:NH1	1.85	0.74
1:B:254:MET:HE2	1:B:265:VAL:HG21	1.70	0.74
1:B:281:ARG:HB3	1:B:307:GLU:OE1	1.91	0.71
1:B:237:ASP:HA	1:B:240:HIS:CD2	2.24	0.70
1:B:75:GLN:NE2	1:B:359:ARG:HH11	1.88	0.69
1:B:243:LYS:HD3	1:B:271:LEU:CD1	2.17	0.68
1:B:210:ILE:HD12	1:B:247:ILE:HD11	1.75	0.68
1:B:254:MET:CE	1:B:261:ASP:HB3	2.20	0.68
1:A:177:ILE:HG13	1:A:209:MET:HE3	1.77	0.66
1:A:146:HIS:HE1	6:A:390:HOH:O	1.80	0.65
1:A:213:ILE:O	1:A:217:THR:HG22	1.97	0.65
1:A:66:TYR:CE2	1:A:93:PRO:HG2	2.34	0.63
1:B:231:ASP:HB3	1:B:234:TYR:HB3	1.81	0.62
1:B:53:TYR:O	1:B:73:ASP:HB3	2.00	0.62
1:A:298:LYS:HD2	1:A:327:MET:HE3	1.82	0.61
1:B:279:LEU:C	1:B:279:LEU:HD23	2.27	0.60
1:B:262:ILE:HG21	1:B:292:PHE:CZ	2.35	0.60
1:B:279:LEU:HD13	1:B:295:ILE:HB	1.83	0.60
1:B:280:GLN:NE2	1:B:301:LYS:HE3	2.16	0.60
1:B:254:MET:HE2	1:B:265:VAL:CG2	2.31	0.60
1:A:63:VAL:HG21	1:A:94:TYR:CE2	2.37	0.59
1:B:232:ARG:HD2	6:B:462:HOH:O	2.02	0.58
1:B:279:LEU:HD21	1:B:311:MET:HE1	1.86	0.58
1:B:232:ARG:HG2	1:B:264:TRP:CE3	2.37	0.58
1:B:227:GLN:HE22	1:B:256:LYS:HG2	1.68	0.58
1:B:327:MET:HA	3:B:385:DGL:HG3	1.86	0.57
1:B:252:GLN:HG2	1:B:277:GLU:OE1	2.04	0.57
1:A:227:GLN:HE21	1:A:256:LYS:H	1.51	0.57
1:A:327:MET:O	1:A:329:GLU:HG3	2.04	0.56
1:A:254:MET:CE	1:A:265:VAL:HG21	2.35	0.56
1:A:214:ARG:HH11	1:A:218:ASP:HA	1.70	0.56
1:B:205:ASN:HB2	1:B:208:GLU:HB3	1.87	0.56
1:A:252:GLN:HG2	1:A:277:GLU:OE1	2.04	0.56
1:B:209:MET:HA	1:B:209:MET:CE	2.35	0.55
1:B:321:ARG:HG3	1:B:345:ASP:OD2	2.06	0.55
1:B:179:THR:OG1	1:B:182:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:HB2	6:B:477:HOH:O	2.06	0.55
1:A:231:ASP:HB3	1:A:234:TYR:CB	2.34	0.55
1:B:279:LEU:HB2	1:B:288:LEU:HD11	1.89	0.55
1:B:225:ALA:HB3	1:B:253:PRO:HA	1.88	0.54
1:B:142:ASP:O	1:B:146:HIS:HD2	1.89	0.54
1:B:239:ILE:HG21	1:B:269:SER:OG	2.08	0.54
1:B:279:LEU:HB2	1:B:288:LEU:CD1	2.37	0.54
1:B:184:ARG:HD2	1:B:216:VAL:HG13	1.89	0.53
1:A:281:ARG:HB3	1:A:307:GLU:OE1	2.08	0.53
1:B:256:LYS:HG3	1:B:257:GLU:OE2	2.07	0.53
1:B:205:ASN:O	1:B:208:GLU:HB3	2.09	0.53
1:B:267:GLN:H	1:B:267:GLN:CD	2.16	0.53
1:A:184:ARG:HD2	1:A:216:VAL:HG13	1.91	0.53
1:B:275:ALA:HB2	1:B:292:PHE:CD2	2.44	0.53
1:B:63:VAL:HG13	1:B:226:ASN:HD21	1.73	0.53
1:A:254:MET:HB2	1:A:255:PRO:HD2	1.90	0.53
1:A:53:TYR:O	1:A:73:ASP:HB3	2.08	0.52
1:B:236:LEU:HD11	1:B:268:GLN:O	2.08	0.52
1:B:254:MET:HE3	1:B:261:ASP:CB	2.25	0.52
1:A:142:ASP:O	1:A:146:HIS:HD2	1.92	0.52
1:A:232:ARG:HB3	1:A:261:ASP:OD2	2.09	0.52
1:B:202:GLY:HA3	1:B:225:ALA:O	2.10	0.52
1:A:75:GLN:NE2	1:A:359:ARG:HH11	1.99	0.52
1:B:261:ASP:HA	6:B:462:HOH:O	2.10	0.52
1:B:276:ASP:O	1:B:301:LYS:NZ	2.43	0.52
1:B:238:MET:O	1:B:242:LEU:HG	2.10	0.51
1:A:46:MET:HE1	1:A:145:LEU:HD21	1.92	0.51
1:B:110:ASN:HB3	1:B:113:GLN:HE21	1.75	0.51
1:B:279:LEU:HD21	1:B:311:MET:CE	2.40	0.51
1:A:261:ASP:O	1:A:264:TRP:HB3	2.11	0.51
1:A:229:TRP:O	1:A:254:MET:HB3	2.11	0.51
1:A:254:MET:HE1	1:A:265:VAL:HG21	1.91	0.51
1:B:161:TRP:CZ3	1:B:340:PHE:HB3	2.46	0.51
1:B:280:GLN:HE22	1:B:301:LYS:HE3	1.75	0.50
1:A:66:TYR:HE2	1:A:93:PRO:HG2	1.76	0.50
1:B:235:ALA:O	1:B:239:ILE:HG13	2.11	0.50
1:A:280:GLN:HE22	1:A:301:LYS:HD2	1.77	0.50
1:B:76:VAL:HG21	1:B:140:ALA:HB1	1.94	0.50
1:A:57:LEU:HD13	1:A:61:PHE:HB2	1.93	0.50
1:A:287:ALA:O	1:A:288:LEU:HD23	2.12	0.50
1:A:341:SER:N	1:A:342:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:HH11	1:A:212:THR:HG23	1.76	0.49
1:A:177:ILE:HD12	1:A:177:ILE:N	2.27	0.49
1:B:277:GLU:HA	6:B:469:HOH:O	2.12	0.49
1:B:146:HIS:HE1	6:B:393:HOH:O	1.95	0.49
1:B:341:SER:N	1:B:342:PRO:CD	2.76	0.49
1:A:92:PRO:O	1:A:94:TYR:N	2.46	0.49
1:B:75:GLN:HE22	1:B:360:PHE:HE2	1.60	0.48
1:B:184:ARG:HD2	1:B:216:VAL:CG1	2.42	0.48
1:B:210:ILE:HG13	1:B:242:LEU:CD2	2.43	0.48
1:A:89:ALA:HB2	1:A:140:ALA:HB2	1.94	0.48
1:A:92:PRO:C	1:A:94:TYR:H	2.21	0.48
1:B:175:ILE:HG21	1:B:213:ILE:CD1	2.42	0.48
1:A:168:THR:O	1:A:369:LYS:HE3	2.14	0.48
1:B:103:MET:O	1:B:107:LYS:HG3	2.13	0.47
1:B:110:ASN:HB3	1:B:113:GLN:NE2	2.29	0.47
1:B:263:ALA:O	1:B:267:GLN:NE2	2.46	0.47
1:A:254:MET:HB2	1:A:255:PRO:CD	2.45	0.47
1:B:227:GLN:NE2	1:B:256:LYS:N	2.41	0.47
1:B:247:ILE:HG22	1:B:271:LEU:HD23	1.97	0.47
1:A:75:GLN:HE21	1:A:359:ARG:NH1	1.98	0.47
1:A:207:LYS:HA	1:A:241:TRP:CH2	2.49	0.47
1:B:91:MET:O	1:B:92:PRO:C	2.58	0.47
1:B:63:VAL:HG13	1:B:226:ASN:ND2	2.30	0.46
1:B:279:LEU:HD11	1:B:285:VAL:HG22	1.97	0.46
1:A:161:TRP:CZ3	1:A:340:PHE:HB3	2.51	0.46
1:B:210:ILE:HG13	1:B:241:TRP:HZ3	1.80	0.46
1:B:301:LYS:NZ	6:B:412:HOH:O	2.44	0.46
1:B:257:GLU:H	1:B:257:GLU:CD	2.22	0.46
1:A:189:GLU:O	1:B:381:MET:HG3	2.16	0.46
1:B:213:ILE:O	1:B:217:THR:HG22	2.16	0.46
1:B:237:ASP:C	1:B:239:ILE:N	2.73	0.46
1:A:177:ILE:HG23	1:A:209:MET:CE	2.46	0.45
1:A:275:ALA:HB2	1:A:292:PHE:CD2	2.51	0.45
1:B:231:ASP:CG	1:B:232:ARG:H	2.24	0.45
1:B:258:GLN:HB3	1:B:261:ASP:OD2	2.16	0.45
1:A:236:LEU:O	1:A:240:HIS:CD2	2.70	0.45
1:B:275:ALA:HB2	1:B:292:PHE:CG	2.51	0.45
1:A:174:THR:HG21	1:A:200:LYS:HE2	1.97	0.45
1:A:341:SER:O	1:A:344:VAL:HG22	2.16	0.45
1:A:184:ARG:HD2	1:A:216:VAL:CG1	2.46	0.45
1:B:226:ASN:O	1:B:227:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:HB	1:A:212:THR:HG21	1.98	0.45
1:B:172:THR:HG22	1:B:196:ILE:HG12	1.99	0.45
1:B:237:ASP:C	1:B:239:ILE:H	2.24	0.45
1:A:99:VAL:O	1:A:103:MET:HG2	2.17	0.45
1:A:238:MET:HA	1:A:238:MET:CE	2.39	0.45
1:B:172:THR:HB	1:B:198:LYS:HB2	1.98	0.45
1:B:180:PRO:O	1:B:184:ARG:NH1	2.51	0.44
1:B:227:GLN:NE2	1:B:255:PRO:HA	2.32	0.44
1:A:68:ARG:HD2	1:A:70:THR:O	2.18	0.44
1:B:231:ASP:CB	1:B:234:TYR:HB3	2.46	0.44
1:A:227:GLN:NE2	1:A:256:LYS:HG2	2.33	0.44
1:A:178:ASP:OD1	1:A:179:THR:N	2.41	0.44
1:A:369:LYS:HE2	1:A:369:LYS:HB3	1.82	0.43
1:A:239:ILE:HG21	1:A:269:SER:OG	2.19	0.43
1:A:91:MET:O	1:A:92:PRO:C	2.60	0.43
1:A:298:LYS:HD2	1:A:327:MET:CE	2.48	0.43
1:B:232:ARG:HG2	1:B:264:TRP:CZ3	2.53	0.43
1:A:175:ILE:HD12	1:A:187:THR:HA	2.01	0.43
1:B:229:TRP:HE3	1:B:235:ALA:HB1	1.83	0.43
1:B:263:ALA:HA	1:B:291:ALA:HA	2.00	0.43
1:A:177:ILE:CG2	1:A:205:ASN:HD21	2.32	0.43
1:A:327:MET:C	1:A:329:GLU:HG3	2.44	0.42
1:A:243:LYS:HD2	1:A:270:PRO:HB2	2.01	0.42
1:B:179:THR:O	1:B:181:ASP:N	2.52	0.42
1:B:227:GLN:HG2	1:B:254:MET:O	2.19	0.42
1:A:72:PRO:HD2	1:A:93:PRO:HD3	2.01	0.42
1:B:202:GLY:HA2	1:B:229:TRP:CD1	2.54	0.42
1:B:267:GLN:CD	1:B:267:GLN:N	2.76	0.42
1:A:237:ASP:O	1:A:240:HIS:HB2	2.20	0.42
1:B:227:GLN:CG	1:B:255:PRO:HA	2.50	0.42
1:B:207:LYS:HA	1:B:241:TRP:CH2	2.54	0.42
1:B:233:GLN:HE22	1:B:236:LEU:HD23	1.85	0.42
1:A:254:MET:HE3	1:A:265:VAL:HG21	2.01	0.42
1:B:158:TYR:CD1	1:B:158:TYR:C	2.98	0.42
1:B:302:CYS:C	1:B:303:THR:HG23	2.45	0.42
1:A:214:ARG:HH22	1:A:221:ILE:HG13	1.84	0.42
1:A:155:ALA:HA	1:A:156:PRO:HD3	1.88	0.42
1:B:223:VAL:HG21	1:B:242:LEU:HD13	2.01	0.42
1:A:229:TRP:HE3	1:A:235:ALA:HB1	1.84	0.41
1:B:170:SER:HA	1:B:369:LYS:HA	2.03	0.41
1:B:296:ASN:HA	1:B:323:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ALA:O	1:A:143:ILE:HG13	2.20	0.41
1:A:61:PHE:HE2	3:A:385:DGL:HG3	1.85	0.41
1:B:280:GLN:CD	1:B:301:LYS:HE3	2.45	0.41
1:A:158:TYR:CD1	1:A:158:TYR:C	2.98	0.41
1:A:322:VAL:HG12	1:A:323:MET:N	2.35	0.41
1:A:188:LYS:NZ	1:A:188:LYS:HB3	2.36	0.41
1:A:326:CYS:C	1:A:327:MET:HE2	2.46	0.41
1:A:381:MET:HE2	1:B:193:LEU:HD12	2.03	0.41
1:B:211:GLU:O	1:B:212:THR:C	2.64	0.41
1:A:133:LYS:HB2	6:A:409:HOH:O	2.20	0.41
1:A:326:CYS:O	1:A:327:MET:HE2	2.21	0.41
1:B:247:ILE:HD12	1:B:247:ILE:N	2.36	0.41
1:B:62:THR:HG21	1:B:203:ARG:HH21	1.85	0.40
1:B:185:ALA:O	1:B:188:LYS:HB3	2.22	0.40
1:B:241:TRP:O	1:B:244:GLU:N	2.49	0.40
1:B:307:GLU:O	1:B:311:MET:HG3	2.21	0.40
1:A:255:PRO:HB2	1:A:258:GLN:NE2	2.36	0.40
1:B:250:ILE:O	1:B:273:VAL:HA	2.21	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	335/338 (99%)	309 (92%)	25 (8%)	1 (0%)	36	35
1	B	335/338 (99%)	307 (92%)	23 (7%)	5 (2%)	8	4
All	All	670/676 (99%)	616 (92%)	48 (7%)	6 (1%)	14	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	LEU
1	B	231	ASP
1	A	93	PRO
1	B	176	GLY
1	B	253	PRO
1	B	180	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/289 (100%)	283 (98%)	5 (2%)	53	60
1	B	288/289 (100%)	278 (96%)	10 (4%)	32	32
All	All	576/578 (100%)	561 (97%)	15 (3%)	40	44

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	142	ASP
1	A	200	LYS
1	A	238	MET
1	A	364	GLU
1	B	119	GLN
1	B	142	ASP
1	B	172	THR
1	B	208	GLU
1	B	209	MET
1	B	250	ILE
1	B	254	MET
1	B	267	GLN
1	B	279	LEU
1	B	321	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	104	ASN
1	A	110	ASN
1	A	146	HIS
1	A	227	GLN
1	A	240	HIS
1	A	258	GLN
1	A	268	GLN
1	A	280	GLN
1	B	75	GLN
1	B	113	GLN
1	B	119	GLN
1	B	146	HIS
1	B	205	ASN
1	B	226	ASN
1	B	227	GLN
1	B	233	GLN
1	B	258	GLN
1	B	267	GLN
1	B	268	GLN
1	B	280	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
5	SO4	B	387	-	4,4,4	0.52	0	6,6,6	0.50	0
2	ALA	B	384	3	3,4,5	0.57	0	2,4,6	0.66	0
3	DGL	A	385	2	8,9,9	1.02	0	8,11,11	0.90	0
3	DGL	B	385	2,4	8,9,9	1.17	0	8,11,11	0.87	0
2	ALA	A	384	3	3,4,5	0.47	0	2,4,6	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	ALA	B	384	3	-	0/1/2/4	-
3	DGL	A	385	2	-	3/9/9/9	-
2	ALA	A	384	3	-	0/1/2/4	-
3	DGL	B	385	2,4	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	385	DGL	C-CA-CB-CG
3	A	385	DGL	OE1-CD-CG-CB
3	A	385	DGL	OE2-CD-CG-CB
3	B	385	DGL	O-C-CA-CB
3	B	385	DGL	OXT-C-CA-CB
3	B	385	DGL	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	385	DGL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	385	DGL	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	337/338 (99%)	0.87	63 (18%) 3 3	24, 44, 76, 83	0
1	B	337/338 (99%)	0.64	58 (17%) 4 3	22, 38, 78, 90	0
All	All	674/676 (99%)	0.75	121 (17%) 3 3	22, 41, 77, 90	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	TRP	6.2
1	B	235	ALA	5.3
1	A	225	ALA	5.3
1	A	229	TRP	5.0
1	B	210	ILE	4.8
1	B	291	ALA	4.6
1	A	234	TYR	4.3
1	B	183	VAL	4.3
1	A	262	ILE	4.3
1	B	240	HIS	4.2
1	B	176	GLY	4.2
1	B	177	ILE	4.2
1	B	234	TYR	4.2
1	A	264	TRP	4.1
1	A	210	ILE	4.0
1	B	242	LEU	4.0
1	A	239	ILE	4.0
1	A	182	VAL	4.0
1	B	270	PRO	3.9
1	B	213	ILE	3.9
1	A	64	ALA	3.9
1	B	236	LEU	3.8
1	B	269	SER	3.8
1	B	271	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	3.6
1	B	241	TRP	3.6
1	B	182	VAL	3.6
1	B	206	ASP	3.5
1	A	65	THR	3.5
1	A	228	GLY	3.5
1	B	202	GLY	3.5
1	A	180	PRO	3.5
1	A	253	PRO	3.5
1	A	236	LEU	3.5
1	A	202	GLY	3.3
1	A	271	LEU	3.3
1	A	183	VAL	3.3
1	A	223	VAL	3.2
1	B	238	MET	3.2
1	A	201	LEU	3.2
1	A	242	LEU	3.1
1	A	235	ALA	3.1
1	B	239	ILE	3.1
1	B	264	TRP	3.1
1	A	176	GLY	3.1
1	A	66	TYR	3.0
1	A	177	ILE	3.0
1	B	266	THR	3.0
1	A	265	VAL	3.0
1	B	265	VAL	3.0
1	B	262	ILE	3.0
1	B	255	PRO	2.9
1	B	175	ILE	2.9
1	A	93	PRO	2.9
1	A	256	LYS	2.9
1	A	291	ALA	2.9
1	A	206	ASP	2.9
1	B	207	LYS	2.9
1	A	241	TRP	2.9
1	B	259	LEU	2.8
1	B	228	GLY	2.8
1	B	231	ASP	2.8
1	A	230	LYS	2.8
1	B	216	VAL	2.8
1	A	213	ILE	2.8
1	B	209	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	267	GLN	2.7
1	A	268	GLN	2.7
1	B	254	MET	2.7
1	A	250	ILE	2.7
1	B	225	ALA	2.6
1	A	187	THR	2.6
1	A	255	PRO	2.6
1	B	180	PRO	2.6
1	B	273	VAL	2.6
1	B	268	GLN	2.6
1	B	212	THR	2.6
1	B	237	ASP	2.6
1	A	240	HIS	2.6
1	A	175	ILE	2.5
1	A	278	SER	2.5
1	A	95	LEU	2.5
1	B	226	ASN	2.5
1	A	238	MET	2.5
1	B	201	LEU	2.4
1	A	231	ASP	2.4
1	A	254	MET	2.4
1	A	270	PRO	2.4
1	A	263	ALA	2.4
1	B	185	ALA	2.4
1	A	105	PHE	2.4
1	B	293	THR	2.4
1	A	252	GLN	2.3
1	A	211	GLU	2.3
1	A	247	ILE	2.3
1	A	63	VAL	2.3
1	B	203	ARG	2.3
1	B	189	GLU	2.3
1	B	285	VAL	2.3
1	A	212	THR	2.3
1	B	272	PRO	2.3
1	A	260	ASP	2.3
1	A	275	ALA	2.3
1	B	290	GLY	2.3
1	A	244	GLU	2.2
1	A	273	VAL	2.2
1	B	187	THR	2.2
1	A	261	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	252	GLN	2.2
1	A	318	LEU	2.1
1	B	247	ILE	2.1
1	A	199	VAL	2.1
1	B	64	ALA	2.1
1	B	230	LYS	2.1
1	A	293	THR	2.1
1	B	250	ILE	2.1
1	B	292	PHE	2.1
1	B	188	LYS	2.1
1	A	269	SER	2.1
1	A	62	THR	2.0
1	B	217	THR	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
5	SO4	B	387	5/5	0.84	0.11	62,63,64,64	0
2	ALA	A	384	5/6	0.85	0.14	46,47,48,49	0
3	DGL	A	385	10/10	0.86	0.13	50,52,55,55	0
4	MG	A	386	1/1	0.87	0.12	53,53,53,53	0
3	DGL	B	385	10/10	0.89	0.10	35,37,38,40	0
2	ALA	B	384	5/6	0.92	0.08	26,29,32,33	0
4	MG	B	386	1/1	0.98	0.03	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.