



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:42 PM UTC

PDB ID : 1TUF / pdb_00001tuf
Title : Crystal structure of Diaminopimelate Decarboxylase from *m. jannaschi*
Authors : Rajashankar, K.; Ray, S.R.; Bonanno, J.B.; Pinho, M.G.; He, G.; De Lencastre, H.; Tomasz, A.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-06-24
Resolution : 2.40 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

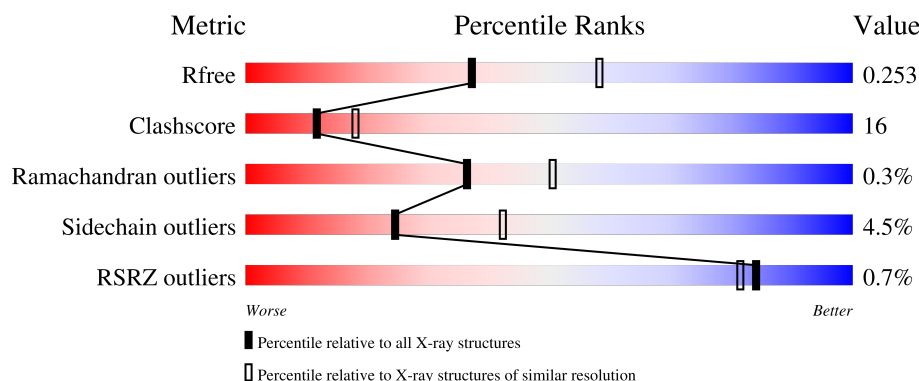
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	434	 64% 34% .
1	B	434	 68% 28% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7142 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.

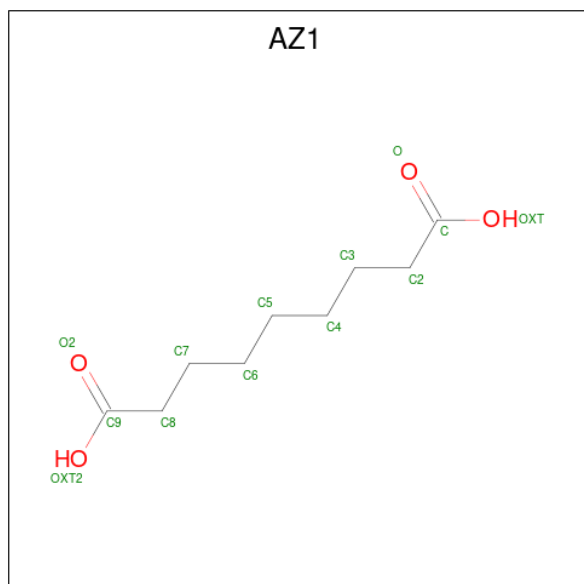
- Molecule 1 is a protein called Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	P	S	0	0	0
			3412	2178	569	644	1	20			
1	B	434	Total	C	N	O	P	S	0	0	0
			3412	2178	569	644	1	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	LLP	LYS	modified residue	UNP Q58497
B	83	LLP	LYS	modified residue	UNP Q58497

- Molecule 2 is AZELAIC ACID (CCD ID: AZ1) (formula: C₉H₁₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	9	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	9	4		

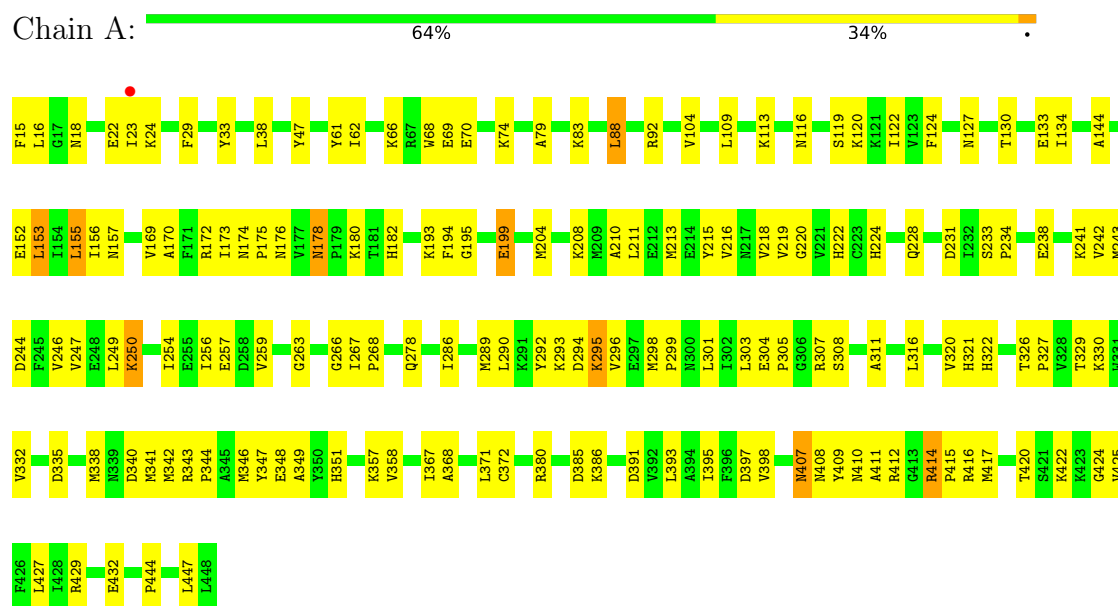
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	179	Total	O	0	0
			179	179		

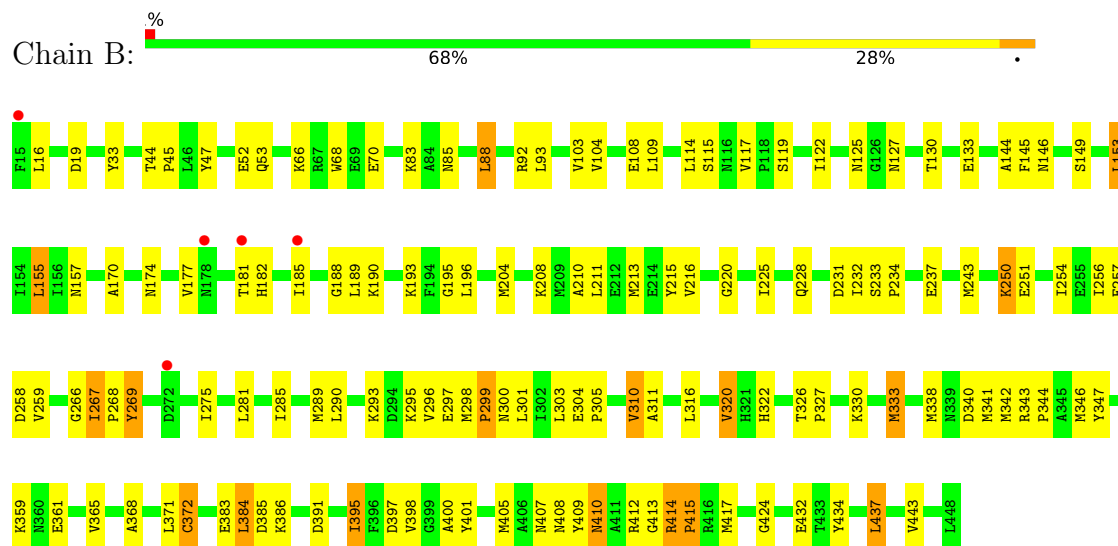
3 Residue-property plots

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: Diaminopimelate decarboxylase



• Molecule 1: Diaminopimelate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.81Å 80.81Å 508.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 25.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.3 (25.00-2.40) 88.3 (25.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.253 0.203 , 0.253	Depositor DCC
R_{free} test set	1804 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7142	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: AZ1, LLP

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	0.42	0/3445	0.90	11/4646 (0.2%)
1	B	0.45	0/3445	0.90	11/4646 (0.2%)
All	All	0.43	0/6890	0.90	22/9292 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	VAL	N-CA-C	5.89	116.61	108.12
1	B	415	PRO	N-CA-C	5.78	119.32	111.22
1	A	342	MET	N-CA-C	5.78	120.06	112.89
1	B	195	GLY	N-CA-C	5.76	122.76	112.22
1	A	170	ALA	N-CA-C	-5.67	101.61	110.17
1	B	225	ILE	N-CA-C	5.55	120.05	113.22
1	B	397	ASP	N-CA-C	5.55	118.90	111.24
1	B	269	TYR	N-CA-C	-5.54	105.32	111.36
1	B	145	PHE	N-CA-C	-5.48	100.37	109.46
1	B	342	MET	N-CA-C	5.40	119.71	113.18
1	B	144	ALA	N-CA-C	5.39	116.71	108.52
1	B	310	VAL	N-CA-C	5.33	118.30	112.96
1	B	117	VAL	N-CA-C	-5.28	104.09	108.63
1	B	170	ALA	N-CA-C	-5.17	101.90	109.81
1	A	178	ASN	CA-C-N	5.15	125.45	119.47
1	A	178	ASN	C-N-CA	5.15	125.45	119.47
1	A	174	ASN	CA-C-N	5.09	125.08	119.89
1	A	174	ASN	C-N-CA	5.09	125.08	119.89
1	A	144	ALA	N-CA-C	5.09	116.80	108.76
1	A	182	HIS	CA-C-N	5.08	124.52	119.24
1	A	182	HIS	C-N-CA	5.08	124.52	119.24
1	A	194	PHE	N-CA-C	5.00	116.98	110.53

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	3412	0	3462	135	0
1	B	3412	0	3461	106	0
2	A	13	0	12	0	0
2	B	13	0	12	0	0
3	A	113	0	0	1	0
3	B	179	0	0	3	0
All	All	7142	0	6947	219	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 16.

All (219) 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:371:LEU:HD21	1:A:412:ARG:HD2	1.44	0.97
1:B:407:ASN:HD22	1:B:409:TYR:H	1.22	0.86
1:A:407:ASN:HD22	1:A:409:TYR:H	1.24	0.85
1:B:401:TYR:HB3	1:B:405:MET:HE2	1.57	0.82
1:A:175:PRO:HB3	1:A:241:LYS:HB3	1.61	0.82
1:B:243:MET:HE1	1:B:259:VAL:HG21	1.61	0.82
1:A:316:LEU:HB3	1:A:395:ILE:CG2	2.14	0.77
1:B:316:LEU:HB3	1:B:395:ILE:HG23	1.68	0.76
1:A:113:LYS:HE2	1:A:113:LYS:HA	1.69	0.75
1:A:153:LEU:HD11	1:A:210:ALA:HB2	1.68	0.74
1:B:371:LEU:HD21	1:B:412:ARG:HD3	1.70	0.72
1:A:47:TYR:HB2	1:A:417:MET:HG2	1.72	0.72
1:B:250:LYS:HG3	1:B:296:VAL:HG22	1.72	0.71
1:B:19:ASP:H	1:B:53:GLN:HE22	1.39	0.71
1:A:338:MET:HG2	1:A:371:LEU:HD12	1.73	0.70
1:A:420:THR:HG22	1:A:425:VAL:HG12	1.71	0.70
1:A:127:ASN:HB2	1:B:333:MET:HE3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:C	1:B:305:PRO:HD3	2.17	0.68
1:B:232:ILE:HD11	1:B:281:LEU:HA	1.75	0.68
1:A:267:ILE:HD11	1:A:308:SER:HA	1.75	0.68
1:B:182:HIS:HB3	1:B:185:ILE:HD13	1.76	0.68
1:A:343:ARG:HD3	1:A:351:HIS:NE2	2.10	0.67
1:A:371:LEU:CD2	1:A:412:ARG:HD2	2.20	0.67
1:A:220:GLY:HA2	1:A:256:ILE:HG23	1.77	0.67
1:A:233:SER:HB3	1:A:234:PRO:HD3	1.76	0.67
1:A:224:HIS:HD2	1:A:263:GLY:H	1.41	0.66
1:B:289:MET:HE2	1:B:301:LEU:HD13	1.77	0.66
1:B:407:ASN:ND2	1:B:409:TYR:H	1.92	0.66
1:B:326:THR:HB	1:B:327:PRO:HD2	1.78	0.64
1:A:157:ASN:ND2	1:A:213:MET:HB3	2.12	0.64
1:B:343:ARG:HB3	1:B:344:PRO:HD3	1.78	0.64
1:A:289:MET:HE2	1:A:301:LEU:HD13	1.80	0.64
1:A:414:ARG:NH2	1:B:408:ASN:HD22	1.96	0.64
1:A:417:MET:HB2	1:A:429:ARG:HB3	1.79	0.64
1:B:341:MET:HE1	1:B:344:PRO:HD3	1.80	0.63
1:B:157:ASN:HD21	1:B:215:TYR:H	1.46	0.63
1:A:303:LEU:C	1:A:305:PRO:HD3	2.23	0.62
1:A:407:ASN:ND2	1:A:409:TYR:H	1.95	0.62
1:A:15:PHE:N	1:A:18:ASN:HD22	1.97	0.61
1:A:127:ASN:HD22	1:B:333:MET:HE3	1.65	0.61
1:A:320:VAL:HG12	1:A:391:ASP:O	2.01	0.61
1:A:267:ILE:HD11	1:A:308:SER:CA	2.31	0.60
1:A:244:ASP:O	1:A:247:VAL:HG22	2.01	0.60
1:A:243:MET:HE1	1:A:259:VAL:HG21	1.82	0.60
1:A:408:ASN:ND2	1:B:414:ARG:NH2	2.49	0.60
1:B:383:GLU:C	1:B:384:LEU:HD23	2.26	0.60
1:A:343:ARG:HB3	1:A:344:PRO:HD3	1.85	0.59
1:A:16:LEU:HD22	1:A:268:PRO:HB3	1.83	0.59
1:A:33:TYR:OH	1:A:424:GLY:HA2	2.02	0.59
1:A:104:VAL:HG21	1:B:372:CYS:HB2	1.83	0.59
1:A:267:ILE:HD13	1:A:307:ARG:HD2	1.83	0.59
1:A:23:ILE:HD11	1:A:358:VAL:HG21	1.85	0.58
1:A:408:ASN:ND2	1:B:414:ARG:HH22	1.99	0.58
1:A:211:LEU:HD21	1:A:218:VAL:HG21	1.85	0.58
1:B:330:LYS:HD3	1:B:365:VAL:HG12	1.86	0.58
1:A:243:MET:HA	1:A:243:MET:HE2	1.84	0.58
1:A:231:ASP:O	1:A:234:PRO:HD2	2.04	0.57
1:A:408:ASN:HD22	1:B:414:ARG:NH2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LEU:CD2	1:B:412:ARG:HD3	2.34	0.56
1:A:340:ASP:OD1	1:A:415:PRO:HD3	2.05	0.56
1:B:267:ILE:HD11	1:B:269:TYR:CE1	2.40	0.56
1:A:157:ASN:HD22	1:A:216:VAL:HG13	1.69	0.56
1:A:298:MET:HA	1:A:298:MET:HE2	1.89	0.55
1:B:92:ARG:HH11	1:B:115:SER:HA	1.72	0.55
1:B:182:HIS:CD2	1:B:234:PRO:HG3	2.41	0.55
1:A:134:ILE:HD12	1:A:155:LEU:HD13	1.89	0.55
1:A:204:MET:HE2	1:A:208:LYS:HG3	1.89	0.54
1:B:157:ASN:HD22	1:B:216:VAL:HG13	1.72	0.54
1:A:243:MET:HE2	1:A:246:VAL:HG21	1.90	0.54
1:A:412:ARG:HD3	3:A:534:HOH:O	2.08	0.54
1:A:385:ASP:O	1:A:386:LYS:C	2.52	0.53
1:B:233:SER:HB3	1:B:234:PRO:HD3	1.90	0.53
1:A:322:HIS:CE1	1:B:155:LEU:HD12	2.42	0.53
1:A:266:GLY:C	1:A:267:ILE:HD12	2.34	0.53
1:A:62:ILE:HG22	1:A:66:LYS:HE3	1.91	0.53
1:B:371:LEU:CD2	1:B:412:ARG:CD	2.87	0.53
1:B:149:SER:HA	1:B:196:LEU:HD21	1.91	0.52
1:A:250:LYS:HG3	1:A:296:VAL:HG12	1.91	0.52
1:B:341:MET:HE2	1:B:398:VAL:HG12	1.91	0.52
1:A:444:PRO:HD2	1:A:447:LEU:HD12	1.91	0.52
1:B:220:GLY:HA2	1:B:256:ILE:HG23	1.90	0.52
1:B:293:LYS:HA	1:B:298:MET:HE3	1.91	0.52
1:A:104:VAL:HG21	1:B:372:CYS:SG	2.50	0.52
1:B:92:ARG:NH1	1:B:114:LEU:O	2.42	0.52
1:B:408:ASN:HA	1:B:412:ARG:O	2.10	0.52
1:B:410:ASN:N	1:B:410:ASN:HD22	2.07	0.52
1:B:213:MET:HB2	1:B:216:VAL:HG22	1.92	0.51
1:A:326:THR:HB	1:A:327:PRO:HD2	1.92	0.51
1:B:66:LYS:O	1:B:70:GLU:HG3	2.10	0.51
1:A:224:HIS:CD2	1:A:263:GLY:H	2.26	0.51
1:A:414:ARG:HD3	1:A:432:GLU:OE1	2.10	0.51
1:A:411:ALA:HB3	1:B:108:GLU:HG2	1.92	0.50
1:B:408:ASN:OD1	1:B:413:GLY:HA2	2.11	0.50
1:B:346:MET:HE2	1:B:347:TYR:OH	2.12	0.50
1:B:414:ARG:HD3	1:B:432:GLU:OE1	2.12	0.50
1:A:155:LEU:HD12	1:B:322:HIS:CE1	2.47	0.50
1:A:332:VAL:HG11	1:A:393:LEU:HD11	1.94	0.50
1:A:243:MET:CE	1:A:246:VAL:HG21	2.42	0.50
1:A:367:ILE:N	1:A:367:ILE:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:O	1:A:92:ARG:HB2	2.12	0.49
1:B:153:LEU:HD11	1:B:210:ALA:HB2	1.94	0.49
1:A:204:MET:HE2	1:A:208:LYS:HE3	1.94	0.49
1:A:68:TRP:CH2	1:A:289:MET:HE3	2.48	0.49
1:A:341:MET:HE2	1:A:398:VAL:HG12	1.93	0.49
1:B:88:LEU:O	1:B:92:ARG:HB2	2.13	0.49
1:B:371:LEU:HD21	1:B:412:ARG:CD	2.42	0.49
1:A:321:HIS:HD2	3:B:551:HOH:O	1.94	0.49
1:B:130:THR:OG1	1:B:133:GLU:HG3	2.12	0.49
1:B:338:MET:HG2	1:B:371:LEU:HD12	1.95	0.49
1:A:368:ALA:HB1	1:B:193:LYS:HD3	1.94	0.49
1:B:434:TYR:HA	1:B:437:LEU:HD23	1.95	0.49
1:A:155:LEU:HD12	1:B:322:HIS:HE1	1.78	0.49
1:A:316:LEU:HB3	1:A:395:ILE:HG22	1.94	0.49
1:B:204:MET:HE2	1:B:208:LYS:HG3	1.95	0.49
1:A:408:ASN:HA	1:A:412:ARG:O	2.13	0.48
1:A:130:THR:OG1	1:A:133:GLU:HG3	2.13	0.48
1:A:295:LYS:HB3	1:A:295:LYS:HZ2	1.78	0.48
1:A:407:ASN:HB2	3:B:572:HOH:O	2.13	0.48
1:B:310:VAL:HG23	1:B:400:ALA:HB2	1.96	0.48
1:B:338:MET:CG	1:B:371:LEU:HD12	2.43	0.48
1:A:290:LEU:C	1:A:292:TYR:H	2.23	0.47
1:A:414:ARG:NH2	1:B:408:ASN:ND2	2.62	0.47
1:A:213:MET:HB2	1:A:216:VAL:HG22	1.96	0.47
1:A:79:ALA:O	1:A:304:GLU:HA	2.14	0.47
1:B:290:LEU:O	1:B:293:LYS:HG2	2.14	0.47
1:B:413:GLY:HA3	1:B:432:GLU:HB2	1.96	0.47
1:A:321:HIS:CE1	1:A:335:ASP:HB3	2.49	0.47
1:A:371:LEU:HD22	1:A:410:ASN:HB2	1.96	0.47
1:B:127:ASN:ND2	1:B:193:LYS:HD2	2.30	0.47
1:A:176:ASN:HD21	1:A:199:GLU:HG3	1.79	0.47
1:A:414:ARG:HH22	1:B:408:ASN:ND2	2.13	0.47
1:A:417:MET:O	1:A:427:LEU:HD12	2.15	0.47
1:B:103:VAL:HB	1:B:108:GLU:HB2	1.97	0.47
1:A:316:LEU:HB3	1:A:395:ILE:HG23	1.96	0.46
1:A:173:ILE:O	1:A:175:PRO:HD3	2.16	0.46
1:B:346:MET:HE2	1:B:347:TYR:CZ	2.50	0.46
1:A:178:ASN:OD1	1:A:180:LYS:HB2	2.16	0.46
1:A:47:TYR:CB	1:A:417:MET:HG2	2.44	0.46
1:A:104:VAL:HG21	1:B:372:CYS:CB	2.46	0.46
1:B:385:ASP:O	1:B:386:LYS:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ILE:O	1:B:289:MET:HG2	2.16	0.46
1:B:177:VAL:HG13	1:B:237:GLU:OE1	2.16	0.45
1:A:238:GLU:O	1:A:242:VAL:HG23	2.15	0.45
1:B:228:GLN:HA	1:B:266:GLY:HA2	1.98	0.45
1:A:61:TYR:CD2	1:A:278:GLN:HG2	2.52	0.45
1:A:88:LEU:HD13	1:B:443:VAL:HG23	1.99	0.45
1:A:88:LEU:HD13	1:B:443:VAL:CG2	2.47	0.45
1:B:119:SER:HA	1:B:122:ILE:HD12	1.98	0.45
1:A:120:LYS:O	1:A:120:LYS:HG2	2.15	0.45
1:A:172:ARG:HA	1:A:222:HIS:O	2.16	0.45
1:B:125:ASN:CG	1:B:146:ASN:HD22	2.25	0.45
1:B:231:ASP:O	1:B:234:PRO:HD2	2.16	0.45
1:A:153:LEU:HD22	1:A:213:MET:SD	2.57	0.45
1:A:249:LEU:HD13	1:A:256:ILE:HD11	1.97	0.45
1:A:414:ARG:HH22	1:B:408:ASN:HD22	1.63	0.45
1:B:257:GLU:O	1:B:299:PRO:HB2	2.17	0.45
1:B:52:GLU:HG2	3:B:597:HOH:O	2.17	0.45
1:B:188:GLY:C	1:B:190:LYS:H	2.25	0.45
1:A:204:MET:HE1	1:A:254:ILE:HD12	1.98	0.45
1:B:44:THR:HA	1:B:45:PRO:C	2.42	0.45
1:A:338:MET:CG	1:A:371:LEU:HD12	2.44	0.44
1:B:211:LEU:HD11	1:B:254:ILE:HG12	1.99	0.44
1:A:295:LYS:HB3	1:A:295:LYS:NZ	2.33	0.44
1:A:119:SER:HA	1:A:122:ILE:HD12	1.99	0.44
1:A:329:THR:HG22	1:A:330:LYS:N	2.32	0.44
1:B:268:PRO:HD3	1:B:275:ILE:HD11	1.98	0.44
1:A:218:VAL:HG23	1:A:218:VAL:O	2.18	0.43
1:B:298:MET:HE2	1:B:298:MET:HA	1.99	0.43
1:A:23:ILE:HG23	1:A:23:ILE:O	2.18	0.43
1:A:74:LYS:HG3	1:A:298:MET:O	2.18	0.43
1:A:66:LYS:O	1:A:70:GLU:HG3	2.19	0.43
1:A:38:LEU:HD21	1:A:425:VAL:HG11	2.01	0.43
1:A:193:LYS:HD3	1:B:368:ALA:HB1	2.00	0.43
1:A:219:VAL:O	1:A:257:GLU:HB3	2.18	0.43
1:B:340:ASP:OD1	1:B:415:PRO:HD3	2.19	0.43
1:A:134:ILE:CD1	1:A:155:LEU:HD13	2.49	0.43
1:B:243:MET:HE3	1:B:259:VAL:HG11	2.01	0.43
1:B:258:ASP:OD1	1:B:300:ASN:HB2	2.18	0.43
1:B:33:TYR:OH	1:B:424:GLY:HA2	2.19	0.43
1:B:174:ASN:HB3	1:B:189:LEU:HB3	2.01	0.43
1:A:127:ASN:HD22	1:B:333:MET:CE	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:O	1:A:290:LEU:HG	2.19	0.43
1:A:347:TYR:O	1:A:348:GLU:HB2	2.19	0.43
1:B:104:VAL:HG12	1:B:125:ASN:HB2	2.00	0.43
1:A:152:GLU:O	1:A:156:ILE:HG13	2.18	0.42
1:A:311:ALA:O	1:A:397:ASP:HA	2.19	0.42
1:A:157:ASN:HD21	1:A:215:TYR:H	1.68	0.42
1:B:251:GLU:HG2	1:B:295:LYS:NZ	2.34	0.42
1:A:62:ILE:O	1:A:66:LYS:HG3	2.19	0.42
1:B:250:LYS:CG	1:B:296:VAL:HG22	2.44	0.42
1:A:22:GLU:CD	1:A:24:LYS:HE3	2.45	0.42
1:B:304:GLU:N	1:B:305:PRO:HD3	2.33	0.42
1:A:416:ARG:HG2	1:A:427:LEU:HD11	2.02	0.42
1:A:69:GLU:HG3	1:A:74:LYS:O	2.20	0.42
1:A:290:LEU:C	1:A:292:TYR:N	2.78	0.42
1:B:19:ASP:N	1:B:53:GLN:HE22	2.13	0.41
1:B:47:TYR:HB2	1:B:417:MET:HG2	2.01	0.41
1:B:232:ILE:HD11	1:B:281:LEU:CA	2.48	0.41
1:A:321:HIS:HE1	1:A:335:ASP:OD2	2.03	0.41
1:B:296:VAL:HG12	1:B:297:GLU:N	2.34	0.41
1:A:228:GLN:O	1:A:228:GLN:HG3	2.20	0.41
1:A:304:GLU:N	1:A:305:PRO:HD3	2.35	0.41
1:A:371:LEU:HD22	1:A:410:ASN:CB	2.50	0.41
1:B:359:LYS:H	1:B:385:ASP:HB3	1.84	0.41
1:B:228:GLN:O	1:B:228:GLN:HG3	2.21	0.41
1:A:29:PHE:HA	1:A:33:TYR:O	2.20	0.41
1:A:267:ILE:HA	1:A:268:PRO:HD3	1.84	0.41
1:A:343:ARG:NH1	1:A:349:ALA:HB1	2.36	0.41
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.85	0.41
1:A:417:MET:HB2	1:A:429:ARG:CB	2.47	0.41
1:B:267:ILE:HD13	1:B:311:ALA:HB1	2.02	0.41
1:B:361:GLU:HG3	1:B:386:LYS:CG	2.51	0.41
1:A:380:ARG:HG3	1:A:380:ARG:NH1	2.37	0.40
1:B:68:TRP:CH2	1:B:289:MET:HE3	2.56	0.40
1:B:320:VAL:HG12	1:B:391:ASP:O	2.21	0.40
1:A:293:LYS:HA	1:A:298:MET:HE3	2.04	0.40
1:A:411:ALA:HB3	1:B:108:GLU:CG	2.51	0.40
1:A:228:GLN:HA	1:A:266:GLY:HA2	2.03	0.40
1:A:124:PHE:CD1	1:A:124:PHE:C	3.00	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	431/434 (99%)	410 (95%)	20 (5%)	1 (0%)	43	58
1	B	431/434 (99%)	413 (96%)	16 (4%)	2 (0%)	24	37
All	All	862/868 (99%)	823 (96%)	36 (4%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	GLY
1	B	85	ASN
1	B	181	THR

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	366/366 (100%)	350 (96%)	16 (4%)	25	43
1	B	366/366 (100%)	349 (95%)	17 (5%)	24	41
All	All	732/732 (100%)	699 (96%)	33 (4%)	24	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	109	LEU
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	153	LEU
1	A	155	LEU
1	A	199	GLU
1	A	250	LYS
1	A	294	ASP
1	A	295	LYS
1	A	299	PRO
1	A	346	MET
1	A	357	LYS
1	A	372	CYS
1	A	407	ASN
1	A	414	ARG
1	A	422	LYS
1	B	16	LEU
1	B	88	LEU
1	B	93	LEU
1	B	109	LEU
1	B	153	LEU
1	B	155	LEU
1	B	250	LYS
1	B	267	ILE
1	B	299	PRO
1	B	320	VAL
1	B	333	MET
1	B	372	CYS
1	B	384	LEU
1	B	395	ILE
1	B	410	ASN
1	B	414	ARG
1	B	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	116	ASN
1	A	141	ASN
1	A	157	ASN
1	A	176	ASN
1	A	192	ASN
1	A	217	ASN
1	A	224	HIS

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Mol	Chain	Res	Type
1	A	321	HIS
1	A	407	ASN
1	A	408	ASN
1	B	18	ASN
1	B	53	GLN
1	B	141	ASN
1	B	146	ASN
1	B	157	ASN
1	B	192	ASN
1	B	217	ASN
1	B	321	HIS
1	B	407	ASN
1	B	408	ASN
1	B	410	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	B	83	1	23,24,25	1.91	6 (26%)	25,32,34	2.23	6 (24%)
1	LLP	A	83	1	23,24,25	2.06	7 (30%)	25,32,34	2.28	7 (28%)

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
1	LLP	B	83	1	-	5/16/17/19	0/1/1/1
1	LLP	A	83	1	-	5/16/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	LLP	C4-C4'	4.96	1.57	1.46
1	B	83	LLP	C4-C4'	4.37	1.55	1.46
1	B	83	LLP	C2-N1	4.23	1.41	1.33
1	A	83	LLP	C4-C5	4.01	1.47	1.42
1	A	83	LLP	C2-N1	3.85	1.40	1.33
1	B	83	LLP	C4-C5	3.82	1.47	1.42
1	A	83	LLP	C4'-NZ	2.96	1.37	1.27
1	A	83	LLP	P-OP3	-2.50	1.45	1.54
1	A	83	LLP	C6-N1	2.50	1.39	1.34
1	B	83	LLP	C4'-NZ	2.44	1.35	1.27
1	B	83	LLP	C6-N1	2.29	1.39	1.34
1	B	83	LLP	P-OP3	-2.27	1.46	1.54
1	A	83	LLP	C3-C2	2.21	1.43	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	LLP	C2'-C2-C3	5.86	127.66	120.80
1	B	83	LLP	C2'-C2-C3	5.34	127.05	120.80
1	B	83	LLP	CE-NZ-C4'	5.30	135.69	118.72
1	A	83	LLP	CE-NZ-C4'	5.22	135.43	118.72
1	B	83	LLP	C4-C4'-NZ	-4.00	105.57	124.04
1	B	83	LLP	C4-C3-C2	3.93	122.36	120.14
1	A	83	LLP	OP4-C5'-C5	3.92	116.69	109.36
1	B	83	LLP	OP4-C5'-C5	3.89	116.66	109.36
1	A	83	LLP	C4-C4'-NZ	-3.76	106.70	124.04
1	A	83	LLP	C4-C3-C2	3.73	122.24	120.14
1	A	83	LLP	C5'-C5-C6	-2.64	115.06	119.36
1	B	83	LLP	C5'-C5-C6	-2.37	115.49	119.36
1	A	83	LLP	C3-C2-N1	-2.25	118.12	120.96

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	83	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	B	83	LLP	C4-C4'-NZ-CE
1	A	83	LLP	CG-CD-CE-NZ
1	B	83	LLP	CG-CD-CE-NZ
1	B	83	LLP	C5-C4-C4'-NZ
1	B	83	LLP	C3-C4-C4'-NZ
1	A	83	LLP	CE-CD-CG-CB
1	A	83	LLP	C3-C4-C4'-NZ
1	A	83	LLP	C5-C4-C4'-NZ
1	B	83	LLP	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	AZ1	A	502	-	12,12,12	1.65	1 (8%)	13,13,13	4.34	6 (46%)
2	AZ1	B	503	-	12,12,12	1.88	1 (8%)	13,13,13	4.33	5 (38%)

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	AZ1	A	502	-	-	5/10/10/10	-
2	AZ1	B	503	-	-	6/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	AZ1	O2-C9	5.46	1.39	1.22
2	A	502	AZ1	O2-C9	4.82	1.37	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	AZ1	C3-C2-C	13.58	149.96	114.51
2	B	503	AZ1	C3-C2-C	13.37	149.41	114.51
2	B	503	AZ1	C4-C3-C2	5.09	131.82	113.13
2	A	502	AZ1	C4-C3-C2	5.01	131.53	113.13
2	B	503	AZ1	C7-C6-C5	3.29	131.00	114.37
2	A	502	AZ1	C7-C6-C5	3.17	130.39	114.37
2	B	503	AZ1	C6-C7-C8	3.08	124.45	113.13
2	A	502	AZ1	C6-C7-C8	2.85	123.59	113.13
2	B	503	AZ1	OXT-C-C2	2.46	121.78	114.00
2	A	502	AZ1	OXT-C-C2	2.29	121.23	114.00
2	A	502	AZ1	C5-C4-C3	2.08	124.86	114.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	AZ1	C2-C3-C4-C5
2	B	503	AZ1	C5-C6-C7-C8
2	A	502	AZ1	C4-C5-C6-C7
2	B	503	AZ1	C2-C3-C4-C5
2	A	502	AZ1	C3-C4-C5-C6
2	B	503	AZ1	C6-C7-C8-C9
2	B	503	AZ1	C4-C5-C6-C7
2	B	503	AZ1	C7-C8-C9-OXT2
2	B	503	AZ1	C7-C8-C9-O2
2	A	502	AZ1	C7-C8-C9-OXT2
2	A	502	AZ1	C7-C8-C9-O2

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	433/434 (99%)	-0.14	1 (0%) 91 89	24, 40, 62, 74	0
1	B	433/434 (99%)	-0.39	5 (1%) 76 73	22, 35, 56, 82	0
All	All	866/868 (99%)	-0.27	6 (0%) 84 81	22, 37, 61, 82	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	THR	2.7
1	B	272	ASP	2.2
1	B	15	PHE	2.2
1	A	23	ILE	2.1
1	B	185	ILE	2.1
1	B	178	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	83	24/25	0.95	0.07	27,33,38,40	0
1	LLP	B	83	24/25	0.96	0.07	22,32,36,38	0

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
2	AZ1	B	503	13/13	0.67	0.25	38,42,49,53	0
2	AZ1	A	502	13/13	0.79	0.21	43,45,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.