



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:18 AM UTC

PDB ID : 3WGQ / pdb_00003wgq
Title : Crystal structure of meso-dapdh Q154L/T173I/R199M/P248S/H249N/N276
S mutant with DAP of from Clostridium tetani E88
Authors : Liu, W.D.; Li, Z.; Huang, C.H.; Guo, R.T.; Wu, Q.Q.; Zhu, D.M.
Deposited on : 2013-08-07
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

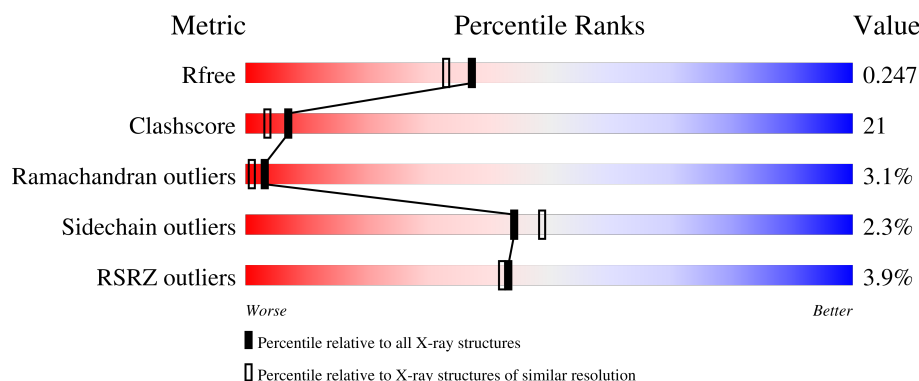
1 Overall quality at a glance

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	326	5% 59% 34% 6%
1	B	326	3% 70% 24% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5820 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.

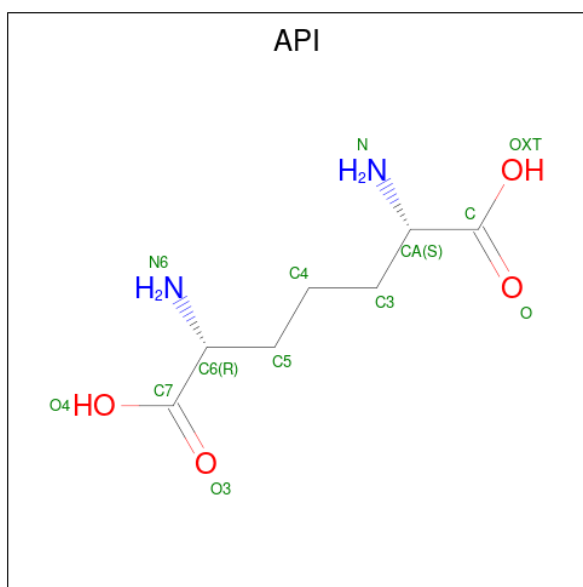
- Molecule 1 is a protein called Meso-diaminopimelate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2525	1591	437	487	10			
1	B	324	Total	C	N	O	S	0	0	0
			2531	1594	438	489	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	LEU	GLN	engineered mutation	UNP Q890V3
A	173	ILE	THR	engineered mutation	UNP Q890V3
A	199	MET	ARG	engineered mutation	UNP Q890V3
A	248	SER	PRO	engineered mutation	UNP Q890V3
A	249	ASN	HIS	engineered mutation	UNP Q890V3
A	276	SER	ASN	engineered mutation	UNP Q890V3
B	154	LEU	GLN	engineered mutation	UNP Q890V3
B	173	ILE	THR	engineered mutation	UNP Q890V3
B	199	MET	ARG	engineered mutation	UNP Q890V3
B	248	SER	PRO	engineered mutation	UNP Q890V3
B	249	ASN	HIS	engineered mutation	UNP Q890V3
B	276	SER	ASN	engineered mutation	UNP Q890V3

- Molecule 2 is 2,6-DIAMINOPIMELIC ACID (CCD ID: API) (formula: C₇H₁₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	2	4		

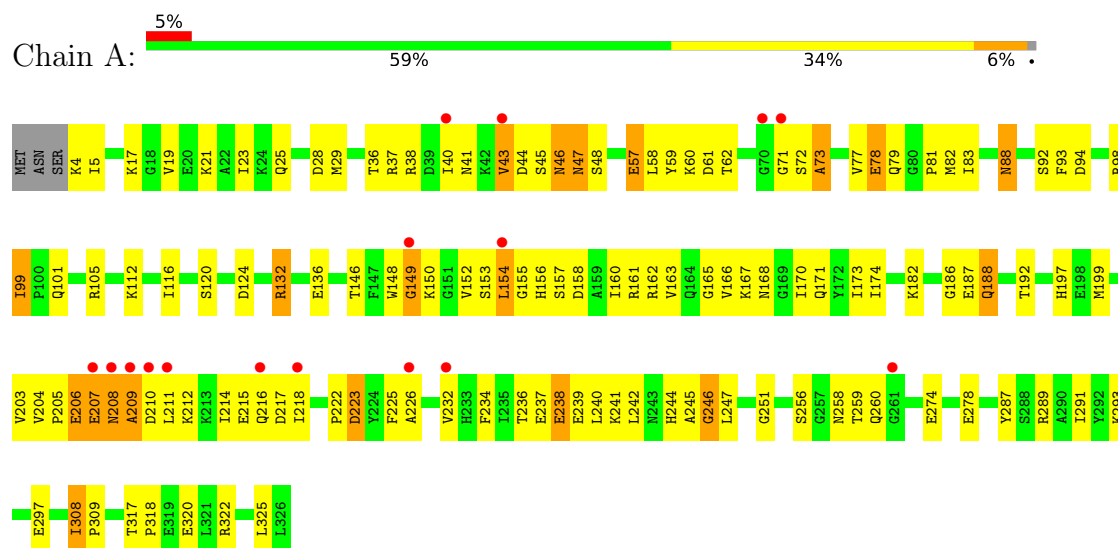
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	343	Total	O	0	0
			343	343		
3	B	408	Total	O	0	0
			408	408		

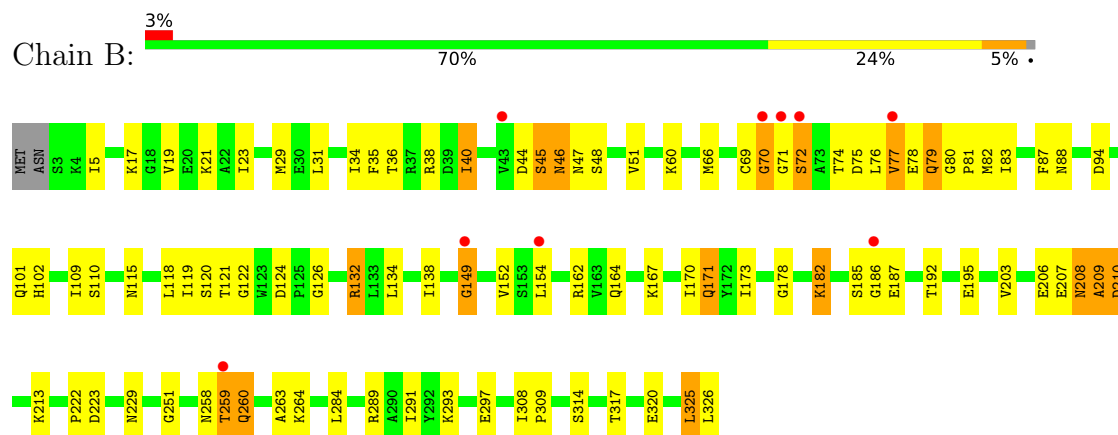
3 Residue-property plots [i](#)

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: Meso-diaminopimelate dehydrogenase



• Molecule 1: Meso-diaminopimelate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.92Å 135.70Å 60.48Å 90.00° 110.43° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (25.00-2.00) 94.8 (25.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.248 0.200 , 0.247	Depositor DCC
R_{free} test set	2269 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5820	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: API

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	0.36	0/2568	0.98	12/3456 (0.3%)
1	B	0.37	0/2574	0.93	11/3464 (0.3%)
All	All	0.37	0/5142	0.96	23/6920 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASN	N-CA-C	-12.21	98.40	113.18
1	A	217	ASP	N-CA-C	-10.18	100.27	112.89
1	B	308	ILE	N-CA-C	9.98	118.95	107.77
1	A	308	ILE	N-CA-C	9.41	118.31	107.77
1	A	206	GLU	N-CA-C	-8.15	101.64	112.72
1	B	88	ASN	N-CA-C	-7.00	99.14	110.20
1	A	88	ASN	N-CA-C	-6.64	100.46	110.28
1	B	185	SER	N-CA-C	-6.25	101.73	110.35
1	A	120	SER	N-CA-C	6.22	119.98	111.39
1	B	325	LEU	N-CA-C	6.08	121.35	113.88
1	B	120	SER	N-CA-C	6.07	119.77	111.39
1	A	244	HIS	N-CA-C	6.05	117.83	109.54
1	B	173	ILE	N-CA-C	-6.01	99.81	108.53
1	B	94	ASP	N-CA-C	5.54	119.03	112.72
1	B	132	ARG	N-CA-C	-5.53	105.17	111.14
1	A	94	ASP	N-CA-C	5.48	119.66	112.92
1	B	229	ASN	N-CA-C	-5.34	101.74	109.59
1	A	99	ILE	CB-CA-C	-5.24	108.79	114.35
1	A	192	THR	N-CA-C	-5.24	102.77	110.52
1	B	209	ALA	N-CA-C	5.21	121.89	110.80
1	B	203	VAL	N-CA-C	5.20	115.96	108.48
1	A	325	LEU	N-CA-C	5.19	119.88	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	N-CA-C	-5.14	105.76	111.36

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	2525	0	2534	132	0
1	B	2531	0	2539	96	0
2	A	13	0	7	0	0
3	A	343	0	0	6	0
3	B	408	0	0	10	0
All	All	5820	0	5080	213	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 21.

All (213) 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:36:THR:HG22	1:A:38:ARG:H	1.26	0.96
1:A:205:PRO:HB2	1:A:207:GLU:HG3	1.47	0.94
1:B:186:GLY:HA3	1:B:264:LYS:HD3	1.48	0.93
1:B:40:ILE:H	1:B:40:ILE:HD13	1.38	0.88
1:B:182:LYS:HE3	1:B:182:LYS:HA	1.60	0.83
1:A:88:ASN:HD22	1:A:116:ILE:H	1.28	0.79
1:B:149:GLY:H	1:B:251:GLY:HA2	1.50	0.76
1:A:241:LYS:HE3	1:A:242:LEU:HD23	1.70	0.73
1:B:118:LEU:HB2	1:B:291:ILE:HD11	1.71	0.73
1:A:148:TRP:H	1:A:197:HIS:HE1	1.38	0.72
1:A:205:PRO:CB	1:A:207:GLU:HG3	2.19	0.71
1:A:260:GLN:HB2	1:B:21:LYS:HB3	1.72	0.71
1:A:81:PRO:HG2	1:A:105:ARG:HE	1.56	0.70
1:A:43:VAL:HG23	1:A:44:ASP:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:O	1:A:214:ILE:HG22	1.92	0.69
1:A:21:LYS:HB3	1:B:260:GLN:HB2	1.72	0.69
1:A:124:ASP:OD2	1:A:132:ARG:NH2	2.26	0.68
1:B:79:GLN:HG2	3:B:451:HOH:O	1.95	0.67
1:B:164:GLN:HE21	1:B:164:GLN:HA	1.58	0.66
1:A:309:PRO:HG3	1:B:309:PRO:HG3	1.77	0.65
1:B:40:ILE:HD13	1:B:40:ILE:N	2.10	0.65
1:A:211:LEU:HD23	1:A:214:ILE:HB	1.77	0.65
1:B:186:GLY:HA3	1:B:264:LYS:CD	2.26	0.65
1:B:289:ARG:HG2	1:B:293:LYS:HE3	1.79	0.65
1:A:204:VAL:HG11	1:A:237:GLU:HG3	1.78	0.64
1:A:204:VAL:HG11	1:A:237:GLU:CG	2.27	0.64
1:B:40:ILE:H	1:B:40:ILE:CD1	2.09	0.64
1:A:4:LYS:HE2	3:A:634:HOH:O	1.97	0.64
1:A:205:PRO:C	1:A:207:GLU:H	2.05	0.64
1:B:81:PRO:HB3	1:B:109:ILE:CD1	2.28	0.64
1:B:187:GLU:O	1:B:187:GLU:HG3	1.98	0.63
1:A:98:ARG:HB3	1:A:98:ARG:NH1	2.12	0.63
1:A:212:LYS:O	1:A:215:GLU:HB2	1.98	0.63
1:A:148:TRP:H	1:A:197:HIS:CE1	2.16	0.62
1:A:225:PHE:O	1:A:226:ALA:HB3	1.99	0.62
1:A:274:GLU:HG3	1:B:264:LYS:HB2	1.82	0.62
1:A:165:GLY:HA3	1:A:210:ASP:OD2	2.00	0.62
1:B:182:LYS:HA	1:B:182:LYS:CE	2.31	0.61
1:A:88:ASN:ND2	1:A:116:ILE:H	1.98	0.61
1:B:124:ASP:CG	1:B:132:ARG:HH22	2.09	0.61
1:A:124:ASP:CG	1:A:132:ARG:HH22	2.08	0.60
1:A:274:GLU:HG3	1:B:264:LYS:O	2.02	0.60
1:A:17:LYS:O	1:A:21:LYS:HD3	2.02	0.60
1:A:157:SER:O	1:A:161:ARG:HG3	2.01	0.59
1:A:293:LYS:O	1:A:297:GLU:HG3	2.02	0.59
1:B:124:ASP:OD2	1:B:132:ARG:NH2	2.34	0.59
1:A:236:THR:HG23	1:A:239:GLU:H	1.66	0.59
1:A:182:LYS:HE3	1:A:187:GLU:CD	2.27	0.59
1:A:186:GLY:HA2	1:A:256:SER:OG	2.02	0.59
1:A:72:SER:O	1:A:73:ALA:HB3	2.04	0.58
1:A:101:GLN:OE1	1:A:101:GLN:N	2.36	0.57
1:A:40:ILE:HG23	1:A:41:ASN:N	2.18	0.57
1:A:241:LYS:O	1:A:241:LYS:HD2	2.04	0.57
1:B:317:THR:OG1	1:B:320:GLU:HG3	2.04	0.57
1:A:149:GLY:H	1:A:251:GLY:HA2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:O	1:A:73:ALA:CB	2.53	0.56
1:B:71:GLY:O	1:B:72:SER:HB3	2.05	0.56
1:B:74:THR:C	1:B:76:LEU:H	2.12	0.56
1:A:203:VAL:O	1:A:205:PRO:HD3	2.05	0.56
1:B:293:LYS:O	1:B:297:GLU:HG3	2.06	0.56
1:A:36:THR:HG22	1:A:38:ARG:N	2.09	0.56
1:A:82:MET:O	1:A:82:MET:HE3	2.06	0.56
1:A:241:LYS:HE3	1:A:242:LEU:CD2	2.36	0.56
1:B:75:ASP:HB2	1:B:79:GLN:CB	2.36	0.55
1:A:57:GLU:HG3	1:A:58:LEU:N	2.21	0.55
1:A:211:LEU:HG	1:A:214:ILE:H	1.72	0.55
1:A:188:GLN:NE2	1:A:258:ASN:ND2	2.55	0.54
1:A:278:GLU:CD	1:B:259:THR:HG21	2.32	0.54
1:B:293:LYS:NZ	1:B:314:SER:O	2.39	0.54
1:A:40:ILE:HG23	1:A:41:ASN:H	1.72	0.54
1:A:278:GLU:HB3	1:B:259:THR:HG21	1.89	0.54
1:A:132:ARG:HH21	1:A:146:THR:HG21	1.71	0.54
1:A:245:ALA:O	1:A:247:LEU:N	2.41	0.53
1:A:28:ASP:OD2	1:A:289:ARG:HD3	2.09	0.53
1:B:209:ALA:O	1:B:210:ASP:HB3	2.08	0.53
1:A:59:TYR:O	1:A:62:THR:HG22	2.09	0.53
1:A:156:HIS:CE1	1:A:199:MET:HE1	2.44	0.53
1:B:192:THR:OG1	1:B:195:GLU:HG3	2.09	0.53
1:A:232:VAL:O	1:A:232:VAL:HG23	2.08	0.53
1:B:44:ASP:O	1:B:45:SER:HB3	2.09	0.53
1:A:187:GLU:O	1:A:188:GLN:HB2	2.08	0.52
1:A:236:THR:HG22	1:A:239:GLU:HG3	1.91	0.52
1:A:77:VAL:HA	1:A:105:ARG:NH2	2.24	0.52
1:B:149:GLY:H	1:B:251:GLY:CA	2.20	0.52
1:B:44:ASP:O	1:B:45:SER:CB	2.58	0.52
1:A:207:GLU:C	1:A:209:ALA:N	2.66	0.52
1:B:134:LEU:O	1:B:138:ILE:HG12	2.10	0.51
1:A:153:SER:O	1:A:155:GLY:N	2.43	0.51
1:A:156:HIS:CB	1:A:171:GLN:HG2	2.40	0.51
1:B:75:ASP:HB2	1:B:79:GLN:HB2	1.93	0.51
1:A:166:VAL:HG13	1:A:203:VAL:HG13	1.93	0.51
1:A:158:ASP:O	1:A:162:ARG:HD3	2.11	0.51
1:A:218:ILE:O	1:A:225:PHE:HB2	2.11	0.51
1:A:44:ASP:O	1:A:45:SER:HB3	2.10	0.51
1:A:246:GLY:HA2	3:A:598:HOH:O	2.10	0.51
1:A:25:GLN:HG3	1:B:260:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:ND2	1:A:116:ILE:HG22	2.26	0.50
1:A:317:THR:OG1	1:A:320:GLU:HG3	2.12	0.50
1:B:46:ASN:O	1:B:48:SER:N	2.41	0.50
1:B:167:LYS:HG2	1:B:206:GLU:CD	2.35	0.50
1:A:163:VAL:HB	1:A:166:VAL:HG21	1.93	0.50
1:A:188:GLN:NE2	1:A:258:ASN:HD22	2.10	0.50
1:A:216:GLN:HE21	1:A:232:VAL:CG2	2.25	0.50
1:A:19:VAL:O	1:A:23:ILE:HG13	2.11	0.50
1:A:92:SER:O	1:A:93:PHE:C	2.55	0.50
1:B:5:ILE:HB	1:B:29:MET:HG2	1.93	0.50
1:A:5:ILE:HB	1:A:29:MET:HG2	1.94	0.50
1:A:152:VAL:CG2	1:A:170:ILE:HD11	2.42	0.50
1:B:259:THR:HG23	3:B:489:HOH:O	2.12	0.49
1:A:260:GLN:CB	1:B:21:LYS:HB3	2.41	0.49
1:B:74:THR:HG22	3:B:731:HOH:O	2.12	0.49
1:B:289:ARG:O	1:B:293:LYS:HG3	2.13	0.49
1:A:182:LYS:HE2	1:A:187:GLU:HB2	1.94	0.49
1:B:79:GLN:O	1:B:83:ILE:HG12	2.13	0.49
1:B:71:GLY:O	1:B:72:SER:CB	2.60	0.48
1:A:211:LEU:O	1:A:215:GLU:HG2	2.14	0.48
1:B:31:LEU:HD21	1:B:34:ILE:HD11	1.95	0.48
1:B:102:HIS:HD2	1:B:119:ILE:CG2	2.27	0.48
1:A:79:GLN:O	1:A:83:ILE:HG12	2.13	0.48
1:A:163:VAL:HG21	1:A:218:ILE:HG12	1.95	0.48
1:A:21:LYS:HB3	1:B:260:GLN:CB	2.43	0.48
1:B:60:LYS:HA	1:B:87:PHE:CE2	2.49	0.48
1:B:119:ILE:N	1:B:119:ILE:HD12	2.29	0.48
1:B:178:GLY:O	1:B:182:LYS:HG2	2.14	0.48
1:A:36:THR:HG21	3:A:797:HOH:O	2.13	0.47
1:A:45:SER:C	1:A:47:ASN:H	2.23	0.47
1:A:60:LYS:O	1:A:61:ASP:HB2	2.14	0.47
1:A:318:PRO:O	1:A:322:ARG:HG3	2.14	0.47
1:B:35:PHE:HA	1:B:51:VAL:O	2.15	0.47
1:B:154:LEU:C	1:B:154:LEU:HD13	2.39	0.47
1:A:236:THR:OG1	1:A:238:GLU:HG2	2.14	0.47
1:B:171:GLN:C	1:B:171:GLN:HE21	2.23	0.47
1:A:225:PHE:O	1:A:226:ALA:CB	2.63	0.47
1:B:44:ASP:HB2	3:B:764:HOH:O	2.13	0.47
1:B:74:THR:C	1:B:76:LEU:N	2.73	0.46
1:A:36:THR:HG22	1:A:37:ARG:N	2.31	0.46
1:A:78:GLU:HA	1:A:78:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASN:ND2	1:A:240:LEU:HD23	2.30	0.46
1:B:69:CYS:O	1:B:70:GLY:C	2.58	0.46
1:A:43:VAL:CG1	3:A:525:HOH:O	2.64	0.46
1:B:77:VAL:HG13	1:B:78:GLU:N	2.31	0.46
1:A:81:PRO:HG2	1:A:105:ARG:NE	2.27	0.46
1:A:43:VAL:HG22	1:A:46:ASN:N	2.31	0.46
1:B:152:VAL:HG21	1:B:170:ILE:HD11	1.98	0.46
1:B:209:ALA:O	1:B:210:ASP:CB	2.62	0.46
1:A:205:PRO:HG3	1:A:234:PHE:CD1	2.51	0.46
1:B:79:GLN:O	1:B:82:MET:HB2	2.15	0.46
1:A:204:VAL:HG11	1:A:237:GLU:HG2	1.96	0.45
1:A:206:GLU:O	1:A:208:ASN:N	2.49	0.45
1:A:208:ASN:O	1:A:209:ALA:HB2	2.15	0.45
1:B:118:LEU:C	1:B:119:ILE:HD12	2.41	0.45
1:A:158:ASP:HA	1:A:161:ARG:HH11	1.80	0.45
1:A:136:GLU:OE2	1:B:325:LEU:HD21	2.17	0.45
1:B:74:THR:O	1:B:77:VAL:HG12	2.16	0.45
1:A:150:LYS:HG3	1:A:174:ILE:HG12	1.99	0.45
1:A:207:GLU:C	1:A:209:ALA:H	2.18	0.45
1:A:208:ASN:O	1:A:209:ALA:CB	2.65	0.45
1:A:163:VAL:HB	1:A:166:VAL:CG2	2.46	0.45
1:B:80:GLY:N	1:B:81:PRO:CD	2.80	0.45
1:A:232:VAL:HG22	3:A:787:HOH:O	2.16	0.45
1:A:47:ASN:HD22	1:A:47:ASN:HA	1.56	0.45
1:B:36:THR:OG1	1:B:38:ARG:HG2	2.17	0.45
1:A:156:HIS:HB2	1:A:171:GLN:HG2	1.99	0.44
1:A:287:TYR:O	1:A:291:ILE:HG12	2.18	0.44
1:B:122:GLY:O	1:B:126:GLY:HA3	2.18	0.44
1:A:105:ARG:HB2	1:A:105:ARG:HH11	1.83	0.44
1:B:79:GLN:H	1:B:81:PRO:HD2	1.82	0.44
1:B:171:GLN:C	1:B:171:GLN:NE2	2.76	0.44
1:B:207:GLU:O	1:B:208:ASN:CB	2.65	0.43
1:B:207:GLU:O	1:B:208:ASN:HB2	2.18	0.43
1:A:216:GLN:HE21	1:A:232:VAL:HG21	1.84	0.43
1:B:258:ASN:HA	1:B:263:ALA:O	2.19	0.43
1:B:164:GLN:HA	1:B:164:GLN:NE2	2.31	0.43
1:B:102:HIS:HD2	1:B:119:ILE:HG23	1.84	0.43
1:B:101:GLN:HB2	3:B:505:HOH:O	2.17	0.43
1:A:211:LEU:HB3	1:A:214:ILE:CG2	2.49	0.43
1:A:274:GLU:CD	1:B:264:LYS:HB2	2.44	0.43
1:A:308:ILE:HA	1:A:309:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:CG	1:B:264:LYS:HB2	2.46	0.43
1:A:156:HIS:HB3	1:A:171:GLN:HG2	2.01	0.42
1:B:115:ASN:ND2	3:B:575:HOH:O	2.52	0.42
1:B:19:VAL:O	1:B:23:ILE:HG13	2.19	0.42
1:A:152:VAL:HG22	1:A:170:ILE:HD11	2.01	0.42
1:A:236:THR:HG22	1:A:239:GLU:OE1	2.18	0.42
1:A:278:GLU:OE1	1:B:259:THR:HG21	2.19	0.42
1:B:260:GLN:NE2	1:B:260:GLN:HA	2.34	0.42
1:A:236:THR:CG2	1:A:239:GLU:HG3	2.50	0.42
1:B:121:THR:CG2	1:B:284:LEU:HD23	2.50	0.42
1:B:222:PRO:O	1:B:223:ASP:HB2	2.20	0.42
1:A:150:LYS:HA	1:A:173:ILE:O	2.19	0.42
1:A:211:LEU:CD2	1:A:214:ILE:HB	2.46	0.42
1:B:259:THR:CG2	1:B:260:GLN:N	2.83	0.42
1:A:152:VAL:HG12	1:A:153:SER:N	2.35	0.42
1:A:148:TRP:N	1:A:197:HIS:HE1	2.12	0.41
1:A:157:SER:O	1:A:160:ILE:HG12	2.20	0.41
1:B:260:GLN:CA	1:B:260:GLN:HE21	2.32	0.41
1:B:118:LEU:HB2	1:B:291:ILE:CD1	2.45	0.41
1:B:213:LYS:HE2	3:B:745:HOH:O	2.21	0.41
1:A:99:ILE:HG21	1:B:326:LEU:HD23	2.02	0.41
1:A:152:VAL:HG12	1:A:154:LEU:H	1.86	0.41
1:A:153:SER:HB3	1:A:171:GLN:NE2	2.36	0.41
1:A:259:THR:O	1:A:260:GLN:C	2.62	0.41
1:A:43:VAL:HG12	3:A:525:HOH:O	2.20	0.41
1:A:105:ARG:CB	1:A:105:ARG:NH1	2.84	0.41
1:A:98:ARG:HB3	1:A:98:ARG:HH11	1.85	0.41
1:B:162:ARG:NH2	3:B:751:HOH:O	2.45	0.41
1:B:17:LYS:HD3	3:B:551:HOH:O	2.20	0.40
1:B:66:MET:HG2	1:B:83:ILE:HG21	2.04	0.40
1:B:149:GLY:N	1:B:251:GLY:HA2	2.28	0.40
1:A:222:PRO:O	1:A:223:ASP:HB2	2.22	0.40
1:B:75:ASP:C	1:B:77:VAL:H	2.28	0.40
1:B:110:SER:HB2	1:B:115:ASN:O	2.21	0.40
1:B:115:ASN:HA	3:B:608:HOH:O	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	321/326 (98%)	289 (90%)	21 (6%)	11 (3%)	3	1
1	B	322/326 (99%)	301 (94%)	12 (4%)	9 (3%)	4	1
All	All	643/652 (99%)	590 (92%)	33 (5%)	20 (3%)	3	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	73	ALA
1	A	154	LEU
1	A	207	GLU
1	A	209	ALA
1	B	45	SER
1	B	72	SER
1	B	79	GLN
1	A	46	ASN
1	A	71	GLY
1	A	149	GLY
1	A	246	GLY
1	B	70	GLY
1	B	149	GLY
1	B	208	ASN
1	A	188	GLN
1	A	223	ASP
1	B	210	ASP
1	B	47	ASN
1	B	77	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	278/281 (99%)	271 (98%)	7 (2%)	42	45
1	B	279/281 (99%)	273 (98%)	6 (2%)	45	50
All	All	557/562 (99%)	544 (98%)	13 (2%)	44	49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	47	ASN
1	A	57	GLU
1	A	78	GLU
1	A	112	LYS
1	A	167	LYS
1	A	238	GLU
1	B	40	ILE
1	B	46	ASN
1	B	171	GLN
1	B	182	LYS
1	B	259	THR
1	B	260	GLN

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	14	ASN
1	A	47	ASN
1	A	79	GLN
1	A	88	ASN
1	A	131	ASN
1	A	145	HIS
1	A	168	ASN
1	A	171	GLN
1	A	188	GLN
1	A	197	HIS
1	A	216	GLN
1	A	258	ASN
1	B	14	ASN

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Mol	Chain	Res	Type
1	B	41	ASN
1	B	115	ASN
1	B	131	ASN
1	B	156	HIS
1	B	164	GLN
1	B	188	GLN
1	B	229	ASN
1	B	233	HIS
1	B	260	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](#)

1 ligand is 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	API	A	400	-	10,12,12	0.90	0	9,15,15	0.71	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	API	A	400	-	-	4/14/14/14	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	API	N6-C6-C7-O3
2	A	400	API	N6-C6-C7-O4
2	A	400	API	C5-C6-C7-O4
2	A	400	API	C5-C6-C7-O3

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

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	323/326 (99%)	0.10	16 (4%) 34 33	20, 37, 76, 96	0
1	B	324/326 (99%)	-0.05	9 (2%) 55 54	19, 36, 67, 91	0
All	All	647/652 (99%)	0.02	25 (3%) 43 42	19, 36, 74, 96	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	VAL	5.2
1	A	149	GLY	4.5
1	A	209	ALA	3.8
1	A	43	VAL	3.8
1	B	259	THR	3.3
1	B	72	SER	3.2
1	B	186	GLY	3.2
1	B	77	VAL	3.1
1	A	154	LEU	3.1
1	B	149	GLY	3.0
1	B	71	GLY	2.9
1	A	216	GLN	2.7
1	B	154	LEU	2.5
1	A	208	ASN	2.5
1	A	218	ILE	2.4
1	A	226	ALA	2.3
1	A	232	VAL	2.3
1	A	70	GLY	2.3
1	A	261	GLY	2.3
1	A	210	ASP	2.2
1	A	207	GLU	2.1
1	B	70	GLY	2.1
1	A	211	LEU	2.1
1	A	40	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLY	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
2	API	A	400	13/13	0.76	0.16	66,71,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.