



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:58 PM UTC

PDB ID : 2EJ6 / pdb_00002ej6
Title : Crystal analysis of delta1-pyrroline-5-carboxylate dehydrogenase from
Thermus thermophilus with bound D-proline
Authors : Inagaki, E.; Sakamoto, K.; Yokoyama, S.; RIKEN Structural Ge-
nomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-15
Resolution : 2.06 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

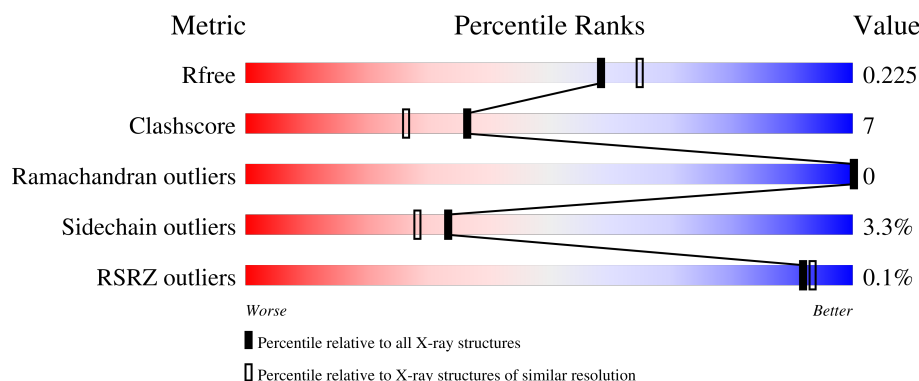
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	516	
1	B	516	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	5520	-	-	X	-
5	MPD	A	1531	X	-	-	-
5	MPD	A	1532	X	-	-	-
5	MPD	B	1534	X	-	-	-
5	MPD	B	5532	X	-	-	-
5	MPD	B	5535	X	-	-	-
5	MPD	B	5537	X	-	-	-

2 Entry composition [i](#)

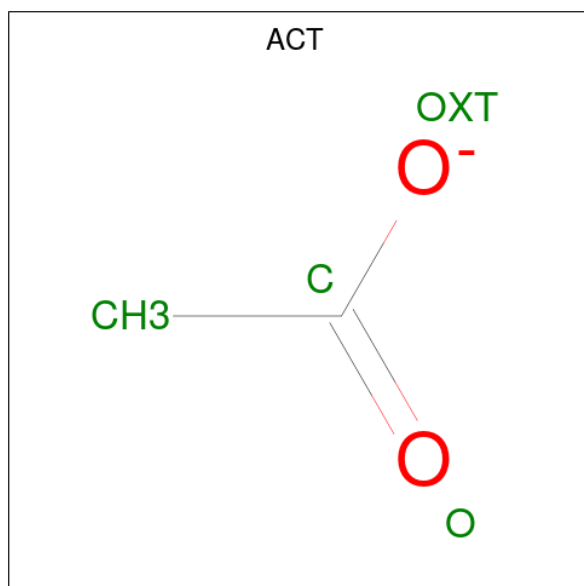
There are 6 unique types of molecules in this entry. The entry contains 8802 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-pyrroline-5-carboxylate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	8	0
			4068	2618	695	745	10			
1	B	516	Total	C	N	O	S	0	8	0
			4066	2615	698	743	10			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

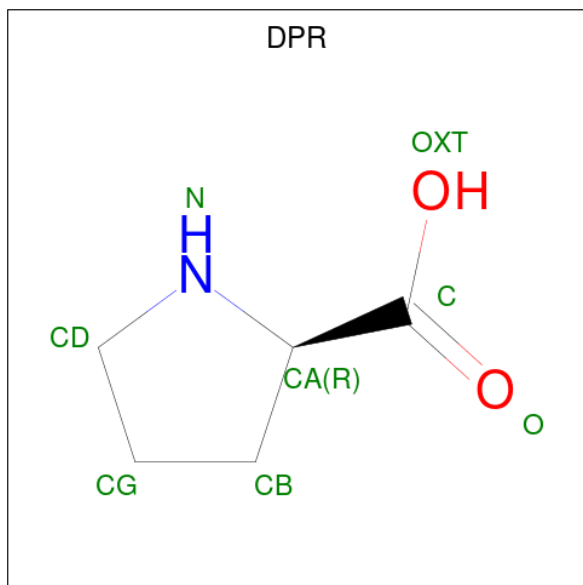


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is D-PROLINE (CCD ID: DPR) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	5	1	2		
4	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	275	Total 275	O 275	0	8
6	B	271	Total 271	O 271	0	3

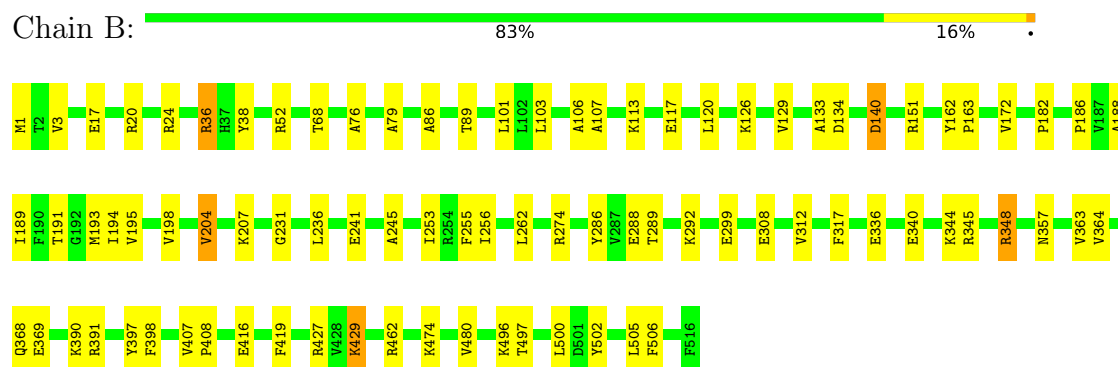
3 Residue-property plots

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: 1-pyrroline-5-carboxylate dehydrogenase



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4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	100.76Å 100.76Å 279.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.68 – 2.06 24.68 – 2.06	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.68-2.06) 96.1 (24.68-2.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.170 , 0.231 0.169 , 0.225	Depositor DCC
R_{free} test set	3333 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.077 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8802	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: ACT, DPR, NA, MPD

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	1.26	6/4204 (0.1%)	1.22	11/5701 (0.2%)
1	B	1.22	6/4206 (0.1%)	1.18	9/5702 (0.2%)
All	All	1.24	12/8410 (0.1%)	1.20	20/11403 (0.2%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	VAL	C-O	7.83	1.31	1.24
1	A	229	PRO	CA-C	7.09	1.58	1.52
1	B	89	THR	CA-CB	6.20	1.62	1.53
1	B	407	VAL	CA-CB	6.11	1.60	1.53
1	B	107	ALA	CA-CB	5.76	1.62	1.53
1	A	157	VAL	CA-CB	-5.48	1.47	1.54
1	A	314	ALA	CA-CB	5.47	1.61	1.53
1	A	106	ALA	CA-CB	5.36	1.61	1.53
1	B	357	ASN	CA-C	5.28	1.57	1.53
1	B	140	ASP	C-O	-5.26	1.18	1.24
1	A	382	GLU	N-CA	5.22	1.52	1.46
1	B	106	ALA	CA-CB	-5.11	1.45	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ALA	CA-C-N	7.64	129.10	120.85
1	A	181	ALA	C-N-CA	7.64	129.10	120.85
1	B	36	ARG	N-CA-C	6.95	120.56	110.28
1	A	172	VAL	CA-C-N	-6.59	113.88	120.21
1	A	172	VAL	C-N-CA	-6.59	113.88	120.21
1	A	441	THR	CA-C-N	-6.18	113.58	120.45
1	A	441	THR	C-N-CA	-6.18	113.58	120.45
1	A	335	TYR	N-CA-C	6.08	118.43	111.02
1	B	408	PRO	CA-C-N	5.98	127.32	119.84
1	B	408	PRO	C-N-CA	5.98	127.32	119.84
1	A	361	GLY	CA-C-N	5.78	125.97	120.31
1	A	361	GLY	C-N-CA	5.78	125.97	120.31
1	B	79	ALA	N-CA-C	-5.74	104.64	111.69
1	B	129	VAL	N-CA-C	5.70	116.44	110.62
1	B	133	ALA	CA-C-N	5.67	128.14	120.44
1	B	133	ALA	C-N-CA	5.67	128.14	120.44
1	B	198	VAL	N-CA-C	5.61	116.34	110.62
1	A	386	VAL	N-CA-C	5.54	119.47	113.43
1	A	463	GLU	N-CA-C	5.13	121.08	114.56
1	B	462	ARG	N-CA-C	5.04	116.85	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	TYR	Peptide

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	4068	0	4054	59	0
1	B	4066	0	4049	56	0
2	A	8	0	6	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	8	0	0
4	B	8	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	40	0	70	5	0
5	B	56	0	98	13	0
6	A	275	0	0	5	0
6	B	271	0	0	7	0
All	All	8802	0	8293	119	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 7.

All (119) 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:36:ARG:HH21	5:B:5537:MPD:HM2	0.94	1.10
1:A:286[B]:TYR:HD2	6:A:5643:HOH:O	1.43	1.01
1:B:36:ARG:NH2	5:B:5537:MPD:HM2	1.79	0.96
1:B:286[B]:TYR:CE1	1:B:506[B]:PHE:CE2	2.65	0.84
2:A:1520:ACT:H2	1:B:172:VAL:HG11	1.59	0.83
1:A:172:VAL:HG11	2:A:5520:ACT:H1	1.63	0.80
5:A:1530:MPD:HM1	5:A:1530:MPD:H52	1.64	0.80
1:A:510:LYS:HD2	2:A:5520:ACT:H3	1.66	0.78
1:A:510:LYS:HD2	2:A:5520:ACT:CH3	2.15	0.77
1:B:286[B]:TYR:CE1	1:B:506[B]:PHE:HE2	2.03	0.75
1:B:427:ARG:HG3	1:B:427:ARG:HH11	1.52	0.75
1:B:24:ARG:HD3	6:B:5725:HOH:O	1.87	0.74
1:B:113:LYS:HE2	6:B:5564:HOH:O	1.88	0.74
1:A:312:VAL:HA	5:A:1531:MPD:HM3	1.72	0.72
1:B:151:ARG:HB3	5:B:5532:MPD:H53	1.72	0.70
1:B:369:GLU:OE2	1:B:391:ARG:NE	2.25	0.69
1:A:368:GLN:O	1:A:372:VAL:HG23	1.94	0.67
1:A:61:PRO:HD2	1:A:395:GLU:HG2	1.75	0.67
1:B:427:ARG:HG3	1:B:427:ARG:NH1	2.07	0.67
1:A:179:VAL:HG13	1:A:193[B]:MET:HE3	1.77	0.66
1:B:245:ALA:HB2	5:B:5534:MPD:H11	1.78	0.65
1:B:207:LYS:HE3	6:B:5648:HOH:O	1.96	0.64
1:B:151:ARG:CB	5:B:5532:MPD:H53	2.28	0.64
1:A:179:VAL:HG13	1:A:193[A]:MET:HE2	1.79	0.63
1:B:312:VAL:HG22	5:B:5536:MPD:H11	1.81	0.62
1:A:364:VAL:HG12	1:A:368:GLN:HG3	1.81	0.62
1:A:286[B]:TYR:CZ	1:A:505:LEU:HB3	2.36	0.61
1:B:390:LYS:HD2	6:B:5685:HOH:O	2.01	0.60
1:A:300:THR:O	1:A:452:ARG:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HA	1:B:289:THR:HB	1.84	0.59
5:B:5536:MPD:H12	5:B:5536:MPD:H52	1.86	0.57
1:B:336:GLU:O	1:B:340:GLU:HG3	2.04	0.57
1:A:210:GLU:HG3	6:A:5662:HOH:O	2.06	0.56
1:B:255:PHE:C	1:B:256:ILE:HD12	2.30	0.56
1:A:138:ALA:CB	1:A:187:VAL:HG12	2.36	0.55
1:B:38:TYR:HB2	1:B:68:THR:HG22	1.88	0.55
1:B:364:VAL:HG12	1:B:368:GLN:HG3	1.89	0.54
1:B:500:LEU:HD13	5:B:5532:MPD:H51	1.90	0.54
1:B:17:GLU:OE1	1:B:20[B]:ARG:NH1	2.40	0.54
1:A:138:ALA:HB2	1:A:188:ALA:HA	1.88	0.54
1:A:144:TYR:CE1	5:A:1530:MPD:HM2	2.44	0.53
1:B:113:LYS:O	1:B:117:GLU:HG3	2.07	0.53
1:B:36:ARG:HH21	5:B:5537:MPD:CM	1.90	0.53
1:B:308:GLU:HG2	1:B:345:ARG:NH1	2.24	0.52
1:B:1[B]:MET:HE1	1:B:103:LEU:HD12	1.91	0.52
1:B:194:ILE:HG23	1:B:204:VAL:HG11	1.93	0.51
1:A:364:VAL:HG12	1:A:368:GLN:CG	2.40	0.51
1:B:308:GLU:O	1:B:312:VAL:HG23	2.12	0.50
1:A:268:ILE:HG13	5:A:1532:MPD:HM3	1.92	0.50
1:A:61:PRO:HD2	1:A:395:GLU:CG	2.43	0.49
1:A:40:LEU:HD11	1:A:75:GLU:HG2	1.94	0.49
1:A:138:ALA:HB2	1:A:187:VAL:HG12	1.93	0.49
1:A:241:GLU:O	1:A:242:GLU:C	2.55	0.49
1:A:510:LYS:HD2	2:A:5520:ACT:H2	1.93	0.49
5:B:5534:MPD:O4	5:B:5534:MPD:H12	2.13	0.49
1:A:3:VAL:HG11	1:A:103:LEU:CD1	2.43	0.48
1:A:286[B]:TYR:CD2	6:A:5643:HOH:O	2.33	0.48
1:A:38:TYR:O	1:A:68:THR:HA	2.14	0.47
1:A:352:GLY:O	1:A:358:PRO:HG3	2.15	0.47
1:B:126:LYS:HG2	1:B:317:PHE:CE1	2.50	0.47
1:A:90:TRP:CZ2	1:A:98:ARG:HG2	2.50	0.46
1:A:264:VAL:HG12	1:A:268:ILE:HD12	1.98	0.46
1:B:3:VAL:HG11	1:B:103:LEU:CD1	2.45	0.46
5:A:1536:MPD:O4	5:A:1536:MPD:H11	2.15	0.46
1:A:384:GLN:NE2	1:A:405:THR:CG2	2.79	0.45
1:A:61:PRO:HD3	1:A:396:GLY:HA2	1.99	0.45
1:B:189:ILE:O	1:B:193[A]:MET:HG3	2.16	0.45
1:A:140:ASP:HB3	1:A:480:VAL:HB	1.98	0.45
1:A:340:GLU:OE1	1:A:344:LYS:NZ	2.49	0.45
1:A:90:TRP:CH2	1:A:98:ARG:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HB	1:A:507:LEU:HD21	1.99	0.45
1:B:120:LEU:CD2	1:B:186:PRO:HG2	2.46	0.45
1:B:1[B]:MET:HE1	1:B:103:LEU:CD1	2.46	0.44
1:B:286[A]:TYR:CZ	1:B:505:LEU:HB3	2.52	0.44
1:A:515:ARG:NH1	6:A:5789:HOH:O	2.40	0.44
1:B:427:ARG:NH1	1:B:427:ARG:CG	2.69	0.44
1:A:1[A]:MET:HE3	1:A:99:SER:HB2	2.00	0.44
1:B:292:LYS:NZ	1:B:416:GLU:O	2.47	0.44
1:A:1[B]:MET:HG2	1:A:96:GLU:HG3	1.99	0.44
1:B:120:LEU:HD21	1:B:186:PRO:HG2	2.00	0.44
1:A:91:LYS:HD2	6:A:5750:HOH:O	2.18	0.44
1:A:298:ASP:OD2	1:A:451:SER:OG	2.22	0.43
1:B:344:LYS:O	1:B:348:ARG:HG3	2.18	0.43
1:B:140:ASP:HB3	1:B:480:VAL:HB	1.98	0.43
1:A:172:VAL:HG11	2:A:5520:ACT:CH3	2.42	0.43
1:B:245:ALA:HB2	5:B:5534:MPD:C1	2.47	0.43
1:A:369:GLU:OE2	1:A:391:ARG:NH1	2.51	0.43
1:A:42:ILE:HG23	1:A:79:ALA:HA	2.01	0.43
1:A:54:VAL:HG13	1:A:64:VAL:HG13	2.01	0.43
1:A:405:THR:HG23	1:A:406:GLU:HG2	2.00	0.43
1:B:429:LYS:HE3	1:B:429:LYS:HB3	1.71	0.43
1:A:126:LYS:HD3	1:A:130:GLU:HB3	2.00	0.42
1:A:80:LEU:HD13	1:A:253:ILE:HD11	2.01	0.42
1:A:253:ILE:HD13	1:A:253:ILE:HA	1.96	0.42
1:A:80:LEU:HD13	1:A:253:ILE:CD1	2.49	0.42
1:B:76:ALA:HA	1:B:236:LEU:HD11	2.01	0.42
1:B:241:GLU:HB3	5:B:5534:MPD:H12	2.01	0.42
1:B:496:LYS:O	1:B:502:TYR:HB2	2.20	0.42
1:A:270:GLU:HG3	1:B:274:ARG:HG2	2.02	0.41
1:A:351:VAL:HG11	1:A:392:LEU:HD12	2.02	0.41
1:A:40:LEU:CD1	1:A:75:GLU:HG2	2.51	0.41
1:B:52:ARG:HG3	6:B:5767:HOH:O	2.19	0.41
1:B:497:THR:HG22	1:B:502:TYR:CE1	2.55	0.41
5:B:5534:MPD:O4	5:B:5534:MPD:C1	2.67	0.41
1:B:86:ALA:HB2	1:B:231:GLY:HA3	2.03	0.41
1:B:162:TYR:CG	1:B:163:PRO:HD2	2.55	0.41
1:B:363:VAL:HG22	1:B:397:TYR:O	2.19	0.41
1:A:43:GLY:HA2	1:A:231:GLY:N	2.36	0.41
1:B:191:THR:O	1:B:195:VAL:HG22	2.21	0.41
1:B:391:ARG:HD2	1:B:398:PHE:O	2.21	0.41
1:B:113:LYS:CE	6:B:5564:HOH:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PRO:HD2	1:A:395:GLU:CD	2.46	0.40
1:B:134:ASP:O	1:B:188:ALA:HB2	2.22	0.40
1:A:181:ALA:HB1	1:A:182:PRO:HD2	2.04	0.40
1:A:369:GLU:HG3	1:A:399:ILE:HD11	2.02	0.40
1:B:182:PRO:HB2	6:B:5699:HOH:O	2.22	0.40
1:A:384:GLN:HE21	1:A:405:THR:CG2	2.34	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	521/516 (101%)	507 (97%)	14 (3%)	0	100	100
1	B	521/516 (101%)	506 (97%)	15 (3%)	0	100	100
All	All	1042/1032 (101%)	1013 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	415/407 (102%)	394 (95%)	21 (5%)	21	14
1	B	415/407 (102%)	406 (98%)	9 (2%)	45	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	830/814 (102%)	800 (96%)	30 (4%)	33	25

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	101	LEU
1	A	207	LYS
1	A	215	VAL
1	A	253	ILE
1	A	286[A]	TYR
1	A	286[B]	TYR
1	A	288	GLU
1	A	299	GLU
1	A	313	SER
1	A	322[A]	CYS
1	A	322[B]	CYS
1	A	340	GLU
1	A	347	GLU
1	A	374	SER
1	A	391	ARG
1	A	393	GLU
1	A	395	GLU
1	A	405	THR
1	A	419	PHE
1	B	101	LEU
1	B	204	VAL
1	B	253	ILE
1	B	288	GLU
1	B	299	GLU
1	B	348	ARG
1	B	419	PHE
1	B	429	LYS
1	B	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	384	GLN

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Mol	Chain	Res	Type
1	B	8	ASN
1	B	332	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
4	DPR	A	1517	-	8,8,8	0.75	0	10,10,10	1.51	2 (20%)
5	MPD	B	5535	-	7,7,7	0.46	0	9,10,10	0.38	0
5	MPD	A	1532	-	7,7,7	0.49	0	9,10,10	0.77	0
4	DPR	B	5517	-	8,8,8	1.18	0	10,10,10	1.42	2 (20%)
5	MPD	B	5534	-	7,7,7	0.58	0	9,10,10	0.85	0
5	MPD	B	5537	-	7,7,7	0.55	0	9,10,10	0.80	0
5	MPD	A	1531	-	7,7,7	0.37	0	9,10,10	0.66	0
5	MPD	A	1530	-	7,7,7	0.46	0	9,10,10	0.99	0
2	ACT	A	5520	-	3,3,3	0.84	0	3,3,3	1.09	0
5	MPD	B	5532	-	7,7,7	0.29	0	9,10,10	0.26	0
5	MPD	B	5536	-	7,7,7	0.42	0	9,10,10	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	A	5531	-	7,7,7	0.35	0	9,10,10	0.40	0
5	MPD	B	5530	-	7,7,7	0.49	0	9,10,10	1.31	0
5	MPD	A	1536	-	7,7,7	0.37	0	9,10,10	0.56	0
5	MPD	B	1534	-	7,7,7	0.43	0	9,10,10	1.09	0
2	ACT	A	1520	-	3,3,3	0.64	0	3,3,3	2.08	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DPR	A	1517	-	-	0/4/11/11	0/1/1/1
5	MPD	B	5535	-	1/1/2/2	0/5/5/5	-
5	MPD	A	1532	-	1/1/2/2	0/5/5/5	-
4	DPR	B	5517	-	-	0/4/11/11	0/1/1/1
5	MPD	B	5534	-	-	5/5/5/5	-
5	MPD	B	5537	-	1/1/2/2	1/5/5/5	-
5	MPD	A	1531	-	1/1/2/2	2/5/5/5	-
5	MPD	A	1530	-	-	2/5/5/5	-
5	MPD	B	5532	-	1/1/2/2	0/5/5/5	-
5	MPD	B	5536	-	-	5/5/5/5	-
5	MPD	A	5531	-	-	2/5/5/5	-
5	MPD	B	5530	-	-	1/5/5/5	-
5	MPD	A	1536	-	-	1/5/5/5	-
5	MPD	B	1534	-	1/1/2/2	1/5/5/5	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1517	DPR	OXT-C-CA	2.73	122.75	113.51
2	A	1520	ACT	OXT-C-CH3	2.57	125.84	115.05
4	B	5517	DPR	OXT-C-CA	2.51	122.01	113.51
2	A	1520	ACT	OXT-C-O	-2.50	112.77	122.03
4	A	1517	DPR	OXT-C-O	-2.35	118.75	124.08
4	B	5517	DPR	OXT-C-O	-2.19	119.12	124.08

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1531	MPD	C4
5	A	1532	MPD	C4
5	B	1534	MPD	C4
5	B	5532	MPD	C4
5	B	5535	MPD	C4
5	B	5537	MPD	C4

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1530	MPD	C2-C3-C4-O4
5	A	1530	MPD	C2-C3-C4-C5
5	B	5530	MPD	C2-C3-C4-C5
5	B	5534	MPD	C1-C2-C3-C4
5	B	5534	MPD	C2-C3-C4-O4
5	B	5536	MPD	C2-C3-C4-O4
5	B	5536	MPD	C2-C3-C4-C5
5	B	1534	MPD	O2-C2-C3-C4
5	A	1531	MPD	CM-C2-C3-C4
5	B	5534	MPD	CM-C2-C3-C4
5	B	5536	MPD	CM-C2-C3-C4
5	B	5534	MPD	C2-C3-C4-C5
5	B	5537	MPD	C2-C3-C4-C5
5	A	1536	MPD	O2-C2-C3-C4
5	B	5534	MPD	O2-C2-C3-C4
5	B	5536	MPD	O2-C2-C3-C4
5	A	1531	MPD	C1-C2-C3-C4
5	A	5531	MPD	C1-C2-C3-C4
5	A	5531	MPD	CM-C2-C3-C4
5	B	5536	MPD	C1-C2-C3-C4

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1532	MPD	1	0
5	B	5534	MPD	5	0
5	B	5537	MPD	3	0
5	A	1531	MPD	1	0
5	A	1530	MPD	2	0
2	A	5520	ACT	5	0
5	B	5532	MPD	3	0
5	B	5536	MPD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1536	MPD	1	0
2	A	1520	ACT	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	516/516 (100%)	-0.66	1 (0%) 91 93	10, 21, 34, 43	8 (1%)
1	B	516/516 (100%)	-0.70	0 100 100	9, 21, 34, 41	8 (1%)
All	All	1032/1032 (100%)	-0.68	1 (0%) 92 93	9, 21, 34, 43	16 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1[A]	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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
5	MPD	B	1534	8/8	0.76	0.14	42,45,46,49	0
5	MPD	B	5536	8/8	0.79	0.16	44,50,53,53	0
5	MPD	A	1536	8/8	0.83	0.17	67,68,69,69	0
5	MPD	B	5537	8/8	0.85	0.13	52,55,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MPD	B	5532	8/8	0.87	0.13	50,54,55,57	0
5	MPD	A	1531	8/8	0.88	0.12	41,44,48,51	0
5	MPD	B	5534	8/8	0.88	0.10	40,42,45,47	0
3	NA	A	1540	1/1	0.90	0.07	31,31,31,31	0
5	MPD	A	1532	8/8	0.90	0.11	44,47,48,50	0
5	MPD	A	5531	8/8	0.91	0.12	52,53,56,57	0
4	DPR	B	5517	8/8	0.91	0.11	33,35,36,37	0
4	DPR	A	1517	8/8	0.92	0.09	32,35,36,36	0
5	MPD	B	5535	8/8	0.92	0.10	33,36,38,38	0
2	ACT	A	5520	4/4	0.93	0.10	39,40,40,41	0
2	ACT	A	1520	4/4	0.93	0.07	26,26,27,29	0
3	NA	B	5540	1/1	0.93	0.09	37,37,37,37	0
5	MPD	B	5530	8/8	0.94	0.08	27,33,34,34	0
5	MPD	A	1530	8/8	0.95	0.07	30,33,36,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.