



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:07 AM GMT

PDB ID : 3R5B
Title : Pseudomonas aeruginosa DapD (PA3666) in complex with L-2-aminopimelate
Authors : Sandalova, T.; Schnell, R.; Schneider, G.
Deposited on : 2011-03-18
Resolution : 2.51 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

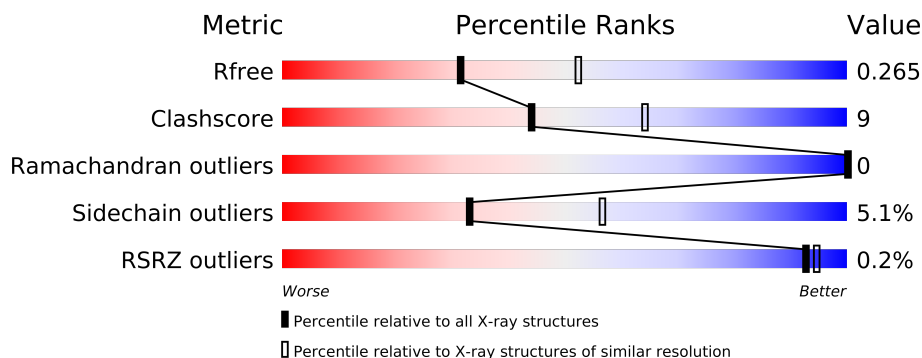
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.51 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	
1	F	347	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NPI	A	381	-	X
2	NPI	E	381	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14397 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TetrahydrodipicolinateN-succinyletransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2364	1506	406	445	7			
1	B	318	Total	C	N	O	S	0	0	0
			2342	1492	403	440	7			
1	C	321	Total	C	N	O	S	0	0	0
			2367	1506	407	447	7			
1	D	321	Total	C	N	O	S	0	0	0
			2364	1506	406	445	7			
1	E	310	Total	C	N	O	S	0	0	0
			2277	1455	386	429	7			
1	F	321	Total	C	N	O	S	0	0	0
			2367	1506	407	447	7			

There are 18 discrepancies between the modelled and reference sequences:

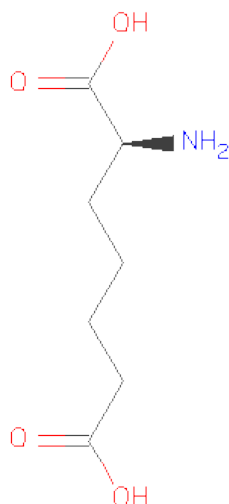
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
A	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
A	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
B	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
B	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
B	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
C	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
C	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
C	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
D	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
D	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
D	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
E	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
E	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
E	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
F	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
F	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2

- Molecule 2 is (2S)-2-AMINOHEPTANEDIOICACID (three-letter code: NPI) (formula: $C_7H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	7	1	4		
2	C	1	Total	C	N	O	0	0
			12	7	1	4		
2	D	1	Total	C	N	O	0	0
			12	7	1	4		
2	E	1	Total	C	N	O	0	0
			12	7	1	4		
2	E	1	Total	C	N	O	0	0
			12	7	1	4		

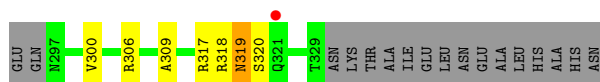
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	53	Total	O	0	0
			53	53		
3	C	44	Total	O	0	0
			44	44		

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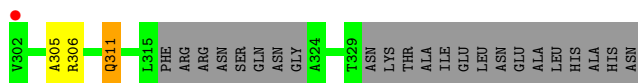
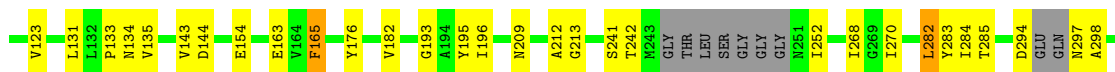
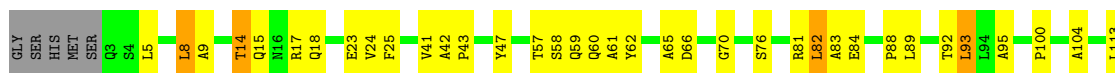
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	36	Total 36	O 36	0	0
3	E	47	Total 47	O 47	0	0
3	F	33	Total 33	O 33	0	0



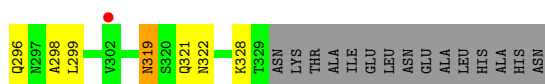
• Molecule 1: TetrahydrodipicolinateN-succinyletransferase

Chain E:



• Molecule 1: TetrahydrodipicolinateN-succinyletransferase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.04Å 102.00Å 134.90Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	36.88 – 2.51 36.88 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.9 (36.88-2.51) 97.3 (36.88-2.51)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.250 , 0.276 0.243 , 0.265	Depositor DCC
R_{free} test set	3763 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 7.1	EDS
Estimated twinning fraction	0.545 for H, K, L 0.455 for H, -K, -L 0.326 for h,-k,-l	Xtriage
Reported twinning fraction	0.545 for H, K, L 0.455 for H, -K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 74974 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14397	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NPI

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	0.51	0/2400	0.63	1/3257 (0.0%)
1	B	0.50	0/2378	0.61	0/3226
1	C	0.50	0/2404	0.66	3/3263 (0.1%)
1	D	0.54	0/2400	0.66	0/3257
1	E	0.54	1/2311 (0.0%)	0.67	0/3137
1	F	0.52	0/2404	0.66	0/3263
All	All	0.52	1/14297 (0.0%)	0.65	4/19403 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	163	GLU	CG-CD	5.69	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	GLN	CB-CA-C	-10.44	89.52	110.40
1	C	296	GLN	N-CA-C	8.64	134.34	111.00
1	C	297	ASN	N-CA-CB	6.55	122.39	110.60
1	A	300	VAL	CG1-CB-CG2	6.26	120.92	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2364	0	2420	39	0
1	B	2342	0	2395	32	0
1	C	2367	0	2417	32	0
1	D	2364	0	2420	46	0
1	E	2277	0	2335	48	0
1	F	2367	0	2417	56	0
2	A	12	0	11	1	0
2	C	12	0	11	1	0
2	D	12	0	11	0	0
2	E	24	0	22	0	0
3	A	43	0	0	3	0
3	B	53	0	0	4	0
3	C	44	0	0	2	0
3	D	36	0	0	2	0
3	E	47	0	0	1	0
3	F	33	0	0	1	0
All	All	14397	0	14459	245	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (245) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:296:GLN:O	1:C:296:GLN:HG3	1.49	1.10
1:D:182:VAL:HG11	1:D:196:ILE:HG21	1.46	0.95
1:D:3:GLN:HE22	1:D:95:ALA:HB1	1.37	0.90
1:C:296:GLN:O	1:C:296:GLN:CG	2.16	0.89
1:E:62:TYR:CE1	1:E:83:ALA:HB1	2.12	0.84
1:B:322:ASN:HD21	1:B:324:ALA:HB2	1.44	0.81
1:D:41:VAL:HG13	1:D:64:LEU:CD2	2.10	0.81
1:D:182:VAL:HG11	1:D:196:ILE:CG2	2.14	0.77
1:B:186:ASP:OD2	3:B:345:HOH:O	2.02	0.76
1:F:14:THR:HG22	1:F:23:GLU:OE1	1.89	0.73
1:E:252:ILE:O	1:E:252:ILE:HD12	1.90	0.71
1:D:252:ILE:O	1:D:252:ILE:HD12	1.90	0.71
1:C:14:THR:HG23	1:C:23:GLU:HG3	1.72	0.71
1:D:41:VAL:HG13	1:D:64:LEU:HD22	1.74	0.70
1:A:14:THR:HG23	1:A:23:GLU:HG3	1.74	0.70
1:B:14:THR:HG23	1:B:23:GLU:HG3	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:154:GLU:HG3	3:B:349:HOH:O	1.91	0.69
1:F:41:VAL:CG1	1:F:45:LEU:HD12	2.22	0.69
1:E:154:GLU:HG3	3:E:354:HOH:O	1.92	0.69
1:D:58:SER:O	1:D:61:ALA:HB3	1.92	0.69
1:F:282:LEU:HD22	1:F:284:ILE:HG23	1.73	0.68
1:F:14:THR:HG23	1:F:23:GLU:HG3	1.75	0.68
1:D:41:VAL:HG13	1:D:64:LEU:HD21	1.77	0.67
1:F:296:GLN:HG3	1:F:296:GLN:O	1.93	0.67
1:F:94:LEU:HD21	1:F:105:GLU:HG3	1.78	0.67
1:E:82:LEU:HG	1:E:89:LEU:HD22	1.76	0.66
1:E:282:LEU:HD22	1:E:284:ILE:HG23	1.77	0.66
1:D:3:GLN:NE2	1:D:95:ALA:HB1	2.09	0.65
1:D:182:VAL:CG1	1:D:196:ILE:HG21	2.25	0.65
1:D:16:ASN:ND2	1:D:18:GLN:HE21	1.95	0.65
1:D:271:PRO:HD2	1:D:309:ALA:HB1	1.78	0.64
1:F:57:THR:HG22	1:F:60:GLN:HG3	1.80	0.64
1:B:252:ILE:HD12	1:B:252:ILE:O	1.98	0.64
1:A:252:ILE:HD12	1:A:252:ILE:O	1.98	0.64
1:F:5:LEU:HD22	1:F:95:ALA:HA	1.79	0.64
1:D:133:PRO:O	1:D:135:VAL:HG23	1.98	0.63
1:D:92:THR:C	1:D:93:LEU:HD23	2.19	0.63
1:C:251:ASN:HB3	1:E:70:GLY:HA2	1.80	0.63
1:D:8:LEU:HD12	1:D:9:ALA:N	2.13	0.63
1:E:133:PRO:O	1:E:135:VAL:HG23	1.98	0.63
1:F:282:LEU:HD22	1:F:284:ILE:CG2	2.28	0.62
1:E:15:GLN:NE2	1:E:88:PRO:HG3	2.15	0.62
1:F:294:ASP:OD2	1:F:298:ALA:HB3	1.99	0.62
1:B:319:ASN:HD22	1:B:322:ASN:H	1.46	0.62
1:B:322:ASN:HD21	1:B:324:ALA:CB	2.12	0.61
1:C:252:ILE:HD12	1:C:252:ILE:O	2.01	0.61
1:D:112:LEU:HD23	1:D:117:LEU:HD12	1.83	0.61
1:E:14:THR:HG23	1:E:23:GLU:HG3	1.82	0.60
1:D:41:VAL:HG12	1:D:45:LEU:HD12	1.84	0.60
1:E:58:SER:O	1:E:61:ALA:HB3	2.01	0.60
1:F:319:ASN:HD22	1:F:321:GLN:H	1.50	0.60
1:E:57:THR:HG22	1:E:60:GLN:HG3	1.83	0.60
2:C:381:NPI:HA	3:C:369:HOH:O	2.01	0.59
1:F:252:ILE:O	1:F:252:ILE:HD12	2.02	0.59
1:D:93:LEU:HD23	1:D:93:LEU:N	2.17	0.59
1:E:15:GLN:HE21	1:E:88:PRO:HG3	1.66	0.59
1:F:293:LEU:HD23	1:F:299:LEU:HA	1.85	0.59
1:A:251:ASN:ND2	3:A:370:HOH:O	2.33	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:112:LEU:HD23	1:D:117:LEU:CD1	2.32	0.58
1:E:100:PRO:O	1:E:131:LEU:HD11	2.03	0.58
1:F:41:VAL:HG13	1:F:45:LEU:HD12	1.85	0.57
1:C:57:THR:HG22	1:C:60:GLN:HG3	1.85	0.57
1:F:62:TYR:CZ	1:F:83:ALA:HB1	2.40	0.57
1:E:62:TYR:CZ	1:E:83:ALA:HB1	2.39	0.57
1:D:64:LEU:HB3	1:D:79:LEU:HD13	1.87	0.56
1:E:57:THR:HG23	1:E:59:GLN:N	2.20	0.56
1:F:8:LEU:HB2	1:F:93:LEU:HD22	1.87	0.56
1:E:311:GLN:HE21	1:E:311:GLN:HA	1.71	0.56
1:B:57:THR:HG22	1:B:60:GLN:HG3	1.86	0.56
1:E:294:ASP:OD2	1:E:298:ALA:HB3	2.07	0.55
1:C:14:THR:HG22	1:C:23:GLU:OE1	2.07	0.55
1:F:92:THR:C	1:F:93:LEU:HD23	2.27	0.55
1:A:41:VAL:HG22	1:A:64:LEU:HD22	1.88	0.55
1:D:174:THR:HG23	3:D:365:HOH:O	2.07	0.55
1:C:311:GLN:HB2	1:C:314:LEU:HD11	1.89	0.55
1:A:293:LEU:O	1:A:329:THR:HG22	2.08	0.54
1:F:62:TYR:CE2	1:F:83:ALA:HB1	2.42	0.54
1:B:87:LYS:NZ	3:B:388:HOH:O	2.33	0.54
1:E:14:THR:CG2	1:E:23:GLU:OE1	2.55	0.54
1:F:138:THR:HG22	1:F:164:VAL:HG22	1.89	0.54
1:E:57:THR:CG2	1:E:60:GLN:H	2.21	0.54
1:F:296:GLN:CG	1:F:296:GLN:O	2.55	0.54
1:A:14:THR:CG2	1:A:23:GLU:OE1	2.56	0.54
1:F:14:THR:CG2	1:F:23:GLU:OE1	2.55	0.54
1:C:14:THR:CG2	1:C:23:GLU:OE1	2.56	0.53
1:B:282:LEU:HD22	1:B:284:ILE:HG23	1.91	0.53
1:D:138:THR:HB	1:D:162:LEU:HD11	1.89	0.53
1:C:282:LEU:HD22	1:C:284:ILE:HG23	1.89	0.53
1:F:98:ALA:O	1:F:109:LYS:NZ	2.42	0.53
1:A:14:THR:HG22	1:A:23:GLU:OE1	2.09	0.53
1:F:120:PRO:HG2	1:F:229:PHE:CD1	2.44	0.53
1:B:14:THR:HG22	1:B:23:GLU:OE1	2.09	0.52
1:F:214:THR:HG22	1:F:230:VAL:HB	1.91	0.52
1:F:189:ARG:HD3	1:F:206:GLY:O	2.09	0.52
1:E:8:LEU:HD12	1:E:8:LEU:C	2.29	0.52
1:E:113:LEU:HD13	1:E:193:GLY:O	2.10	0.52
1:F:92:THR:HG21	1:F:104:ALA:HB1	1.91	0.52
1:B:14:THR:CG2	1:B:23:GLU:OE1	2.58	0.51
1:F:41:VAL:HG13	1:F:45:LEU:CD1	2.40	0.51
1:F:295:GLU:O	1:F:296:GLN:HB3	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:THR:HG22	1:A:60:GLN:HG3	1.91	0.51
1:E:182:VAL:HG11	1:E:196:ILE:HG21	1.93	0.51
1:C:26:TYR:OH	1:C:92:THR:HG21	2.11	0.51
1:A:157:LEU:HD21	1:C:82:LEU:HD12	1.93	0.51
1:D:282:LEU:HD22	1:D:284:ILE:HG23	1.93	0.50
1:D:8:LEU:C	1:D:8:LEU:HD12	2.31	0.50
1:E:165:PHE:CE2	1:F:163:GLU:HG3	2.46	0.50
1:D:42:ALA:HB3	1:D:43:PRO:HD3	1.91	0.50
1:F:28:LEU:HD12	1:F:78:LEU:HD22	1.94	0.50
1:A:82:LEU:HD23	1:B:157:LEU:HD21	1.94	0.50
1:F:252:ILE:HD13	1:F:254:ILE:HD11	1.94	0.50
1:B:133:PRO:O	1:B:135:VAL:HG23	2.12	0.50
1:C:41:VAL:HG22	1:C:64:LEU:HD22	1.93	0.50
1:A:41:VAL:CG1	1:A:45:LEU:HD12	2.42	0.49
1:F:87:LYS:HB3	1:F:88:PRO:HD2	1.95	0.49
1:A:319:ASN:HD22	1:A:321:GLN:H	1.58	0.49
1:C:5:LEU:HD22	1:C:95:ALA:HA	1.93	0.49
1:F:147:GLU:HG3	3:F:357:HOH:O	2.12	0.49
1:A:57:THR:HG23	1:A:59:GLN:N	2.27	0.49
1:A:271:PRO:HD2	1:A:309:ALA:HB1	1.93	0.49
1:B:174:THR:HG23	3:B:378:HOH:O	2.12	0.49
1:C:319:ASN:HD22	1:C:322:ASN:H	1.60	0.49
1:B:322:ASN:ND2	1:B:324:ALA:HB2	2.19	0.48
1:D:57:THR:HG22	1:D:60:GLN:HG3	1.94	0.48
1:D:100:PRO:O	1:D:131:LEU:HD11	2.12	0.48
1:B:57:THR:HG23	1:B:59:GLN:N	2.29	0.48
1:C:57:THR:HG23	1:C:59:GLN:N	2.29	0.48
1:B:285:THR:O	1:B:305:ALA:HB3	2.14	0.48
1:B:41:VAL:HG22	1:B:64:LEU:HD22	1.95	0.48
1:B:26:TYR:OH	1:B:92:THR:HG21	2.12	0.48
1:D:16:ASN:ND2	1:D:18:GLN:NE2	2.59	0.48
1:F:62:TYR:O	1:F:65:ALA:HB3	2.13	0.48
1:F:153:LEU:HD22	1:F:157:LEU:CD1	2.43	0.48
1:A:31:LEU:N	3:A:386:HOH:O	2.32	0.48
1:A:41:VAL:HG13	1:A:45:LEU:HD12	1.96	0.47
1:D:183:ARG:HB2	1:D:201:THR:HG23	1.96	0.47
1:C:319:ASN:HD21	1:C:321:GLN:HB2	1.79	0.47
1:E:143:VAL:HG12	1:E:144:ASP:O	2.14	0.47
1:C:146:ALA:HB3	3:C:363:HOH:O	2.12	0.47
1:E:57:THR:HG22	1:E:60:GLN:H	1.78	0.47
1:C:47:TYR:CG	1:C:93:LEU:HD12	2.50	0.47
1:F:14:THR:HB	1:F:87:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:5:LEU:HD22	1:B:95:ALA:HA	1.96	0.47
1:E:209:ASN:O	1:E:212:ALA:HB3	2.15	0.47
1:C:41:VAL:CG1	1:C:45:LEU:HD12	2.45	0.47
1:A:5:LEU:HD22	1:A:95:ALA:HA	1.97	0.47
1:E:92:THR:HG21	1:E:104:ALA:HB1	1.95	0.47
1:A:282:LEU:HD22	1:A:284:ILE:HG23	1.96	0.47
1:C:93:LEU:HD23	1:C:93:LEU:N	2.29	0.47
1:F:135:VAL:HG13	1:F:143:VAL:O	2.16	0.46
1:C:47:TYR:CD2	1:C:93:LEU:HD12	2.51	0.46
1:F:64:LEU:CB	1:F:79:LEU:HD13	2.46	0.46
1:C:296:GLN:O	1:C:297:ASN:ND2	2.48	0.46
1:A:42:ALA:HB3	1:A:43:PRO:HD3	1.97	0.46
1:F:174:THR:HG22	1:F:178:VAL:HG22	1.98	0.46
1:D:57:THR:HG23	1:D:59:GLN:H	1.80	0.46
1:D:57:THR:HG23	1:D:59:GLN:N	2.30	0.45
1:C:294:ASP:OD2	1:C:298:ALA:HB3	2.16	0.45
1:E:24:VAL:HG12	1:E:25:PHE:N	2.31	0.45
1:A:26:TYR:OH	1:A:92:THR:HG21	2.16	0.45
1:B:41:VAL:HG13	1:B:45:LEU:HD12	1.97	0.45
1:E:65:ALA:O	1:E:76:SER:OG	2.23	0.45
1:B:41:VAL:CG1	1:B:45:LEU:HD12	2.46	0.45
1:A:47:TYR:CD2	1:A:93:LEU:HD12	2.52	0.45
1:E:81:ARG:NH2	1:F:154:GLU:OE1	2.50	0.45
1:F:93:LEU:N	1:F:93:LEU:HD23	2.32	0.45
1:A:268:ILE:HG21	1:A:272:LEU:HD11	1.98	0.45
1:B:93:LEU:HD23	1:B:93:LEU:N	2.32	0.45
1:A:133:PRO:O	1:A:135:VAL:HG23	2.17	0.45
1:D:185:ALA:HB1	1:D:204:HIS:CE1	2.52	0.45
1:D:116:ARG:NH2	1:D:179:PRO:HB2	2.32	0.45
1:F:14:THR:HB	1:F:87:LYS:CE	2.47	0.44
1:D:135:VAL:HG11	1:D:142:ALA:HB1	1.99	0.44
1:F:64:LEU:HB3	1:F:79:LEU:HD13	1.99	0.44
1:A:47:TYR:CG	1:A:93:LEU:HD12	2.52	0.44
1:E:285:THR:O	1:E:305:ALA:HB3	2.17	0.44
1:D:182:VAL:CG1	1:D:196:ILE:CG2	2.91	0.44
1:B:47:TYR:CG	1:B:93:LEU:HD12	2.52	0.44
1:A:225:SER:HB3	2:A:381:NPI:OXT	2.18	0.44
1:D:132:LEU:O	1:D:169:LYS:NZ	2.32	0.44
1:B:294:ASP:OD2	1:B:298:ALA:HB3	2.18	0.44
1:A:294:ASP:OD2	1:A:298:ALA:HB3	2.18	0.44
1:A:319:ASN:ND2	1:A:321:GLN:H	2.16	0.44
1:E:17:ARG:HB2	1:E:18:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:110:LEU:HD22	1:D:193:GLY:HA3	2.00	0.44
1:B:47:TYR:CD2	1:B:93:LEU:HD12	2.52	0.44
1:D:15:GLN:NE2	1:D:88:PRO:HG3	2.33	0.44
1:C:292:LEU:O	1:C:293:LEU:HD23	2.18	0.44
1:C:42:ALA:HB3	1:C:43:PRO:HD3	2.00	0.44
1:B:57:THR:HG23	1:B:59:GLN:H	1.82	0.43
1:E:8:LEU:HD12	1:E:9:ALA:N	2.33	0.43
1:A:317:ARG:HG3	1:A:318:ARG:N	2.31	0.43
1:A:93:LEU:HD23	1:A:93:LEU:N	2.33	0.43
1:D:157:LEU:HD23	1:F:85:SER:HB2	2.00	0.43
1:A:185:ALA:N	3:A:377:HOH:O	2.51	0.43
1:F:321:GLN:O	1:F:322:ASN:ND2	2.51	0.43
1:F:252:ILE:HD13	1:F:254:ILE:CD1	2.48	0.43
1:A:156:ARG:NH1	1:C:23:GLU:OE2	2.51	0.43
1:C:57:THR:HG23	1:C:59:GLN:H	1.82	0.43
1:A:166:SER:HA	1:C:187:THR:HG23	2.00	0.43
1:F:108:LEU:O	1:F:108:LEU:HD12	2.19	0.43
1:F:42:ALA:N	1:F:43:PRO:CD	2.81	0.43
1:A:57:THR:HG23	1:A:59:GLN:H	1.84	0.43
1:E:57:THR:HG23	1:E:59:GLN:H	1.81	0.43
1:B:42:ALA:HB3	1:B:43:PRO:HD3	2.00	0.43
1:F:177:VAL:HG22	1:F:178:VAL:N	2.33	0.42
1:D:243:MET:HG2	1:D:269:GLY:HA2	2.01	0.42
1:E:42:ALA:N	1:E:43:PRO:CD	2.82	0.42
1:F:294:ASP:OD1	1:F:295:GLU:O	2.37	0.42
1:F:116:ARG:NH2	1:F:180:ALA:O	2.48	0.42
1:F:294:ASP:O	1:F:295:GLU:C	2.57	0.42
1:E:24:VAL:O	1:E:176:TYR:HE2	2.01	0.42
1:B:62:TYR:CE1	1:B:83:ALA:HB1	2.54	0.42
1:C:133:PRO:O	1:C:135:VAL:HG23	2.19	0.42
1:D:319:ASN:HD22	1:D:320:SER:N	2.17	0.42
1:E:14:THR:HG23	1:E:23:GLU:OE1	2.19	0.42
1:A:292:LEU:O	1:A:293:LEU:HD23	2.19	0.42
1:F:41:VAL:CG1	1:F:45:LEU:CD1	2.95	0.42
1:A:300:VAL:HG22	1:A:301:LYS:HG2	2.02	0.42
1:F:182:VAL:HG12	1:F:197:GLY:O	2.19	0.42
1:E:62:TYR:CD1	1:E:83:ALA:HB1	2.52	0.42
1:B:322:ASN:C	1:B:322:ASN:ND2	2.74	0.41
1:A:62:TYR:CE1	1:A:83:ALA:HB1	2.55	0.41
1:D:223:ARG:HG3	3:D:363:HOH:O	2.19	0.41
1:D:92:THR:HG21	1:D:104:ALA:HB1	2.03	0.41
1:D:14:THR:HG23	1:D:23:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:8:LEU:C	1:C:8:LEU:HD12	2.40	0.41
1:E:134:ASN:HD22	1:E:135:VAL:H	1.68	0.41
1:C:41:VAL:HG13	1:C:45:LEU:HD12	2.02	0.41
1:A:87:LYS:HB3	1:A:88:PRO:HD2	2.03	0.41
1:E:57:THR:H	1:E:60:GLN:NE2	2.19	0.41
1:E:270:ILE:HD13	1:E:305:ALA:HB1	2.01	0.41
1:E:195:TYR:O	1:E:213:GLY:HA3	2.20	0.41
1:E:47:TYR:CD2	1:E:93:LEU:HD12	2.56	0.41
1:E:47:TYR:CG	1:E:93:LEU:HD12	2.56	0.41
1:D:222:GLY:HA3	1:D:240:CYS:SG	2.61	0.41
1:A:92:THR:OG1	1:A:108:LEU:HD22	2.21	0.41
1:E:242:THR:HG22	1:E:268:ILE:CG1	2.51	0.40
1:A:57:THR:CG2	1:A:60:GLN:H	2.35	0.40
1:E:92:THR:CG2	1:E:104:ALA:HB1	2.52	0.40
1:F:272:LEU:HD22	1:F:276:ASN:HD22	1.86	0.40
1:D:125:LEU:O	1:D:128:ILE:HB	2.21	0.40
1:E:165:PHE:CZ	1:F:163:GLU:HG3	2.57	0.40
1:B:57:THR:CG2	1:B:60:GLN:H	2.35	0.40
1:E:5:LEU:HD22	1:E:95:ALA:HA	2.02	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	315/347 (91%)	310 (98%)	5 (2%)	0	100	100
1	B	312/347 (90%)	308 (99%)	4 (1%)	0	100	100
1	C	317/347 (91%)	313 (99%)	4 (1%)	0	100	100
1	D	315/347 (91%)	297 (94%)	18 (6%)	0	100	100
1	E	302/347 (87%)	291 (96%)	11 (4%)	0	100	100
1	F	317/347 (91%)	304 (96%)	13 (4%)	0	100	100
All	All	1878/2082 (90%)	1823 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	244/263 (93%)	231 (95%)	13 (5%)	32	54
1	B	241/263 (92%)	229 (95%)	12 (5%)	34	58
1	C	244/263 (93%)	234 (96%)	10 (4%)	41	67
1	D	244/263 (93%)	230 (94%)	14 (6%)	29	50
1	E	235/263 (89%)	220 (94%)	15 (6%)	25	43
1	F	244/263 (93%)	234 (96%)	10 (4%)	41	67
All	All	1452/1578 (92%)	1378 (95%)	74 (5%)	33	57

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	14	THR
1	A	59	GLN
1	A	92	THR
1	A	93	LEU
1	A	123	VAL
1	A	153	LEU
1	A	163	GLU
1	A	282	LEU
1	A	297	ASN
1	A	306	ARG
1	A	317	ARG
1	A	319	ASN
1	B	8	LEU
1	B	14	THR
1	B	82	LEU
1	B	92	THR
1	B	93	LEU
1	B	123	VAL
1	B	163	GLU
1	B	282	LEU

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Mol	Chain	Res	Type
1	B	297	ASN
1	B	306	ARG
1	B	317	ARG
1	B	322	ASN
1	C	8	LEU
1	C	14	THR
1	C	82	LEU
1	C	92	THR
1	C	93	LEU
1	C	123	VAL
1	C	153	LEU
1	C	163	GLU
1	C	282	LEU
1	C	296	GLN
1	D	8	LEU
1	D	14	THR
1	D	93	LEU
1	D	153	LEU
1	D	163	GLU
1	D	198	GLU
1	D	245	THR
1	D	253	VAL
1	D	282	LEU
1	D	300	VAL
1	D	306	ARG
1	D	317	ARG
1	D	318	ARG
1	D	319	ASN
1	E	8	LEU
1	E	14	THR
1	E	41	VAL
1	E	66	ASP
1	E	82	LEU
1	E	84	GLU
1	E	93	LEU
1	E	123	VAL
1	E	165	PHE
1	E	241	SER
1	E	282	LEU
1	E	283	TYR
1	E	297	ASN
1	E	306	ARG

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Mol	Chain	Res	Type
1	E	311	GLN
1	F	14	THR
1	F	59	GLN
1	F	84	GLU
1	F	92	THR
1	F	153	LEU
1	F	163	GLU
1	F	165	PHE
1	F	282	LEU
1	F	319	ASN
1	F	328	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	GLN
1	A	60	GLN
1	A	134	ASN
1	A	319	ASN
1	B	15	GLN
1	B	60	GLN
1	B	115	HIS
1	B	134	ASN
1	B	319	ASN
1	B	322	ASN
1	C	3	GLN
1	C	15	GLN
1	C	60	GLN
1	C	134	ASN
1	C	297	ASN
1	C	319	ASN
1	D	3	GLN
1	D	15	GLN
1	D	18	GLN
1	D	52	GLN
1	D	60	GLN
1	D	319	ASN
1	E	15	GLN
1	E	59	GLN
1	E	60	GLN
1	E	115	HIS

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Mol	Chain	Res	Type
1	E	134	ASN
1	E	311	GLN
1	F	3	GLN
1	F	15	GLN
1	F	18	GLN
1	F	134	ASN
1	F	276	ASN
1	F	311	GLN
1	F	319	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NPI	A	381	-	11,11,11	0.87	0	13,13,13	1.01	0
2	NPI	C	381	-	11,11,11	1.08	1 (9%)	13,13,13	0.93	1 (7%)
2	NPI	D	381	-	11,11,11	1.04	0	13,13,13	1.08	0
2	NPI	E	345	-	11,11,11	1.15	0	13,13,13	0.95	1 (7%)
2	NPI	E	381	-	11,11,11	1.07	0	13,13,13	1.07	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	NPI	A	381	-	-	0/11/11/11	0/0/0/0
2	NPI	C	381	-	-	0/11/11/11	0/0/0/0
2	NPI	D	381	-	-	0/11/11/11	0/0/0/0
2	NPI	E	345	-	-	0/11/11/11	0/0/0/0
2	NPI	E	381	-	-	0/11/11/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	381	NPI	C6-C7	2.34	1.56	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	345	NPI	C-CA-N	-2.24	105.66	109.36
2	C	381	NPI	C-CA-N	2.05	112.75	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	321/347 (92%)	-0.20	0	100 100	12, 17, 48, 68	0
1	B	318/347 (91%)	-0.24	0	100 100	11, 16, 43, 56	0
1	C	321/347 (92%)	-0.16	1 (0%)	91 93	12, 18, 46, 55	0
1	D	321/347 (92%)	-0.11	1 (0%)	91 93	12, 18, 50, 76	0
1	E	310/347 (89%)	-0.21	1 (0%)	91 93	11, 17, 44, 59	0
1	F	321/347 (92%)	-0.14	1 (0%)	91 93	13, 19, 50, 58	0
All	All	1912/2082 (91%)	-0.18	4 (0%)	93 94	11, 18, 48, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	321	GLN	3.2
1	F	302	VAL	2.1
1	E	302	VAL	2.0
1	C	3	GLN	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NPI	E	381	12/12	0.17	2.90	2,2,5,5	0
2	NPI	A	381	12/12	0.17	2.04	7,8,10,10	0
2	NPI	C	381	12/12	0.16	1.32	6,11,20,22	0
2	NPI	E	345	12/12	0.15	0.82	8,16,19,20	0
2	NPI	D	381	12/12	0.15	0.24	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.