



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 09:16 PM UTC

PDB ID : 3R5D / pdb_00003r5d
Title : Pseudomonas aeruginosa DapD (PA3666) apoprotein
Authors : Sandalova, T.; Schnell, R.; Schneider, G.
Deposited on : 2011-03-18
Resolution : 1.80 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

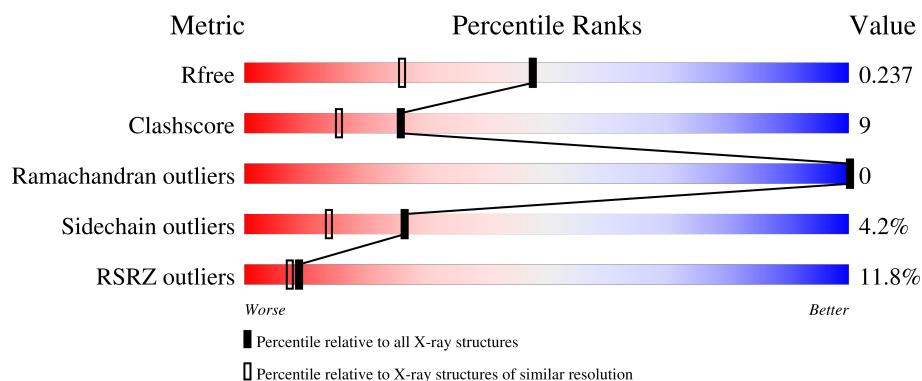
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	347	10% 77% 14% • 8%
1	B	347	13% 78% 14% • 8%
1	C	347	11% 69% 20% • 8%
1	D	347	10% 75% 16% • 8%
1	E	347	10% 74% 16% • 8%

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Mol	Chain	Length	Quality of chain
1	F	347	

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	GOL	E	345	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14905 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 Tetrahydrodipicolinate N-succinyletransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	2	0
			2366	1507	405	447	7			
1	B	320	Total	C	N	O	S	0	2	0
			2366	1507	405	447	7			
1	C	319	Total	C	N	O	S	0	1	0
			2358	1502	404	445	7			
1	D	320	Total	C	N	O	S	0	2	0
			2370	1509	408	446	7			
1	E	320	Total	C	N	O	S	0	2	0
			2366	1507	405	447	7			
1	F	320	Total	C	N	O	S	0	1	0
			2362	1504	405	446	7			

There are 18 discrepancies between the modelled and reference sequences:

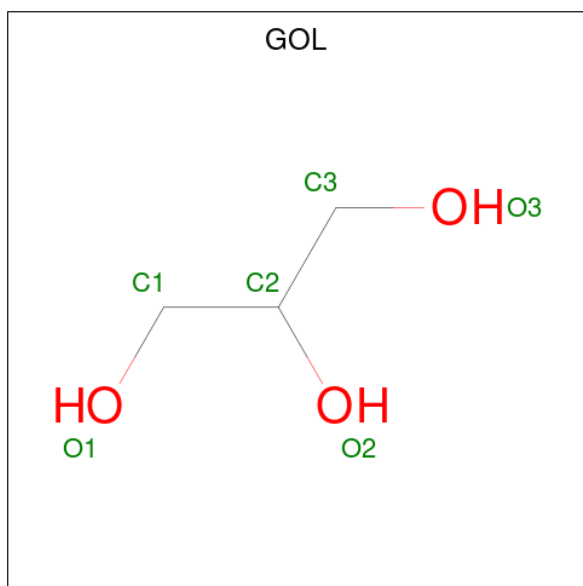
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9Z9H2
A	-1	SER	-	expression tag	UNP Q9Z9H2
A	0	HIS	-	expression tag	UNP Q9Z9H2
B	-2	GLY	-	expression tag	UNP Q9Z9H2
B	-1	SER	-	expression tag	UNP Q9Z9H2
B	0	HIS	-	expression tag	UNP Q9Z9H2
C	-2	GLY	-	expression tag	UNP Q9Z9H2
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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

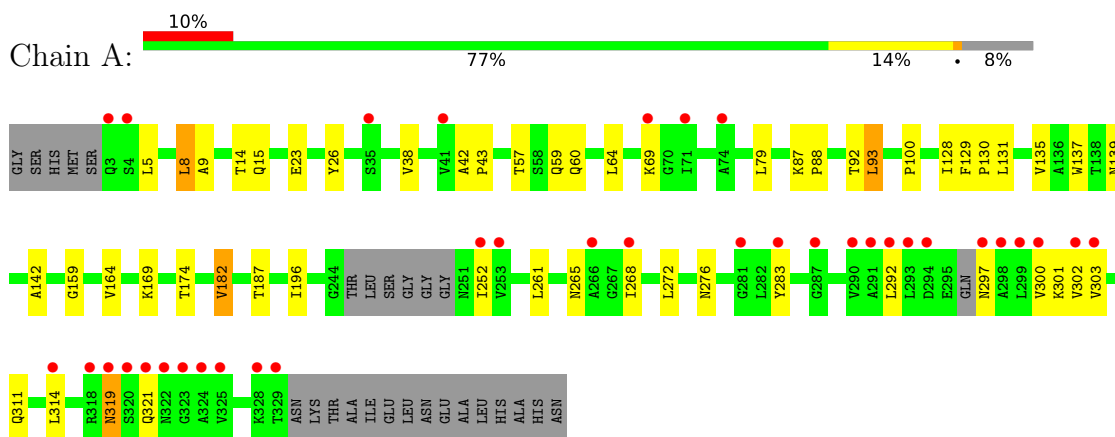
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	143	Total	O	0	0
			143	143		
3	C	89	Total	O	0	0
			89	89		
3	D	120	Total	O	0	0
			120	120		
3	E	147	Total	O	0	0
			147	147		
3	F	94	Total	O	0	0
			94	94		

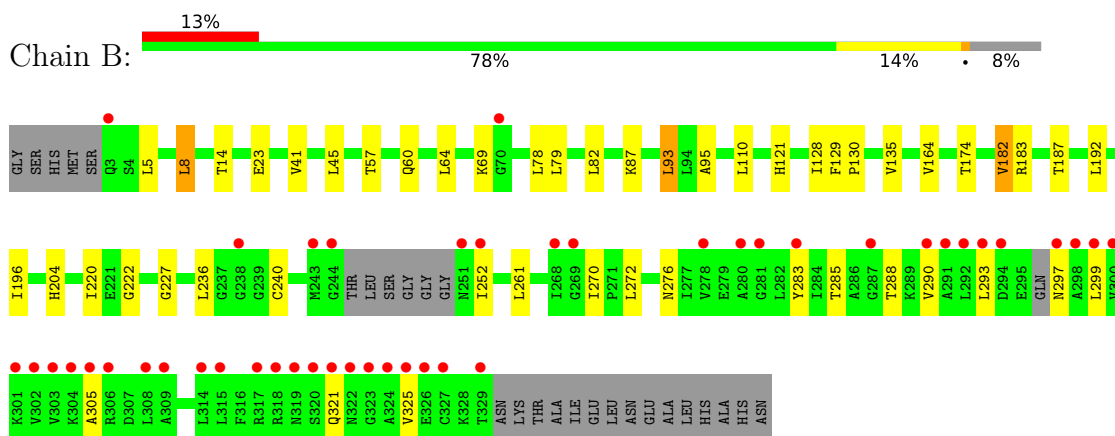
3 Residue-property plots

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.

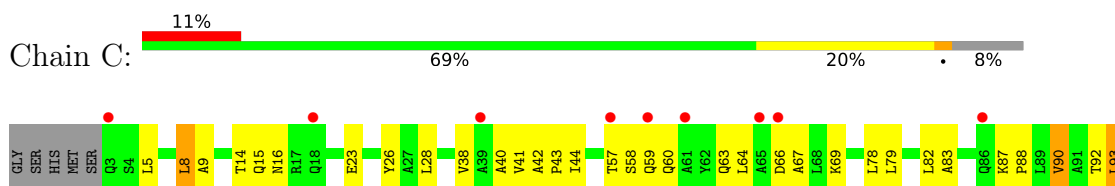
- Molecule 1: Tetrahydrodipicolinate N-succinyletransferase

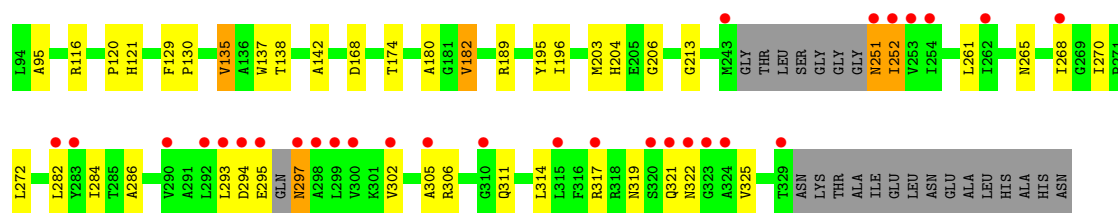


- Molecule 1: Tetrahydrodipicolinate N-succinyletransferase

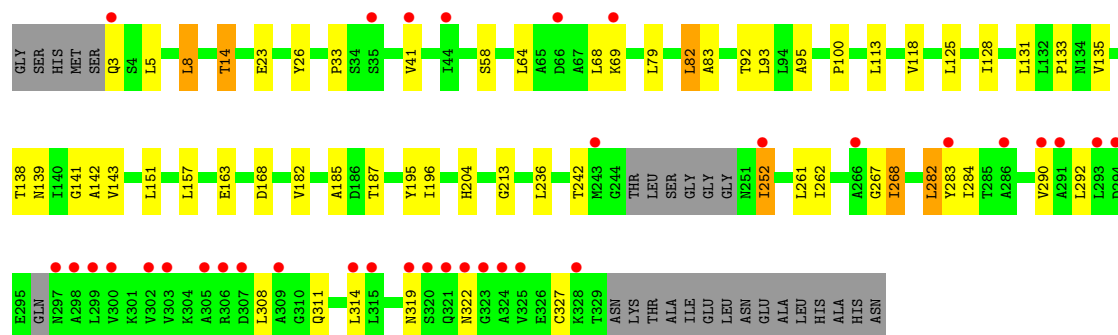
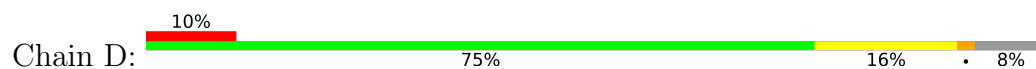


- Molecule 1: Tetrahydrodipicolinate N-succinyletransferase

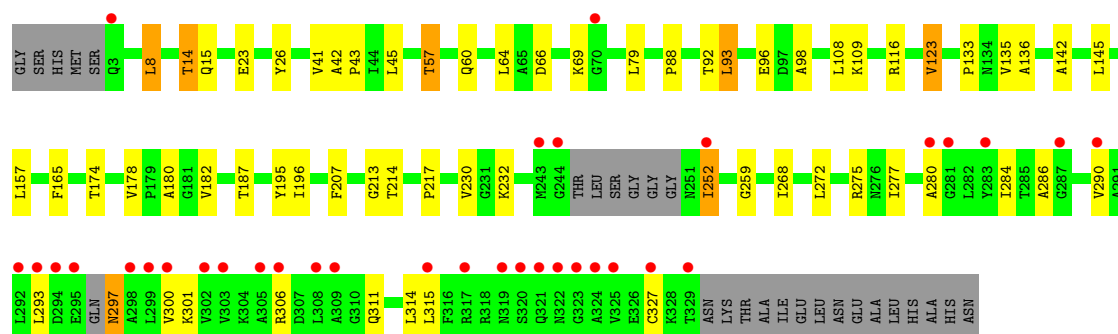
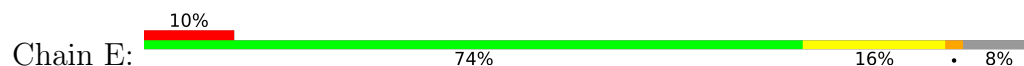




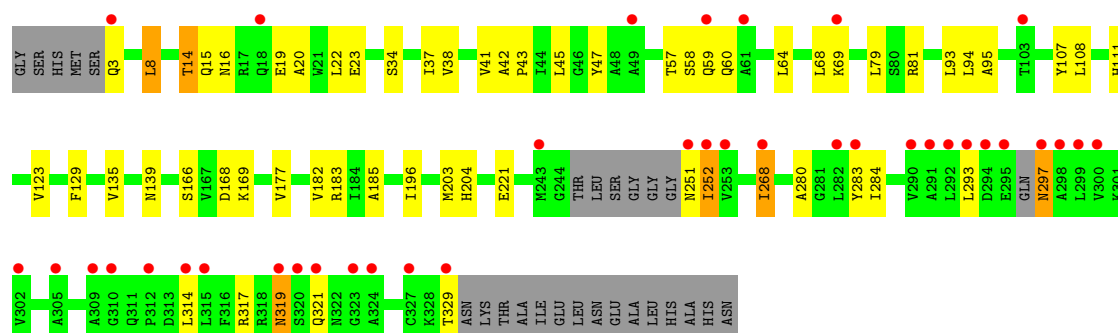
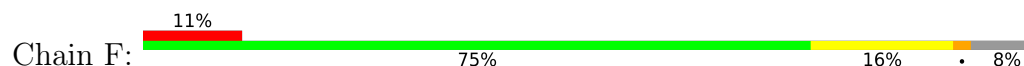
● Molecule 1: Tetrahydrodipicolinate N-succinyletransferase



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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)	24.38 – 1.80 24.38 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (24.38-1.80) 94.9 (24.38-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.236 0.208 , 0.237	Depositor DCC
R_{free} test set	10007 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.277 for h,-k,-l	Xtriage
Reported twinning fraction	0.507 for H, K, L 0.493 for h,-k,-l	Depositor
Outliers	0 of 197589 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14905	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: GOL

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	0.49	0/2408	0.71	0/3268
1	B	0.51	0/2408	0.70	0/3268
1	C	0.50	0/2397	0.72	0/3253
1	D	0.48	0/2412	0.72	0/3272
1	E	0.50	0/2408	0.69	0/3268
1	F	0.50	0/2401	0.74	0/3258
All	All	0.50	0/14434	0.71	0/19587

There are no bond length outliers.

There are no bond angle outliers.

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	2366	0	2422	46	0
1	B	2366	0	2422	40	0
1	C	2358	0	2412	63	0
1	D	2370	0	2428	48	0
1	E	2366	0	2422	50	0
1	F	2362	0	2415	45	0
2	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	6	0	8	4	0
3	A	112	0	0	0	0
3	B	143	0	0	1	0
3	C	89	0	0	3	0
3	D	120	0	0	2	0
3	E	147	0	0	1	0
3	F	94	0	0	0	0
All	All	14905	0	14537	272	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 9.

All (272) 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:14:THR:HG22	1:A:87:LYS:HZ1	1.18	1.02
1:A:14:THR:HG22	1:A:87:LYS:NZ	1.73	1.01
1:B:14:THR:HG22	1:B:87:LYS:HZ1	1.31	0.95
1:A:139:ASN:HB2	2:A:345:GOL:H12	1.54	0.88
1:C:8:LEU:HD13	1:C:93:LEU:HD22	1.58	0.86
1:C:26:TYR:OH	1:C:92:THR:HG21	1.74	0.86
1:B:14:THR:HG22	1:B:87:LYS:NZ	1.91	0.85
1:F:57:THR:HG22	1:F:59:GLN:H	1.43	0.83
1:C:8:LEU:HD13	1:C:93:LEU:CD2	2.09	0.82
1:F:45:LEU:HD21	1:F:64:LEU:HD11	1.62	0.82
1:B:14:THR:HG23	1:B:23:GLU:OE1	1.82	0.80
1:E:174:THR:HG22	1:E:178:VAL:HG22	1.66	0.76
1:B:174[A]:THR:HG21	1:B:187:THR:HG21	1.68	0.76
1:C:14:THR:HG23	1:C:23:GLU:OE1	1.87	0.74
1:A:57:THR:HG22	1:A:60:GLN:HE21	1.52	0.74
1:E:41:VAL:HG13	1:E:64:LEU:CD2	2.18	0.73
1:D:100:PRO:O	1:D:131:LEU:HD11	1.89	0.72
1:B:5:LEU:HD22	1:B:95:ALA:HA	1.72	0.71
1:C:41:VAL:HG13	1:C:64:LEU:HD22	1.72	0.70
1:F:38:VAL:O	1:F:42:ALA:HB2	1.91	0.70
1:A:129:PHE:O	1:A:169:LYS:NZ	2.23	0.70
1:F:3:GLN:OE1	1:F:95:ALA:HB1	1.93	0.69
1:F:182:VAL:HG11	1:F:196:ILE:HG21	1.73	0.69
1:C:8:LEU:HD12	1:C:9:ALA:N	2.09	0.68
1:A:164:VAL:O	1:C:174[B]:THR:HG21	1.94	0.68
1:C:78:LEU:O	1:C:82:LEU:HD13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174[B]:THR:HG21	1:B:164:VAL:O	1.95	0.66
1:B:272:LEU:HD22	1:B:276:ASN:HD22	1.61	0.66
1:C:42:ALA:HB3	1:C:43:PRO:HD3	1.77	0.65
1:C:14:THR:HG22	1:C:87:LYS:NZ	2.10	0.65
1:D:135:VAL:HG11	1:D:142:ALA:HB1	1.79	0.64
1:F:319:ASN:HD22	1:F:321:GLN:H	1.45	0.64
1:D:8:LEU:C	1:D:8:LEU:HD12	2.22	0.64
1:E:41:VAL:HG13	1:E:64:LEU:HD22	1.78	0.64
1:E:92[A]:THR:OG1	1:E:108:LEU:HD22	1.98	0.64
1:E:280:ALA:HB1	1:F:283:TYR:CE1	2.33	0.64
1:F:14:THR:HG23	1:F:23:GLU:OE1	1.97	0.64
1:E:57[B]:THR:H	1:E:60:GLN:HE21	1.46	0.63
1:E:57[A]:THR:H	1:E:60:GLN:HE21	1.46	0.63
1:A:26:TYR:OH	1:A:92[B]:THR:HG21	1.98	0.63
1:F:34:SER:O	1:F:38:VAL:HG23	1.98	0.62
1:C:203:MET:HE3	1:C:204:HIS:HD2	1.64	0.62
1:C:14:THR:OG1	1:C:23:GLU:HG3	2.01	0.60
1:D:267:GLY:HA3	1:D:283:TYR:CD1	2.36	0.60
1:E:41:VAL:HG12	1:E:45:LEU:HD12	1.84	0.60
1:F:8:LEU:HB2	1:F:93:LEU:CD2	2.32	0.59
1:A:14:THR:CG2	1:A:87:LYS:HZ1	2.05	0.59
1:A:139:ASN:CB	2:A:345:GOL:H12	2.30	0.59
1:C:15:GLN:HE21	1:C:88:PRO:HG3	1.67	0.59
1:E:41:VAL:HG13	1:E:64:LEU:HD21	1.84	0.59
1:C:57:THR:HG22	1:C:60:GLN:HG3	1.85	0.59
1:C:251:ASN:N	1:C:251:ASN:HD22	2.00	0.59
1:A:174[B]:THR:CG2	1:B:164:VAL:O	2.51	0.58
1:A:265:ASN:ND2	1:B:283:TYR:OH	2.30	0.58
1:B:182:VAL:HG22	1:B:196:ILE:HG22	1.84	0.58
1:D:267:GLY:HA3	1:D:283:TYR:CE1	2.39	0.58
1:E:41:VAL:HG12	1:E:45:LEU:CD1	2.34	0.58
1:E:98:ALA:O	1:E:109:LYS:NZ	2.36	0.58
1:C:14:THR:HG22	1:C:87:LYS:HZ3	1.65	0.58
1:B:41:VAL:HG22	1:B:64:LEU:HD22	1.85	0.58
1:A:14:THR:HG23	1:A:23:GLU:OE1	2.04	0.57
1:D:5:LEU:HD22	1:D:95:ALA:HA	1.85	0.57
1:B:174[A]:THR:HG21	1:B:187:THR:CG2	2.34	0.57
1:D:290:VAL:HG11	1:D:327:CYS:HB2	1.88	0.56
1:E:116:ARG:NH2	1:E:180:ALA:O	2.34	0.56
1:C:41:VAL:HG13	1:C:64:LEU:CD2	2.35	0.56
1:E:182:VAL:HG11	1:E:196:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:PHE:HB2	1:C:130:PRO:HD3	1.87	0.56
1:D:182:VAL:HG11	1:D:196:ILE:HG21	1.88	0.56
1:D:252:ILE:HD12	1:D:252:ILE:O	2.05	0.56
1:F:252:ILE:HD12	1:F:252:ILE:O	2.06	0.56
1:C:14:THR:HG21	3:C:437:HOH:O	2.06	0.56
1:C:137:TRP:CZ3	1:C:142:ALA:HB2	2.41	0.55
1:E:187:THR:HG23	1:F:166:SER:HA	1.89	0.55
1:A:42:ALA:HB3	1:A:43:PRO:HD3	1.89	0.55
1:A:164:VAL:O	1:C:174[B]:THR:CG2	2.55	0.55
1:F:8:LEU:HB2	1:F:93:LEU:HD22	1.88	0.55
1:A:311:GLN:HB2	1:A:314:LEU:HD11	1.90	0.54
1:B:290:VAL:HG22	1:B:325:VAL:HG12	1.88	0.54
1:D:133:PRO:O	1:D:135:VAL:HG23	2.06	0.54
1:D:100:PRO:HB2	1:D:131:LEU:CD1	2.38	0.54
1:B:129:PHE:HB2	1:B:130:PRO:HD3	1.89	0.54
1:C:40:ALA:HB1	1:C:67:ALA:HB1	1.89	0.54
1:F:182:VAL:HG11	1:F:196:ILE:CG2	2.38	0.54
1:A:57:THR:H	1:A:60:GLN:HE21	1.54	0.54
1:A:8:LEU:HB2	1:A:93:LEU:HD22	1.90	0.54
1:B:57:THR:H	1:B:60:GLN:HE21	1.55	0.54
1:C:182:VAL:HG22	1:C:196:ILE:HG22	1.89	0.54
1:E:57[B]:THR:H	1:E:60:GLN:NE2	2.06	0.54
1:D:41:VAL:HG22	1:D:64:LEU:HD22	1.90	0.53
1:E:14:THR:HG23	1:E:23:GLU:HG3	1.89	0.53
1:A:14:THR:HG22	1:A:87:LYS:HZ3	1.72	0.53
1:B:8:LEU:C	1:B:8:LEU:HD12	2.33	0.53
1:E:57[A]:THR:H	1:E:60:GLN:NE2	2.06	0.53
1:D:113:LEU:HD23	1:D:118:VAL:HG23	1.91	0.53
1:F:57:THR:CG2	1:F:58:SER:N	2.71	0.53
1:D:82:LEU:HD12	1:E:157:LEU:HD21	1.90	0.53
1:F:68:LEU:HD12	1:F:79:LEU:CD1	2.39	0.53
1:C:203:MET:HE3	1:C:204:HIS:CD2	2.43	0.53
1:E:290:VAL:HG11	1:E:327:CYS:HB2	1.90	0.53
1:F:47:TYR:CG	1:F:93:LEU:HD12	2.44	0.53
1:B:8:LEU:HB2	1:B:93:LEU:HD22	1.90	0.53
1:D:14:THR:HG21	3:D:382:HOH:O	2.09	0.52
1:C:319:ASN:HD22	1:C:322:ASN:H	1.56	0.52
1:D:58:SER:OG	1:D:83:ALA:O	2.26	0.52
1:E:314:LEU:HD22	1:E:327:CYS:SG	2.48	0.52
1:A:292:LEU:O	1:A:300:VAL:HG12	2.10	0.52
1:E:133:PRO:O	1:E:135:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLN:HE21	1:C:302:VAL:HG11	1.74	0.52
1:E:26:TYR:OH	1:E:92[A]:THR:HG21	2.10	0.52
1:C:189:ARG:HD3	1:C:206:GLY:O	2.10	0.52
1:C:57:THR:HG23	1:C:59:GLN:N	2.24	0.51
1:C:92:THR:C	1:C:93:LEU:HD23	2.35	0.51
1:D:292:LEU:HD13	1:D:308:LEU:HD21	1.92	0.51
1:E:286:ALA:HB1	1:E:306:ARG:HB3	1.92	0.51
1:B:290:VAL:HG22	1:B:325:VAL:CG1	2.40	0.51
1:C:268:ILE:HG21	1:C:272:LEU:HD11	1.93	0.51
1:F:185:ALA:HB1	1:F:204:HIS:CE1	2.46	0.51
1:A:100:PRO:O	1:A:131:LEU:HD11	2.11	0.50
1:D:185:ALA:HB1	1:D:204:HIS:CE1	2.47	0.50
1:A:265:ASN:HD22	1:B:283:TYR:HH	1.54	0.50
1:C:116:ARG:HD3	3:C:376:HOH:O	2.11	0.50
1:E:136:ALA:HB2	1:E:145:LEU:HD23	1.91	0.50
1:F:94:LEU:HD11	1:F:108:LEU:HD23	1.92	0.50
1:A:57:THR:HG23	1:A:60:GLN:H	1.77	0.50
1:C:28:LEU:HD11	3:C:480:HOH:O	2.12	0.50
1:D:26:TYR:OH	1:D:92[A]:THR:HG21	2.12	0.50
1:C:189:ARG:HD2	1:C:204:HIS:O	2.12	0.50
1:D:187:THR:OG1	1:E:165:PHE:HA	2.12	0.50
1:C:116:ARG:NH2	1:C:180:ALA:O	2.43	0.50
1:D:139:ASN:HB2	2:E:345:GOL:H31	1.94	0.50
1:D:282:LEU:HD11	1:D:284:ILE:HG23	1.93	0.49
1:C:90:VAL:HG13	1:C:92:THR:HG23	1.94	0.49
1:F:268:ILE:HG13	1:F:268:ILE:O	2.11	0.49
1:C:5:LEU:HD12	1:C:38:VAL:CG2	2.42	0.49
1:B:78:LEU:O	1:B:82:LEU:HD13	2.13	0.49
1:D:8:LEU:HB2	1:D:93:LEU:HD22	1.94	0.49
1:D:143:VAL:HG11	1:D:151:LEU:HD12	1.94	0.49
1:D:261:LEU:HD13	1:D:261:LEU:O	2.13	0.49
1:F:41:VAL:HG22	1:F:64:LEU:HD22	1.94	0.49
1:E:41:VAL:CG1	1:E:45:LEU:CD1	2.91	0.49
1:F:8:LEU:HD21	1:F:37:ILE:CG2	2.42	0.49
1:C:5:LEU:HD23	1:C:95:ALA:HA	1.94	0.49
1:D:283:TYR:CE1	1:F:280:ALA:HB1	2.47	0.49
1:C:44:ILE:HD13	1:C:63:GLN:HB3	1.95	0.48
1:A:8:LEU:HD12	1:A:9:ALA:N	2.28	0.48
1:A:159:GLY:HA2	1:C:87:LYS:HZ2	1.79	0.48
1:C:135:VAL:HG12	1:C:137:TRP:CE2	2.48	0.48
1:C:120:PRO:O	1:C:121:HIS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:PRO:HD2	1:E:232:LYS:HG3	1.96	0.48
1:E:293:LEU:HD13	1:E:297:ASN:HB2	1.95	0.47
1:F:57:THR:H	1:F:60:GLN:HE21	1.62	0.47
1:A:265:ASN:HB2	1:B:283:TYR:OH	2.15	0.47
1:B:204:HIS:CD2	1:B:204:HIS:H	2.31	0.47
1:F:57:THR:HG22	1:F:58:SER:N	2.29	0.47
1:B:110:LEU:HB3	1:B:192:LEU:HG	1.96	0.47
1:D:319:ASN:HD22	1:D:322:ASN:H	1.61	0.47
1:A:319:ASN:HD22	1:A:321:GLN:H	1.61	0.47
1:C:93:LEU:HD23	1:C:93:LEU:N	2.30	0.47
1:F:16:ASN:ND2	1:F:20:ALA:HB3	2.30	0.47
1:D:311:GLN:HB2	1:D:314:LEU:HD11	1.96	0.47
1:D:125:LEU:HD22	1:D:128:ILE:HD12	1.96	0.47
1:C:252:ILE:O	1:C:252:ILE:HD12	2.15	0.46
1:A:128:ILE:HG23	1:A:129:PHE:HD1	1.80	0.46
1:A:137:TRP:CZ3	1:A:142:ALA:HB2	2.49	0.46
1:C:195:TYR:O	1:C:213:GLY:HA3	2.15	0.46
1:C:293:LEU:HD13	1:C:297:ASN:HB2	1.96	0.46
1:D:282:LEU:HD12	1:D:283:TYR:N	2.30	0.46
1:E:64:LEU:HB3	1:E:79:LEU:HD13	1.98	0.46
1:E:214:THR:HG22	1:E:230:VAL:HB	1.96	0.46
1:A:283:TYR:OH	1:C:265:ASN:ND2	2.46	0.46
1:F:42:ALA:HB3	1:F:43:PRO:HD3	1.98	0.46
1:A:8:LEU:HD12	1:A:8:LEU:C	2.41	0.46
1:D:68:LEU:HD12	1:D:79:LEU:CD1	2.46	0.45
1:F:22:LEU:HD22	1:F:135:VAL:HG22	1.97	0.45
1:B:174[A]:THR:HG21	1:B:187:THR:CB	2.46	0.45
1:B:183:ARG:HD2	1:C:168:ASP:OD1	2.17	0.45
1:C:64:LEU:HB3	1:C:79:LEU:HD13	1.97	0.45
1:E:311:GLN:HB2	1:E:314:LEU:HD11	1.98	0.45
2:E:345:GOL:H12	1:F:139:ASN:HB3	1.98	0.45
1:A:64:LEU:HB3	1:A:79:LEU:HD13	1.97	0.45
1:F:293:LEU:HD13	1:F:297:ASN:HB2	1.98	0.45
1:A:272:LEU:HD22	1:A:276:ASN:HD22	1.81	0.45
1:B:252:ILE:HD12	1:B:252:ILE:O	2.16	0.45
1:D:157:LEU:HD11	1:F:81:ARG:HB3	1.99	0.45
1:E:109:LYS:HE2	1:E:123:VAL:HG13	1.99	0.45
1:D:204:HIS:CD2	1:E:207:PHE:CE2	3.05	0.45
1:A:93:LEU:HD23	1:A:93:LEU:N	2.32	0.45
1:B:121:HIS:CE1	1:B:227:GLY:O	2.70	0.45
1:D:236:LEU:HG	1:D:262:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:LEU:HD21	1:E:64:LEU:HD11	1.98	0.45
1:D:138:THR:HA	1:D:163:GLU:O	2.17	0.44
1:D:242:THR:HG22	1:D:268:ILE:CD1	2.46	0.44
1:E:277:ILE:HB	1:E:315:LEU:HD13	2.00	0.44
1:C:282:LEU:HD11	1:C:325:VAL:HG22	1.99	0.44
1:D:139:ASN:CB	2:E:345:GOL:H31	2.47	0.44
1:D:195:TYR:O	1:D:213:GLY:HA3	2.17	0.44
1:E:259:GLY:O	1:E:275:ARG:HA	2.17	0.44
1:D:100:PRO:C	1:D:131:LEU:HD11	2.42	0.44
1:A:129:PHE:HB2	1:A:130:PRO:HD3	1.99	0.44
1:A:182:VAL:HG22	1:A:196:ILE:HG22	1.99	0.44
1:B:270:ILE:CD1	1:B:305:ALA:HB1	2.48	0.44
1:B:174[A]:THR:CG2	1:B:187:THR:HB	2.48	0.44
1:B:222:GLY:HA3	1:B:240:CYS:SG	2.58	0.44
1:F:252:ILE:O	1:F:252:ILE:CD1	2.65	0.44
1:F:94:LEU:CD1	1:F:108:LEU:HD23	2.48	0.43
1:C:182:VAL:CG2	1:C:196:ILE:HG22	2.48	0.43
1:C:311:GLN:HB2	1:C:314:LEU:HD11	2.00	0.43
1:B:87:LYS:NZ	3:B:358:HOH:O	2.45	0.43
1:F:16:ASN:HD21	1:F:20:ALA:HB3	1.83	0.43
1:B:293:LEU:HD23	1:B:299:LEU:HA	2.01	0.43
1:C:294:ASP:O	1:C:295:GLU:C	2.60	0.43
1:E:8:LEU:HD12	1:E:8:LEU:C	2.42	0.43
1:F:107:TYR:O	1:F:111:HIS:ND1	2.46	0.43
1:A:301:LYS:HG3	1:A:303:VAL:HG13	2.01	0.43
1:C:5:LEU:HD12	1:C:38:VAL:HG21	2.00	0.43
1:C:286:ALA:HB1	1:C:306:ARG:CZ	2.49	0.43
1:D:252:ILE:O	1:D:252:ILE:CD1	2.67	0.43
1:F:3:GLN:CD	1:F:95:ALA:HB1	2.44	0.43
1:D:3:GLN:NE2	1:D:95:ALA:HB1	2.34	0.43
1:C:64:LEU:CB	1:C:79:LEU:HD13	2.49	0.43
1:E:300:VAL:HG12	1:E:301:LYS:HG2	2.00	0.43
1:F:314:LEU:CD2	1:F:329:THR:HG22	2.49	0.43
1:A:174[B]:THR:HG21	1:A:187:THR:CB	2.49	0.42
1:A:302:VAL:HG11	1:C:321:GLN:NE2	2.34	0.42
1:C:57:THR:HG23	1:C:60:GLN:H	1.84	0.42
1:D:64:LEU:HB3	1:D:79:LEU:HD13	2.01	0.42
1:F:168:ASP:OD1	1:F:169:LYS:N	2.48	0.42
1:F:203:MET:HB2	1:F:221:GLU:HG2	2.01	0.42
1:A:5:LEU:HD12	1:A:38:VAL:CG2	2.49	0.42
1:B:41:VAL:CG1	1:B:45:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:THR:HA	1:D:268:ILE:HG12	2.01	0.42
1:A:268:ILE:HG21	1:A:272:LEU:HD11	2.01	0.42
1:C:57:THR:HG23	1:C:59:GLN:H	1.83	0.42
1:D:14:THR:HG23	1:D:23:GLU:HG3	2.01	0.42
1:E:15:GLN:HE21	1:E:88:PRO:HG3	1.85	0.42
1:C:8:LEU:HA	1:C:92:THR:O	2.20	0.42
1:E:42:ALA:HB3	1:E:43:PRO:HD3	2.01	0.42
1:E:57[A]:THR:HG22	3:E:378:HOH:O	2.20	0.42
1:F:59:GLN:HE21	1:F:59:GLN:N	2.18	0.41
1:B:285:THR:H	1:B:288:THR:HG1	1.67	0.41
1:C:58:SER:OG	1:C:83:ALA:O	2.38	0.41
1:C:251:ASN:N	1:C:251:ASN:ND2	2.62	0.41
1:E:195:TYR:O	1:E:213:GLY:HA3	2.20	0.41
1:C:16:ASN:OD1	1:C:16:ASN:C	2.63	0.41
1:D:8:LEU:HD23	1:D:33:PRO:CB	2.51	0.41
1:E:135:VAL:HG11	1:E:142:ALA:HB1	2.02	0.41
1:B:64:LEU:HB3	1:B:79:LEU:HD13	2.03	0.41
1:B:128:ILE:HG23	1:B:129:PHE:HD1	1.85	0.41
1:C:270:ILE:HD13	1:C:305:ALA:HB1	2.03	0.41
1:D:168:ASP:OD1	1:F:183:ARG:HD2	2.21	0.41
1:E:268:ILE:HD12	1:E:272:LEU:HG	2.03	0.41
1:F:129:PHE:O	1:F:169:LYS:NZ	2.52	0.41
1:E:268:ILE:HG21	1:E:272:LEU:HD11	2.03	0.40
2:E:345:GOL:H12	1:F:139:ASN:CB	2.51	0.40
1:D:204:HIS:CD2	1:D:204:HIS:H	2.40	0.40
1:A:15:GLN:HE21	1:A:88:PRO:HG3	1.86	0.40
1:D:141:GLY:HA2	3:D:664:HOH:O	2.20	0.40
1:E:174:THR:CG2	1:E:178:VAL:HG22	2.42	0.40
1:E:252:ILE:HD12	1:E:252:ILE:O	2.22	0.40
1:A:5:LEU:HD12	1:A:38:VAL:HG22	2.03	0.40
1:B:270:ILE:HD13	1:B:305:ALA:HB1	2.03	0.40
1:E:182:VAL:HG11	1:E:196:ILE:CG2	2.51	0.40
1:F:15:GLN:HB3	1:F:19:GLU:HA	2.02	0.40
1:A:182:VAL:CG2	1:A:196:ILE:HG22	2.52	0.40
1:B:220:ILE:HD13	1:B:236:LEU:HD13	2.04	0.40
1:E:136:ALA:HB2	1:E:145:LEU:CD2	2.49	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	316/347 (91%)	309 (98%)	7 (2%)	0	100	100
1	B	316/347 (91%)	312 (99%)	4 (1%)	0	100	100
1	C	314/347 (90%)	307 (98%)	7 (2%)	0	100	100
1	D	316/347 (91%)	310 (98%)	6 (2%)	0	100	100
1	E	316/347 (91%)	309 (98%)	7 (2%)	0	100	100
1	F	315/347 (91%)	309 (98%)	6 (2%)	0	100	100
All	All	1893/2082 (91%)	1856 (98%)	37 (2%)	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	245/263 (93%)	235 (96%)	10 (4%)	27	15
1	B	245/263 (93%)	238 (97%)	7 (3%)	37	25
1	C	244/263 (93%)	230 (94%)	14 (6%)	18	8
1	D	245/263 (93%)	238 (97%)	7 (3%)	37	25
1	E	245/263 (93%)	233 (95%)	12 (5%)	22	10
1	F	244/263 (93%)	232 (95%)	12 (5%)	22	10
All	All	1468/1578 (93%)	1406 (96%)	62 (4%)	26	14

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	59	GLN
1	A	69	LYS
1	A	93	LEU
1	A	135	VAL
1	A	182	VAL
1	A	252	ILE
1	A	261	LEU
1	A	297	ASN
1	A	319	ASN
1	B	8	LEU
1	B	69	LYS
1	B	93	LEU
1	B	135	VAL
1	B	182	VAL
1	B	261	LEU
1	B	297	ASN
1	C	8	LEU
1	C	66	ASP
1	C	69	LYS
1	C	90	VAL
1	C	93	LEU
1	C	135	VAL
1	C	138	THR
1	C	182	VAL
1	C	251	ASN
1	C	252	ILE
1	C	261	LEU
1	C	284	ILE
1	C	297	ASN
1	C	317	ARG
1	D	8	LEU
1	D	14	THR
1	D	69	LYS
1	D	82	LEU
1	D	252	ILE
1	D	268	ILE
1	D	282	LEU
1	E	8	LEU
1	E	14	THR
1	E	57[A]	THR
1	E	57[B]	THR

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Mol	Chain	Res	Type
1	E	66	ASP
1	E	69	LYS
1	E	93	LEU
1	E	96	GLU
1	E	123	VAL
1	E	252	ILE
1	E	284	ILE
1	E	297	ASN
1	F	8	LEU
1	F	14	THR
1	F	69	LYS
1	F	123	VAL
1	F	177	VAL
1	F	251	ASN
1	F	252	ILE
1	F	268	ILE
1	F	284	ILE
1	F	297	ASN
1	F	317	ARG
1	F	319	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	18	GLN
1	A	52	GLN
1	A	60	GLN
1	A	63	GLN
1	A	86	GLN
1	A	115	HIS
1	A	134	ASN
1	A	204	HIS
1	A	251	ASN
1	A	276	ASN
1	A	319	ASN
1	B	3	GLN
1	B	15	GLN
1	B	18	GLN
1	B	52	GLN
1	B	60	GLN
1	B	121	HIS

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Mol	Chain	Res	Type
1	B	204	HIS
1	B	251	ASN
1	B	265	ASN
1	B	276	ASN
1	B	319	ASN
1	B	321	GLN
1	C	15	GLN
1	C	52	GLN
1	C	86	GLN
1	C	115	HIS
1	C	204	HIS
1	C	276	ASN
1	C	297	ASN
1	C	319	ASN
1	C	321	GLN
1	D	52	GLN
1	D	60	GLN
1	D	115	HIS
1	D	134	ASN
1	D	204	HIS
1	D	251	ASN
1	D	319	ASN
1	D	322	ASN
1	E	15	GLN
1	E	18	GLN
1	E	52	GLN
1	E	60	GLN
1	E	115	HIS
1	E	121	HIS
1	E	134	ASN
1	E	251	ASN
1	E	265	ASN
1	E	276	ASN
1	E	297	ASN
1	E	319	ASN
1	F	15	GLN
1	F	52	GLN
1	F	59	GLN
1	F	60	GLN
1	F	115	HIS
1	F	121	HIS
1	F	134	ASN

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Mol	Chain	Res	Type
1	F	204	HIS
1	F	297	ASN
1	F	319	ASN

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 ⓘ

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	GOL	A	345	-	5,5,5	0.52	0	5,5,5	1.43	1 (20%)
2	GOL	E	345	-	5,5,5	0.39	0	5,5,5	0.92	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	GOL	A	345	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	345	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	345	GOL	O2-C2-C1	2.51	119.59	109.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	345	GOL	O2-C2-C3-O3
2	E	345	GOL	C1-C2-C3-O3
2	A	345	GOL	C1-C2-C3-O3
2	E	345	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	345	GOL	2	0
2	E	345	GOL	4	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	320/347 (92%)	0.59	36 (11%) 10 8	9, 23, 49, 51	2 (0%)
1	B	320/347 (92%)	0.63	45 (14%) 6 5	9, 23, 49, 51	2 (0%)
1	C	319/347 (91%)	0.63	38 (11%) 9 7	9, 24, 48, 51	1 (0%)
1	D	320/347 (92%)	0.58	35 (10%) 10 9	11, 22, 49, 52	2 (0%)
1	E	320/347 (92%)	0.55	34 (10%) 11 9	10, 22, 48, 52	2 (0%)
1	F	320/347 (92%)	0.62	38 (11%) 9 7	12, 23, 48, 51	1 (0%)
All	All	1919/2082 (92%)	0.60	226 (11%) 9 7	9, 23, 48, 52	10 (0%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	GLY	6.3
1	E	324	ALA	5.9
1	E	323	GLY	5.9
1	B	324	ALA	5.9
1	D	298	ALA	5.9
1	D	321	GLN	5.8
1	D	283	TYR	5.7
1	E	294	ASP	5.7
1	A	299	LEU	5.6
1	D	299	LEU	5.6
1	E	283	TYR	5.4
1	B	294	ASP	5.1
1	A	300	VAL	5.0
1	B	302	VAL	5.0
1	E	302	VAL	4.9
1	D	302	VAL	4.8
1	D	291	ALA	4.8
1	D	323	GLY	4.8
1	D	290	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	298	ALA	4.6
1	E	3	GLN	4.3
1	B	283	TYR	4.3
1	C	329	THR	4.3
1	C	61	ALA	4.3
1	C	251	ASN	4.3
1	E	252	ILE	4.3
1	A	283	TYR	4.3
1	B	3	GLN	4.2
1	C	86	GLN	4.2
1	A	302	VAL	4.2
1	B	298	ALA	4.2
1	F	315	LEU	4.2
1	D	319	ASN	4.1
1	E	329	THR	4.1
1	B	320	SER	4.1
1	D	320	SER	4.1
1	F	320	SER	4.1
1	E	300	VAL	4.0
1	B	299	LEU	4.0
1	A	298	ALA	4.0
1	D	300	VAL	4.0
1	E	303	VAL	4.0
1	F	252	ILE	3.9
1	A	323	GLY	3.9
1	A	290	VAL	3.8
1	A	320	SER	3.8
1	C	253	VAL	3.8
1	D	303	VAL	3.7
1	E	280	ALA	3.7
1	E	320	SER	3.6
1	C	324	ALA	3.5
1	B	252	ILE	3.5
1	D	293	LEU	3.5
1	B	303	VAL	3.5
1	B	308	LEU	3.5
1	A	321	GLN	3.5
1	D	252	ILE	3.4
1	C	66	ASP	3.4
1	A	293	LEU	3.4
1	A	329	THR	3.4
1	B	287	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	319	ASN	3.4
1	F	300	VAL	3.3
1	F	324	ALA	3.3
1	B	315	LEU	3.3
1	A	291	ALA	3.3
1	C	300	VAL	3.3
1	F	329	THR	3.2
1	C	322	ASN	3.2
1	F	243	MET	3.2
1	F	294	ASP	3.2
1	B	325	VAL	3.2
1	D	243	MET	3.2
1	C	321	GLN	3.2
1	C	293	LEU	3.2
1	E	309	ALA	3.1
1	F	283	TYR	3.1
1	E	244	GLY	3.1
1	F	292	LEU	3.1
1	A	322	ASN	3.1
1	A	252	ILE	3.1
1	A	325	VAL	3.1
1	D	294	ASP	3.1
1	D	297	ASN	3.1
1	C	320	SER	3.1
1	C	315	LEU	3.0
1	A	4	SER	3.0
1	C	18	GLN	3.0
1	A	324	ALA	3.0
1	B	280	ALA	3.0
1	E	299	LEU	3.0
1	A	297	ASN	3.0
1	B	319	ASN	3.0
1	F	314	LEU	2.9
1	F	268	ILE	2.9
1	B	291	ALA	2.9
1	C	252	ILE	2.9
1	D	35	SER	2.9
1	E	308	LEU	2.9
1	B	244	GLY	2.9
1	F	297	ASN	2.9
1	B	321	GLN	2.9
1	B	243	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	293	LEU	2.9
1	F	293	LEU	2.9
1	F	299	LEU	2.9
1	D	325	VAL	2.8
1	A	3	GLN	2.8
1	E	293	LEU	2.8
1	E	281	GLY	2.8
1	F	18	GLN	2.8
1	D	307	ASP	2.8
1	A	314	LEU	2.8
1	F	321	GLN	2.8
1	C	297	ASN	2.8
1	E	322	ASN	2.8
1	E	287	GLY	2.8
1	B	305	ALA	2.7
1	D	266	ALA	2.7
1	E	327	CYS	2.7
1	C	282	LEU	2.7
1	E	315	LEU	2.7
1	C	323	GLY	2.7
1	A	294	ASP	2.7
1	E	292	LEU	2.7
1	B	297	ASN	2.7
1	F	253	VAL	2.7
1	F	302	VAL	2.7
1	E	317	ARG	2.7
1	A	303	VAL	2.7
1	F	61	ALA	2.6
1	E	325	VAL	2.6
1	D	328	LYS	2.6
1	C	243	MET	2.6
1	A	281	GLY	2.6
1	E	305	ALA	2.6
1	A	292	LEU	2.6
1	B	269	GLY	2.6
1	E	290	VAL	2.6
1	F	298	ALA	2.6
1	D	315	LEU	2.5
1	A	268	ILE	2.5
1	E	70	GLY	2.5
1	A	318	ARG	2.5
1	C	283	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	251	ASN	2.5
1	C	310	GLY	2.5
1	D	322	ASN	2.5
1	B	300	VAL	2.5
1	F	312	PRO	2.5
1	B	327	CYS	2.4
1	D	314	LEU	2.4
1	B	268	ILE	2.4
1	B	304	LYS	2.4
1	D	324	ALA	2.4
1	F	103	THR	2.4
1	E	295	GLU	2.4
1	D	305	ALA	2.4
1	D	3	GLN	2.4
1	F	323	GLY	2.4
1	C	299	LEU	2.4
1	C	294	ASP	2.4
1	B	306	ARG	2.4
1	E	306	ARG	2.4
1	F	305	ALA	2.4
1	B	290	VAL	2.4
1	C	302	VAL	2.4
1	B	301	LYS	2.4
1	F	327	CYS	2.4
1	B	317	ARG	2.3
1	B	309	ALA	2.3
1	B	281	GLY	2.3
1	F	295	GLU	2.3
1	B	314	LEU	2.3
1	F	282	LEU	2.3
1	B	318	ARG	2.3
1	F	290	VAL	2.3
1	B	329	THR	2.3
1	A	266	ALA	2.3
1	F	49	ALA	2.3
1	F	309	ALA	2.3
1	C	254	ILE	2.3
1	A	35	SER	2.3
1	A	41	VAL	2.3
1	C	292	LEU	2.3
1	A	287	GLY	2.2
1	B	70	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	251	ASN	2.2
1	E	243	MET	2.2
1	A	74	ALA	2.2
1	C	39	ALA	2.2
1	C	262	ILE	2.2
1	B	322	ASN	2.2
1	F	319	ASN	2.2
1	A	69	LYS	2.2
1	D	69	LYS	2.2
1	C	65	ALA	2.2
1	E	321	GLN	2.1
1	B	278	VAL	2.1
1	C	317	ARG	2.1
1	C	298	ALA	2.1
1	C	268	ILE	2.1
1	B	326	GLU	2.1
1	D	309	ALA	2.1
1	B	238	GLY	2.1
1	E	319	ASN	2.1
1	C	3	GLN	2.1
1	F	3	GLN	2.1
1	B	292	LEU	2.1
1	F	291	ALA	2.1
1	D	66	ASP	2.1
1	D	306	ARG	2.1
1	F	69	LYS	2.0
1	C	57	THR	2.0
1	C	290	VAL	2.0
1	D	41	VAL	2.0
1	C	305	ALA	2.0
1	D	286	ALA	2.0
1	C	295	GLU	2.0
1	A	328	LYS	2.0
1	A	71	ILE	2.0
1	D	44	ILE	2.0
1	C	59	GLN	2.0
1	F	59	GLN	2.0
1	F	310	GLY	2.0
1	A	253	VAL	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	GOL	A	345	6/6	0.70	0.20	19,20,23,23	0
2	GOL	E	345	6/6	0.70	0.17	25,27,27,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.