



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:08 pm GMT

PDB ID : 3PB2
Title : Characterisation of the first monomeric dihydrodipicolinate synthase variant reveals evolutionary insights
Authors : Pearce, F.G.; Dobson, R.C.J.; Jameson, G.B.
Deposited on : 2010-10-20
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

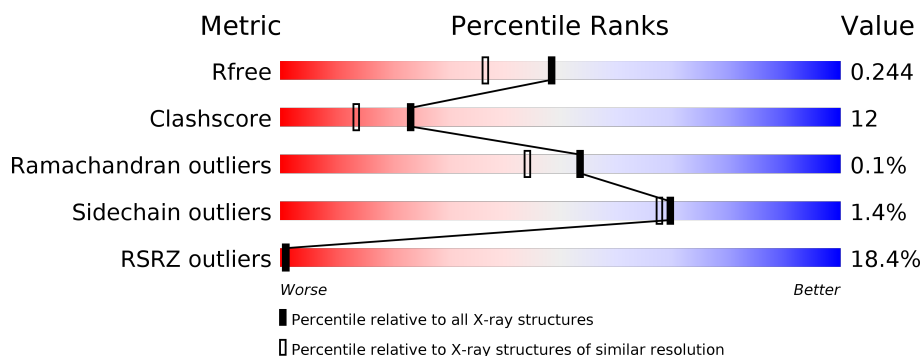
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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. 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	300	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 90%, yellow 90%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 90% 9% </div> </div>
1	B	300	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 85%, yellow 85%, yellow 14%, grey 14%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 95%; margin: 0 auto;"> 85% 14% </div> </div>
1	C	300	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 83%, yellow 83%, yellow 16%, grey 16%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 95%; margin: 0 auto;"> 83% 16% </div> </div>
1	D	300	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 20%, green 20%, green 78%, yellow 78%, yellow 20%, grey 20%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 95%; margin: 0 auto;"> 20% 78% 20% </div> </div>
1	E	300	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 11%, green 11%, green 75%, yellow 75%, yellow 23%, grey 23%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 95%; margin: 0 auto;"> 75% 23% </div> </div>
1	F	300	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 52%, green 52%, green 45%, yellow 45%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 95%; margin: 0 auto;"> 52% 45% </div> </div>

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	A	296	-	-	X	-
2	GOL	B	298	-	-	X	-
2	GOL	C	296	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14945 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 Dihydropicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	2	0
			2321	1475	391	448	7			
1	B	298	Total	C	N	O	S	0	2	0
			2306	1467	392	440	7			
1	C	297	Total	C	N	O	S	0	3	0
			2296	1461	388	440	7			
1	D	298	Total	C	N	O	S	0	0	0
			2295	1457	389	442	7			
1	E	296	Total	C	N	O	S	0	4	0
			2299	1460	390	442	7			
1	F	295	Total	C	N	O	S	0	2	0
			2265	1437	382	438	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q9X1K9
A	-4	ILE	-	EXPRESSION TAG	UNP Q9X1K9
A	-3	ASP	-	EXPRESSION TAG	UNP Q9X1K9
A	-2	PRO	-	EXPRESSION TAG	UNP Q9X1K9
A	-1	PHE	-	EXPRESSION TAG	UNP Q9X1K9
A	0	THR	-	EXPRESSION TAG	UNP Q9X1K9
A	233	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
A	237	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
B	-5	GLY	-	EXPRESSION TAG	UNP Q9X1K9
B	-4	ILE	-	EXPRESSION TAG	UNP Q9X1K9
B	-3	ASP	-	EXPRESSION TAG	UNP Q9X1K9
B	-2	PRO	-	EXPRESSION TAG	UNP Q9X1K9
B	-1	PHE	-	EXPRESSION TAG	UNP Q9X1K9
B	0	THR	-	EXPRESSION TAG	UNP Q9X1K9
B	233	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
B	237	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
C	-5	GLY	-	EXPRESSION TAG	UNP Q9X1K9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ILE	-	EXPRESSION TAG	UNP Q9X1K9
C	-3	ASP	-	EXPRESSION TAG	UNP Q9X1K9
C	-2	PRO	-	EXPRESSION TAG	UNP Q9X1K9
C	-1	PHE	-	EXPRESSION TAG	UNP Q9X1K9
C	0	THR	-	EXPRESSION TAG	UNP Q9X1K9
C	233	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
C	237	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
D	-5	GLY	-	EXPRESSION TAG	UNP Q9X1K9
D	-4	ILE	-	EXPRESSION TAG	UNP Q9X1K9
D	-3	ASP	-	EXPRESSION TAG	UNP Q9X1K9
D	-2	PRO	-	EXPRESSION TAG	UNP Q9X1K9
D	-1	PHE	-	EXPRESSION TAG	UNP Q9X1K9
D	0	THR	-	EXPRESSION TAG	UNP Q9X1K9
D	233	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
D	237	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
E	-5	GLY	-	EXPRESSION TAG	UNP Q9X1K9
E	-4	ILE	-	EXPRESSION TAG	UNP Q9X1K9
E	-3	ASP	-	EXPRESSION TAG	UNP Q9X1K9
E	-2	PRO	-	EXPRESSION TAG	UNP Q9X1K9
E	-1	PHE	-	EXPRESSION TAG	UNP Q9X1K9
E	0	THR	-	EXPRESSION TAG	UNP Q9X1K9
E	233	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
E	237	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
F	-5	GLY	-	EXPRESSION TAG	UNP Q9X1K9
F	-4	ILE	-	EXPRESSION TAG	UNP Q9X1K9
F	-3	ASP	-	EXPRESSION TAG	UNP Q9X1K9
F	-2	PRO	-	EXPRESSION TAG	UNP Q9X1K9
F	-1	PHE	-	EXPRESSION TAG	UNP Q9X1K9
F	0	THR	-	EXPRESSION TAG	UNP Q9X1K9
F	233	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9
F	237	ALA	ARG	ENGINEERED MUTATION	UNP Q9X1K9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

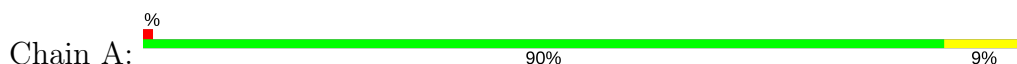
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	271	Total	O	0	0
			271	271		
3	B	285	Total	O	0	0
			285	285		
3	C	227	Total	O	0	0
			227	227		
3	D	137	Total	O	0	0
			137	137		
3	E	119	Total	O	0	0
			119	119		
3	F	34	Total	O	0	0
			34	34		

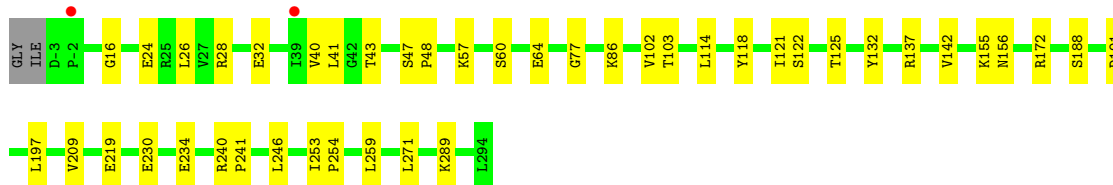
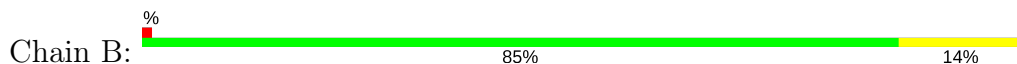
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

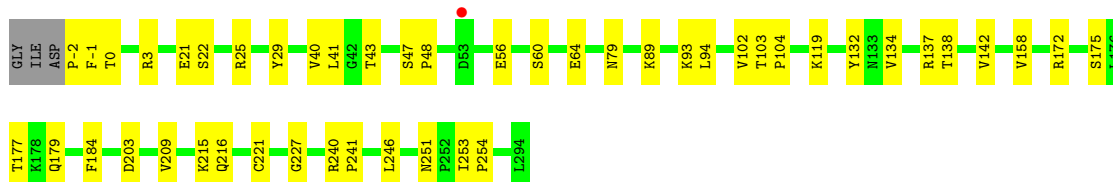
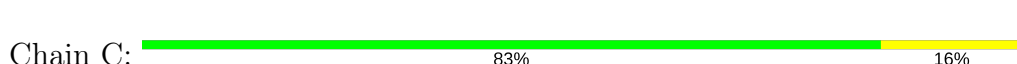
• Molecule 1: Dihydrodipicolinate synthase



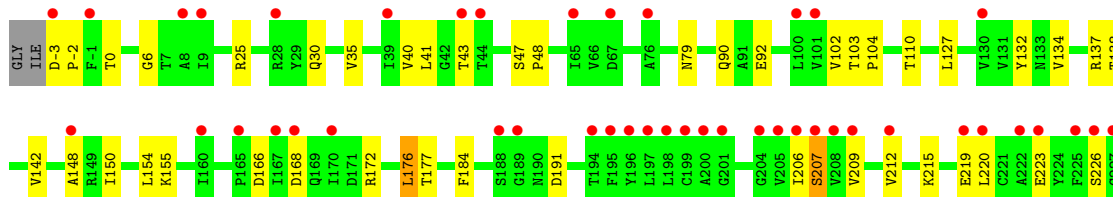
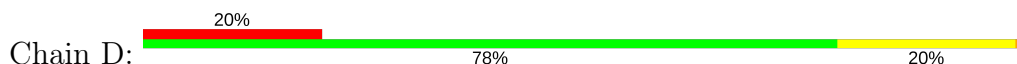
• Molecule 1: Dihydrodipicolinate synthase

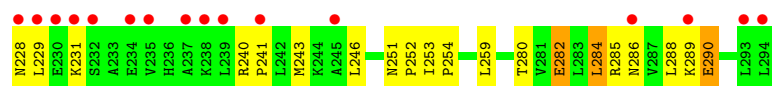


• Molecule 1: Dihydrodipicolinate synthase

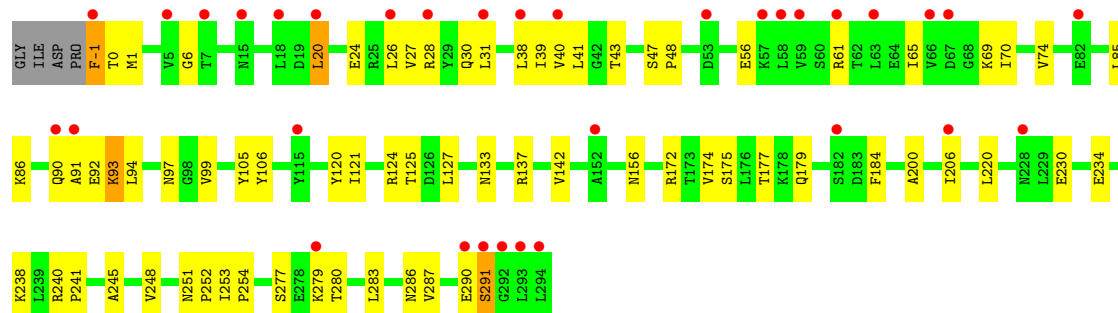
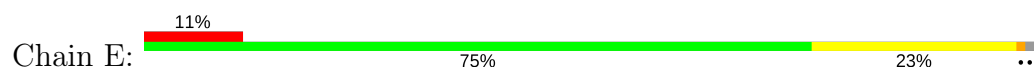


• Molecule 1: Dihydrodipicolinate synthase

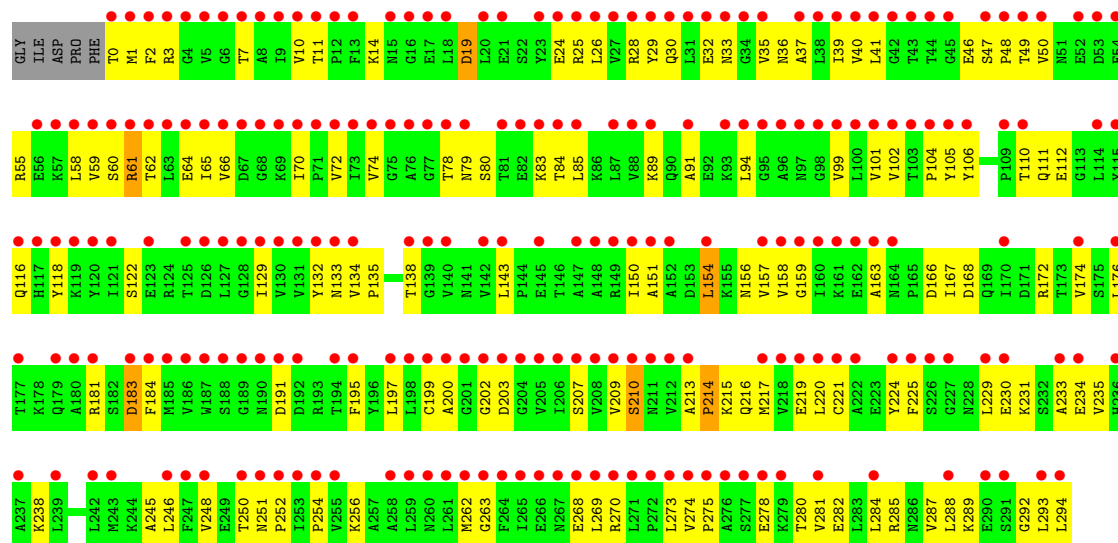
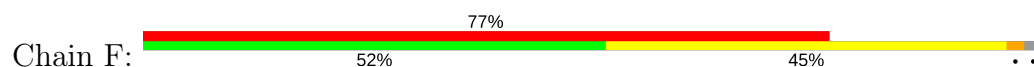




● Molecule 1: Dihydrodipicolinate synthase



● Molecule 1: Dihydrodipicolinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.20Å 125.34Å 78.43Å 90.00° 103.54° 90.00°	Depositor
Resolution (Å)	33.19 – 1.90 33.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.19-1.90) 100.0 (33.26-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.169 , 0.210 0.217 , 0.244	Depositor DCC
R_{free} test set	7115 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14945	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 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	0.43	0/2363	0.55	0/3207
1	B	0.44	0/2348	0.56	0/3186
1	C	0.38	0/2341	0.51	0/3177
1	D	0.31	0/2331	0.48	0/3164
1	E	0.31	0/2345	0.48	0/3182
1	F	0.25	0/2302	0.45	0/3126
All	All	0.36	0/14030	0.51	0/19042

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	2321	0	2385	22	0
1	B	2306	0	2376	29	0
1	C	2296	0	2364	35	0
1	D	2295	0	2352	51	0
1	E	2299	0	2364	61	0
1	F	2265	0	2311	144	0
2	A	36	0	48	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	32	8	0
2	C	24	0	32	8	0
2	D	6	0	8	1	0
3	A	271	0	0	5	0
3	B	285	0	0	6	1
3	C	227	0	0	5	0
3	D	137	0	0	4	0
3	E	119	0	0	0	0
3	F	34	0	0	6	0
All	All	14945	0	14272	342	1

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 12.

All (342) 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:E:20:LEU:CD1	1:E:61:ARG:HG2	1.78	1.11
1:E:20:LEU:HD11	1:E:61:ARG:CG	1.82	1.06
1:E:93:LYS:HE2	1:E:93:LYS:HA	1.34	1.02
3:A:368:HOH:O	2:B:297:GOL:H2	1.57	1.02
1:E:28:ARG:HG3	1:E:28:ARG:HH11	1.24	1.01
1:C:227:GLY:HA2	2:C:295:GOL:H11	1.42	1.00
1:F:213:ALA:HB1	1:F:216:GLN:CG	1.92	0.99
1:F:213:ALA:CB	1:F:216:GLN:HG3	1.91	0.99
1:F:101:VAL:CG1	1:F:129:ILE:HD11	1.93	0.97
1:F:213:ALA:HB1	1:F:216:GLN:HG3	0.97	0.95
1:F:102:VAL:HA	1:F:132:TYR:HB3	1.48	0.95
1:F:99:VAL:HG23	1:F:129:ILE:HG13	1.45	0.95
1:F:11:THR:HG23	1:F:58:LEU:HD21	1.50	0.93
1:D:-3:ASP:HB2	1:D:-2:PRO:HD3	1.52	0.92
1:E:20:LEU:HD11	1:E:61:ARG:HG2	0.91	0.91
1:D:-3:ASP:HB2	1:D:-2:PRO:CD	2.00	0.90
1:D:229:LEU:CD1	1:F:229:LEU:HD21	2.01	0.89
1:F:101:VAL:HG11	1:F:129:ILE:HD11	1.53	0.87
1:D:229:LEU:HD12	1:F:229:LEU:HD21	1.57	0.86
1:F:24:GLU:HG3	1:F:65:ILE:HD13	1.56	0.85
1:D:191:ASP:OD2	1:D:207:SER:HB2	1.77	0.84
1:F:234:GLU:O	1:F:238:LYS:HG2	1.78	0.83
1:F:274:VAL:HG12	1:F:275:PRO:HD2	1.63	0.81
1:F:59:VAL:HG11	1:F:94:LEU:HD13	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLU:HG3	1:E:65:ILE:HD13	1.63	0.81
1:F:101:VAL:HG13	1:F:118:TYR:HE1	1.45	0.80
2:A:298:GOL:H11	1:E:230:GLU:OE2	1.80	0.80
1:E:234:GLU:O	1:E:238:LYS:HD3	1.81	0.80
1:F:74:VAL:HG11	1:F:91:ALA:HB1	1.65	0.79
1:F:274:VAL:CG1	1:F:275:PRO:HD2	2.14	0.78
1:D:285:ARG:HG2	1:D:289:LYS:HE2	1.64	0.78
1:F:284:LEU:O	1:F:288:LEU:HD23	1.83	0.78
1:C:221:CYS:HB2	2:C:297:GOL:H32	1.66	0.77
1:D:286:ASN:O	1:D:290:GLU:HG2	1.84	0.77
1:E:124:ARG:HG3	1:E:124:ARG:HH11	1.48	0.77
1:E:28:ARG:NH1	1:E:28:ARG:HG3	1.98	0.77
1:F:207:SER:HB2	1:F:210:SER:HB2	1.67	0.77
1:F:129:ILE:CG2	1:F:157:VAL:HG12	2.14	0.76
1:F:24:GLU:HG3	1:F:65:ILE:CD1	2.15	0.75
2:B:295:GOL:H11	3:B:1063:HOH:O	1.86	0.74
1:C:89:LYS:O	1:C:93:LYS:HG2	1.89	0.73
1:E:27:VAL:O	1:E:31:LEU:HD13	1.89	0.73
1:D:284:LEU:O	1:D:288:LEU:HD13	1.88	0.73
1:F:151:ALA:O	1:F:181:ARG:HD3	1.89	0.73
1:F:250:THR:HG23	3:F:1015:HOH:O	1.90	0.71
1:F:122:SER:OG	1:F:156:ASN:HB2	1.91	0.71
1:F:1[B]:MET:CE	1:F:1[B]:MET:HA	2.19	0.71
1:F:215:LYS:O	1:F:219:GLU:HG2	1.89	0.71
1:F:28:ARG:O	1:F:32:GLU:HG3	1.89	0.71
1:F:49:THR:HG21	1:F:270:ARG:HB2	1.72	0.71
1:E:24:GLU:HG3	1:E:65:ILE:CD1	2.21	0.70
1:E:74:VAL:HG11	1:E:91:ALA:HB1	1.73	0.70
1:B:77:GLY:O	2:B:297:GOL:H11	1.91	0.70
1:F:251:ASN:OD1	1:F:252:PRO:HA	1.92	0.70
1:F:284:LEU:HA	1:F:287:VAL:HG12	1.75	0.69
1:F:40:VAL:HG12	1:F:41:LEU:HG	1.75	0.69
1:B:57:LYS:NZ	2:B:298:GOL:H12	2.08	0.69
1:F:199:CYS:HA	1:F:224:TYR:OH	1.93	0.69
1:A:124:ARG:NH2	2:A:296:GOL:O1	2.25	0.68
1:F:60:SER:O	1:F:64:GLU:HG3	1.94	0.68
1:D:215:LYS:O	1:D:219:GLU:HG3	1.94	0.67
1:F:101:VAL:HG11	1:F:129:ILE:CD1	2.25	0.67
1:F:101:VAL:HG12	1:F:129:ILE:HD11	1.74	0.67
1:F:256:LYS:HE2	1:F:268:GLU:O	1.94	0.67
1:F:47:SER:OG	1:F:48:PRO:HD3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ARG:HG3	1:E:124:ARG:NH1	2.08	0.66
1:F:231:LYS:O	1:F:235:VAL:HG23	1.94	0.66
1:C:251:ASN:HD22	2:C:296:GOL:H11	1.60	0.66
1:F:167:ILE:HG22	3:F:434:HOH:O	1.94	0.66
1:F:101:VAL:CG1	1:F:129:ILE:CD1	2.73	0.65
1:E:20:LEU:HD12	1:E:61:ARG:HE	1.61	0.64
1:D:-3:ASP:O	1:D:0:THR:HG22	1.97	0.64
1:D:110:THR:HA	2:D:295:GOL:H2	1.81	0.63
1:D:229:LEU:HD11	1:F:229:LEU:HD21	1.80	0.63
1:F:263:GLY:HA2	3:F:518:HOH:O	1.97	0.63
1:C:102:VAL:HA	1:C:132:TYR:HB3	1.81	0.63
1:F:10:VAL:HG12	1:F:11:THR:N	2.14	0.62
1:F:157:VAL:O	1:F:157:VAL:HG23	1.99	0.62
1:D:223:GLU:OE1	1:D:231:LYS:HD3	2.00	0.62
1:D:229:LEU:HD12	1:F:229:LEU:CD2	2.29	0.62
1:D:102:VAL:HA	1:D:132:TYR:HB3	1.80	0.62
1:F:11:THR:HG23	1:F:58:LEU:CD2	2.27	0.62
1:F:112:GLU:O	1:F:116:GLN:HG2	1.99	0.62
1:C:172:ARG:HD3	3:C:801:HOH:O	1.99	0.62
1:E:277:SER:OG	1:E:279:LYS:HG2	2.01	0.61
1:F:55:ARG:O	1:F:59:VAL:HG12	2.00	0.61
1:C:22:SER:HA	1:C:25:ARG:NH1	2.16	0.61
1:B:32:GLU:O	2:B:296:GOL:H31	2.00	0.61
1:F:174:VAL:HG11	1:F:200:ALA:O	2.01	0.61
1:A:102:VAL:HA	1:A:132:TYR:HB3	1.82	0.60
1:D:30:GLN:HB3	1:D:35:VAL:HG21	1.83	0.60
1:F:135:PRO:HD2	3:F:795:HOH:O	2.00	0.60
1:E:92:GLU:HG3	1:E:127:LEU:HD13	1.83	0.60
1:F:197:LEU:CD2	1:F:202:GLY:HA3	2.33	0.59
1:F:292:GLY:C	1:F:293:LEU:HD12	2.22	0.59
1:C:240:ARG:HB3	1:C:241:PRO:HD3	1.84	0.59
1:F:3:ARG:HD2	1:F:203:ASP:HB3	1.83	0.59
1:D:240:ARG:CZ	1:F:172:ARG:HD3	2.32	0.59
1:B:230:GLU:O	1:B:234:GLU:HG3	2.03	0.59
1:B:57:LYS:HZ2	2:B:298:GOL:H12	1.64	0.59
1:F:273:LEU:N	1:F:273:LEU:HD12	2.18	0.58
1:B:219:GLU:HG3	3:B:728:HOH:O	2.02	0.58
1:A:124:ARG:HH12	2:A:296:GOL:H32	1.69	0.58
1:C:40:VAL:HG12	1:C:41:LEU:HG	1.86	0.58
1:E:28:ARG:CG	1:E:28:ARG:HH11	2.06	0.58
1:F:59:VAL:CG1	1:F:94:LEU:HD13	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HB3	1:A:241:PRO:HD3	1.87	0.57
1:F:172:ARG:CZ	1:F:176:LEU:HD21	2.34	0.57
1:B:155:LYS:HD2	3:B:850:HOH:O	2.03	0.57
1:B:86:LYS:HD2	3:B:950:HOH:O	2.05	0.57
1:B:172:ARG:HD3	1:C:240:ARG:NE	2.20	0.57
1:F:101:VAL:CG1	1:F:118:TYR:HE1	2.17	0.57
1:F:197:LEU:HD23	1:F:202:GLY:HA3	1.84	0.57
1:F:287:VAL:HG13	1:F:288:LEU:HD22	1.87	0.57
1:E:125:THR:HG23	1:E:156:ASN:HD21	1.69	0.56
1:F:154:LEU:N	1:F:154:LEU:CD1	2.68	0.56
1:F:274:VAL:HG12	1:F:275:PRO:CD	2.34	0.56
1:E:0:THR:HG21	1:E:97:ASN:O	2.06	0.56
1:F:47:SER:N	1:F:48:PRO:CD	2.68	0.56
1:E:28:ARG:CG	1:E:28:ARG:NH1	2.67	0.56
1:F:278:GLU:O	1:F:282:GLU:HG2	2.05	0.56
1:D:-3:ASP:CB	1:D:-2:PRO:CD	2.79	0.55
1:E:43:THR:HG21	1:E:137:ARG:CZ	2.36	0.55
1:C:253:ILE:HB	1:C:254:PRO:HD3	1.89	0.55
1:F:289:LYS:HG2	1:F:294:LEU:OXT	2.06	0.55
1:C:21:GLU:CD	1:C:21:GLU:H	2.10	0.55
1:E:-1:PHE:HD2	1:E:-1:PHE:H3	1.52	0.55
1:F:129:ILE:HG22	1:F:157:VAL:HA	1.87	0.55
2:B:298:GOL:H12	3:B:604:HOH:O	2.06	0.55
1:C:56:GLU:HB2	3:C:458:HOH:O	2.06	0.55
1:D:229:LEU:HD23	1:D:229:LEU:C	2.28	0.55
1:D:229:LEU:O	1:D:229:LEU:HD23	2.06	0.54
1:F:74:VAL:HG11	1:F:91:ALA:CB	2.35	0.54
1:C:22:SER:HA	1:C:25:ARG:HH12	1.71	0.54
1:B:121:ILE:O	1:B:125:THR:HG22	2.07	0.54
1:E:287:VAL:O	1:E:291:SER:HB2	2.07	0.54
1:F:66:VAL:HG11	1:F:72:VAL:HG21	1.89	0.54
1:F:154:LEU:N	1:F:154:LEU:HD12	2.22	0.54
1:D:251:ASN:OD1	1:D:252:PRO:HA	2.08	0.54
1:F:191:ASP:CG	1:F:209:VAL:HG12	2.28	0.54
1:F:246:LEU:O	1:F:254:PRO:HG2	2.08	0.54
1:F:154:LEU:O	1:F:157:VAL:HG22	2.07	0.54
1:E:93:LYS:HA	1:E:93:LYS:CE	2.16	0.53
1:F:3:ARG:NH2	1:F:225:PHE:CD1	2.77	0.53
1:B:102:VAL:HA	1:B:132:TYR:HB3	1.90	0.53
1:F:287:VAL:HG13	1:F:288:LEU:N	2.23	0.53
1:E:74:VAL:HG13	1:E:99:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LEU:C	1:D:220:LEU:HD23	2.28	0.52
1:A:36:ASN:HB2	3:A:580:HOH:O	2.09	0.52
1:C:56:GLU:HG3	1:C:94:LEU:HD21	1.92	0.52
1:E:93:LYS:HE2	1:E:93:LYS:CA	2.24	0.52
1:F:14:LYS:CB	1:F:19:ASP:OD1	2.58	0.52
1:E:175:SER:O	1:E:179:GLN:HG3	2.10	0.52
1:F:37:ALA:HA	1:F:70:ILE:HD13	1.92	0.52
1:C:3:ARG:NH1	1:C:203:ASP:OD1	2.43	0.52
1:F:1[B]:MET:HA	1:F:1[B]:MET:HE2	1.93	0.51
1:A:228:ASN:ND2	1:A:231:LYS:HD2	2.26	0.51
1:C:47:SER:N	1:C:48:PRO:CD	2.73	0.51
1:D:148:ALA:HB2	1:D:176:LEU:HB3	1.91	0.51
1:A:240:ARG:NH2	1:E:172:ARG:HD3	2.25	0.51
1:F:0:THR:HG23	1:F:0:THR:O	2.11	0.51
1:A:151:ALA:O	1:A:181:ARG:HD3	2.11	0.51
1:D:150:ILE:HG23	1:D:154:LEU:HD12	1.90	0.51
1:D:212:VAL:HG12	1:D:259:LEU:HD23	1.93	0.51
1:F:10:VAL:CG1	1:F:11:THR:N	2.74	0.51
1:F:172:ARG:NH2	1:F:176:LEU:HD21	2.25	0.51
1:A:124:ARG:HH22	2:A:296:GOL:C1	2.24	0.51
1:C:251:ASN:HD22	2:C:296:GOL:C1	2.23	0.51
1:F:262:MET:CE	1:F:293:LEU:HD23	2.41	0.51
1:F:30:GLN:OE1	1:F:35:VAL:HG21	2.11	0.51
1:F:209:VAL:CG1	1:F:217:MET:SD	2.99	0.50
1:B:103:THR:HG21	1:B:142:VAL:HG23	1.92	0.50
1:F:78:THR:HG23	1:F:80:SER:O	2.11	0.50
1:B:114:LEU:HD13	1:B:142:VAL:HG22	1.94	0.50
1:F:150:ILE:HG22	1:F:157:VAL:HG21	1.93	0.50
1:E:125:THR:HG23	1:E:156:ASN:ND2	2.25	0.50
1:C:103:THR:HG21	1:C:142:VAL:HG23	1.93	0.50
1:F:133:ASN:O	1:F:163:ALA:HB3	2.11	0.50
1:F:284:LEU:HA	1:F:287:VAL:CG1	2.40	0.50
1:D:43:THR:HG21	1:D:137:ARG:CZ	2.41	0.49
1:E:61:ARG:O	1:E:65:ILE:HG13	2.12	0.49
1:F:101:VAL:HG12	1:F:129:ILE:CD1	2.40	0.49
1:F:166:ASP:OD2	1:F:168:ASP:HB3	2.12	0.49
1:F:0:THR:HB	1:F:183:ASP:OD1	2.11	0.49
1:E:251:ASN:OD1	1:E:252:PRO:HA	2.12	0.49
1:E:6:GLY:O	1:E:206:ILE:HA	2.12	0.49
1:E:86:LYS:O	1:E:90:GLN:HG3	2.12	0.49
1:F:278:GLU:HA	1:F:281:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:GLU:OE1	1:D:282:GLU:HA	2.12	0.49
1:E:220:LEU:C	1:E:220:LEU:HD23	2.32	0.49
1:E:279:LYS:HG3	1:E:280:THR:N	2.28	0.49
1:C:209:VAL:HG22	1:C:246:LEU:HD12	1.95	0.49
1:C:0:THR:HG21	1:C:158:VAL:HG11	1.95	0.48
1:C:134:VAL:HG13	1:C:138:THR:HG23	1.95	0.48
1:F:221:CYS:HB3	1:F:225:PHE:CZ	2.48	0.48
1:F:33:ASN:HB2	1:F:214:PRO:HB2	1.95	0.48
1:C:175:SER:O	1:C:179:GLN:HG3	2.13	0.48
1:D:285:ARG:O	1:D:289:LYS:HG3	2.13	0.48
1:F:62:THR:O	1:F:66:VAL:HG12	2.14	0.48
1:A:47:SER:N	1:A:48:PRO:CD	2.76	0.48
1:B:26[B]:LEU:HD11	1:B:259:LEU:HD13	1.96	0.48
1:E:-1:PHE:C	1:E:1:MET:H	2.16	0.48
1:F:274:VAL:CG1	1:F:275:PRO:CD	2.87	0.48
1:D:228:ASN:HB3	1:D:231:LYS:HB3	1.94	0.48
1:F:105:TYR:O	1:F:106:TYR:HB3	2.14	0.48
1:E:26:LEU:O	1:E:30:GLN:HG2	2.14	0.48
1:F:101:VAL:HG13	1:F:101:VAL:O	2.13	0.48
1:F:33:ASN:CB	1:F:214:PRO:HB2	2.44	0.48
1:C:-2:PRO:HD2	1:C:-1:PHE:H	1.78	0.47
1:E:133:ASN:OD1	1:E:142:VAL:HG23	2.14	0.47
1:F:292:GLY:O	1:F:293:LEU:HD12	2.15	0.47
1:D:280:THR:HG22	1:D:284:LEU:CD2	2.43	0.47
1:F:157:VAL:HG23	1:F:184:PHE:HE1	1.79	0.47
1:F:129:ILE:HG21	1:F:157:VAL:HG12	1.96	0.47
1:B:43:THR:HG21	1:B:137:ARG:CZ	2.45	0.47
1:E:121:ILE:O	1:E:125:THR:HG22	2.14	0.47
1:E:174:VAL:HG11	1:E:200:ALA:O	2.15	0.47
1:D:166:ASP:OD2	1:D:168:ASP:HB3	2.14	0.47
1:E:277:SER:OG	1:E:279:LYS:CG	2.62	0.47
1:F:110:THR:HG22	1:F:111:GLN:N	2.29	0.47
1:F:230:GLU:O	1:F:234:GLU:HB2	2.14	0.47
1:F:25:ARG:HH11	1:F:25:ARG:HB2	1.80	0.47
1:F:39:ILE:N	1:F:39:ILE:HD12	2.30	0.47
1:C:29:TYR:OH	2:C:298:GOL:H32	2.15	0.47
1:A:-5:GLY:O	1:A:156:ASN:OD1	2.34	0.47
1:E:248[A]:VAL:HG21	1:E:283:LEU:CD2	2.45	0.47
1:F:10:VAL:HG13	3:F:306:HOH:O	2.15	0.46
1:C:119:LYS:HE3	3:C:360:HOH:O	2.14	0.46
1:F:61:ARG:NH1	1:F:64:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:300:GOL:H32	3:A:461:HOH:O	2.14	0.46
1:C:134:VAL:HG13	1:C:134:VAL:O	2.15	0.46
1:D:253:ILE:HB	1:D:254:PRO:HD3	1.97	0.46
1:F:70:ILE:C	1:F:70:ILE:HD12	2.36	0.46
1:E:69:LYS:HD3	1:E:69:LYS:HA	1.76	0.46
1:D:79:ASN:HA	1:D:104:PRO:HB3	1.97	0.46
1:E:38:LEU:HG	1:E:70:ILE:HD11	1.97	0.46
1:E:99:VAL:HG13	1:E:127:LEU:HD23	1.96	0.46
1:F:284:LEU:CA	1:F:287:VAL:HG12	2.43	0.46
1:C:177:THR:HB	1:C:184:PHE:CD2	2.51	0.46
1:F:256:LYS:HD3	1:F:269:LEU:HG	1.97	0.46
1:D:240:ARG:HB3	1:D:241:PRO:HD3	1.97	0.45
1:B:47:SER:N	1:B:48:PRO:CD	2.79	0.45
1:C:251:ASN:ND2	2:C:296:GOL:H11	2.29	0.45
1:D:155:LYS:HG2	3:D:735:HOH:O	2.16	0.45
1:E:-1:PHE:C	1:E:1:MET:N	2.70	0.45
1:E:253:ILE:HB	1:E:254:PRO:HD3	1.97	0.45
1:D:134:VAL:HG13	1:D:138:THR:HG23	1.98	0.45
1:D:280:THR:O	1:D:284:LEU:HD22	2.17	0.45
1:D:47:SER:N	1:D:48:PRO:CD	2.80	0.45
1:E:47:SER:OG	1:E:48:PRO:HD3	2.17	0.45
1:A:43:THR:HG21	1:A:137:ARG:CZ	2.46	0.45
1:F:1[B]:MET:HB3	1:F:2:PHE:H	1.57	0.45
1:A:26:LEU:HA	1:A:26:LEU:HD12	1.85	0.45
1:D:220:LEU:O	1:D:220:LEU:HD23	2.17	0.45
1:E:286:ASN:O	1:E:290:GLU:HG3	2.17	0.45
1:F:209:VAL:HG13	1:F:217:MET:SD	2.56	0.45
1:A:200:ALA:O	2:A:300:GOL:H2	2.17	0.45
1:F:7:THR:HG23	1:F:210:SER:HB3	1.98	0.45
1:F:159:GLY:HA2	1:F:184:PHE:CZ	2.52	0.44
1:F:47:SER:N	1:F:48:PRO:HD2	2.32	0.44
1:B:16:GLY:HA2	3:B:501:HOH:O	2.17	0.44
1:A:38:LEU:HD12	1:A:38:LEU:HA	1.89	0.44
1:F:274:VAL:HG13	1:F:275:PRO:HD2	1.94	0.44
1:F:278:GLU:O	1:F:281:VAL:HG12	2.18	0.44
1:A:191:ASP:OD2	1:A:209:VAL:HG23	2.18	0.44
1:D:177:THR:HB	1:D:184:PHE:CD2	2.51	0.44
1:D:92:GLU:HA	1:D:127:LEU:HD11	2.00	0.44
1:E:245:ALA:O	1:E:248[A]:VAL:HG23	2.18	0.44
1:F:85:LEU:O	1:F:89:LYS:HG2	2.18	0.44
1:C:43:THR:HG21	1:C:137:ARG:CZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:LEU:C	1:F:220:LEU:HD23	2.38	0.44
1:F:207:SER:HB2	1:F:210:SER:CB	2.43	0.44
1:F:195:PHE:CZ	1:F:233:ALA:HB2	2.52	0.44
1:E:105:TYR:O	1:E:106:TYR:HB3	2.18	0.43
1:E:74:VAL:HG11	1:E:91:ALA:CB	2.45	0.43
1:F:111:GLN:HG3	1:F:143:LEU:HD22	1.99	0.43
1:B:209:VAL:HG22	1:B:246:LEU:HD12	1.99	0.43
1:E:24:GLU:OE1	1:E:61:ARG:NH2	2.51	0.43
1:F:50:VAL:O	1:F:50:VAL:HG23	2.19	0.43
1:D:209:VAL:HG21	1:D:243:MET:HG2	1.99	0.43
1:E:177:THR:HB	1:E:184:PHE:CD2	2.53	0.43
1:F:26:LEU:O	1:F:29:TYR:HB3	2.18	0.43
1:D:40:VAL:HG12	1:D:41:LEU:HG	2.00	0.43
1:F:0:THR:N	1:F:158:VAL:HG23	2.34	0.43
1:F:78:THR:HG22	1:F:84:THR:OG1	2.18	0.43
1:D:176:LEU:HG	3:D:875:HOH:O	2.17	0.43
1:F:102:VAL:CA	1:F:132:TYR:HB3	2.35	0.43
2:A:299:GOL:H2	3:A:485:HOH:O	2.17	0.43
1:E:47:SER:N	1:E:48:PRO:CD	2.82	0.43
1:D:6:GLY:O	1:D:206:ILE:HA	2.19	0.43
2:A:295:GOL:H11	1:B:271:LEU:HD12	2.01	0.43
1:D:103:THR:HG21	1:D:142:VAL:HG23	2.00	0.43
1:E:240:ARG:HB3	1:E:241:PRO:HD3	2.01	0.42
1:F:101:VAL:HA	3:F:411:HOH:O	2.19	0.42
1:F:79:ASN:HA	1:F:104:PRO:HB3	2.00	0.42
1:B:24:GLU:O	1:B:28:ARG:HG3	2.18	0.42
1:D:290:GLU:H	1:D:290:GLU:HG2	1.52	0.42
1:F:245:ALA:HA	1:F:248:VAL:HG13	2.00	0.42
1:C:215:LYS:HE2	1:C:216:GLN:HE22	1.83	0.42
1:C:21:GLU:N	1:C:21:GLU:CD	2.71	0.42
1:F:157:VAL:CG2	1:F:157:VAL:O	2.64	0.42
1:F:59:VAL:HG11	1:F:94:LEU:CD1	2.43	0.42
1:F:46:GLU:C	1:F:48:PRO:HD2	2.39	0.42
1:A:137:ARG:HH11	2:A:297:GOL:C1	2.32	0.42
1:A:56:GLU:HG3	1:A:94:LEU:HD21	2.01	0.42
1:B:188:SER:HA	1:B:197:LEU:HD13	1.99	0.42
1:B:40:VAL:HG12	1:B:41:LEU:HG	2.01	0.42
1:B:60:SER:O	1:B:64:GLU:HG3	2.19	0.42
2:C:296:GOL:C2	3:C:727:HOH:O	2.67	0.42
1:F:280:THR:O	1:F:284:LEU:HG	2.20	0.42
1:D:25:ARG:NH1	3:D:955:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:N	1:E:39:ILE:HD12	2.35	0.42
1:D:90:GLN:HG3	3:D:673:HOH:O	2.20	0.42
1:A:47:SER:OG	1:A:48:PRO:HD3	2.20	0.41
1:E:56:GLU:HG2	1:E:94:LEU:HD11	2.02	0.41
1:F:1[B]:MET:HA	1:F:1[B]:MET:HE3	1.99	0.41
1:F:262:MET:HE1	1:F:293:LEU:HD23	2.02	0.41
1:A:36:ASN:ND2	3:A:580:HOH:O	2.52	0.41
1:F:150:ILE:CG2	1:F:157:VAL:HG21	2.50	0.41
1:F:287:VAL:CG1	1:F:288:LEU:N	2.83	0.41
1:A:103:THR:HG21	1:A:142:VAL:HG23	2.03	0.41
1:B:118:TYR:O	1:B:122:SER:HB3	2.21	0.41
1:B:253:ILE:HB	1:B:254:PRO:HD3	2.03	0.41
1:B:57:LYS:HZ3	2:B:298:GOL:H12	1.84	0.41
1:B:240:ARG:N	1:B:241:PRO:CD	2.84	0.41
2:C:296:GOL:H2	3:C:727:HOH:O	2.19	0.41
1:E:85:LEU:HD22	1:E:120:TYR:CE2	2.55	0.41
1:C:103:THR:HG21	1:C:142:VAL:CG2	2.50	0.41
1:F:158:VAL:HG22	1:F:158:VAL:O	2.20	0.41
1:D:246:LEU:HA	1:D:246:LEU:HD23	1.89	0.41
1:F:101:VAL:HG13	1:F:118:TYR:CE1	2.37	0.41
1:F:78:THR:HG21	1:F:83:LYS:HB3	2.02	0.41
1:B:191:ASP:OD2	1:B:209:VAL:HG23	2.22	0.40
1:C:60:SER:O	1:C:64:GLU:HG3	2.20	0.40
1:C:79:ASN:HA	1:C:104:PRO:HB3	2.02	0.40
1:A:177:THR:HB	1:A:184:PHE:CD2	2.56	0.40
1:F:134:VAL:HG13	1:F:138:THR:HG23	2.04	0.40
1:D:30:GLN:O	1:D:35:VAL:HG22	2.21	0.40
1:E:40:VAL:HG12	1:E:41:LEU:HG	2.03	0.40
1:F:284:LEU:O	1:F:288:LEU:CD2	2.61	0.40
1:F:285:ARG:HG2	1:F:294:LEU:HD21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:296:GOL:O1	3:B:487:HOH:O[2_555]	2.09	0.11

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	300/300 (100%)	296 (99%)	4 (1%)	0	100	100
1	B	298/300 (99%)	295 (99%)	3 (1%)	0	100	100
1	C	298/300 (99%)	293 (98%)	5 (2%)	0	100	100
1	D	296/300 (99%)	293 (99%)	3 (1%)	0	100	100
1	E	298/300 (99%)	291 (98%)	7 (2%)	0	100	100
1	F	294/300 (98%)	282 (96%)	11 (4%)	1 (0%)	43	33
All	All	1784/1800 (99%)	1750 (98%)	33 (2%)	1 (0%)	53	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	214	PRO

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	258/256 (101%)	255 (99%)	3 (1%)	74	73
1	B	255/256 (100%)	254 (100%)	1 (0%)	92	92
1	C	255/256 (100%)	255 (100%)	0	100	100
1	D	254/256 (99%)	247 (97%)	7 (3%)	47	39
1	E	256/256 (100%)	252 (98%)	4 (2%)	65	62
1	F	249/256 (97%)	243 (98%)	6 (2%)	52	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1527/1536 (99%)	1506 (99%)	21 (1%)	69	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ARG
1	A	238	LYS
1	A	240	ARG
1	B	156	ASN
1	D	172	ARG
1	D	176	LEU
1	D	207	SER
1	D	226	SER
1	D	282	GLU
1	D	284	LEU
1	D	290	GLU
1	E	-1	PHE
1	E	20	LEU
1	E	93	LYS
1	E	291	SER
1	F	19	ASP
1	F	36	ASN
1	F	61	ARG
1	F	154	LEU
1	F	183	ASP
1	F	210	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	B	228	ASN
1	C	90	GLN
1	C	179	GLN
1	C	228	ASN
1	C	251	ASN
1	E	156	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	295	-	5,5,5	0.41	0	5,5,5	0.24	0
2	GOL	A	296	-	5,5,5	0.45	0	5,5,5	0.45	0
2	GOL	A	297	-	5,5,5	0.38	0	5,5,5	0.53	0
2	GOL	A	298	-	5,5,5	0.31	0	5,5,5	0.43	0
2	GOL	A	299	-	5,5,5	0.37	0	5,5,5	0.25	0
2	GOL	A	300	-	5,5,5	0.35	0	5,5,5	0.22	0
2	GOL	B	295	-	5,5,5	0.31	0	5,5,5	0.42	0
2	GOL	B	296	-	5,5,5	0.36	0	5,5,5	0.30	0
2	GOL	B	297	-	5,5,5	0.51	0	5,5,5	0.13	0
2	GOL	B	298	-	5,5,5	0.35	0	5,5,5	0.44	0
2	GOL	C	295	-	5,5,5	0.40	0	5,5,5	0.28	0
2	GOL	C	296	-	5,5,5	0.30	0	5,5,5	0.28	0
2	GOL	C	297	-	5,5,5	0.35	0	5,5,5	0.51	0
2	GOL	C	298	-	5,5,5	0.45	0	5,5,5	0.59	0
2	GOL	D	295	-	5,5,5	0.42	0	5,5,5	0.33	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	295	-	-	0/4/4/4	0/0/0/0
2	GOL	A	296	-	-	0/4/4/4	0/0/0/0
2	GOL	A	297	-	-	0/4/4/4	0/0/0/0
2	GOL	A	298	-	-	0/4/4/4	0/0/0/0
2	GOL	A	299	-	-	0/4/4/4	0/0/0/0
2	GOL	A	300	-	-	0/4/4/4	0/0/0/0
2	GOL	B	295	-	-	0/4/4/4	0/0/0/0
2	GOL	B	296	-	-	0/4/4/4	0/0/0/0
2	GOL	B	297	-	-	0/4/4/4	0/0/0/0
2	GOL	B	298	-	-	0/4/4/4	0/0/0/0
2	GOL	C	295	-	-	0/4/4/4	0/0/0/0
2	GOL	C	296	-	-	0/4/4/4	0/0/0/0
2	GOL	C	297	-	-	0/4/4/4	0/0/0/0
2	GOL	C	298	-	-	0/4/4/4	0/0/0/0
2	GOL	D	295	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	295	GOL	1	0
2	A	296	GOL	3	1
2	A	297	GOL	1	0
2	A	298	GOL	1	0
2	A	299	GOL	1	0
2	A	300	GOL	2	0
2	B	295	GOL	1	0
2	B	296	GOL	1	0
2	B	297	GOL	2	0
2	B	298	GOL	4	0
2	C	295	GOL	1	0
2	C	296	GOL	5	0
2	C	297	GOL	1	0
2	C	298	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	295	GOL	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	300/300 (100%)	-0.17	2 (0%) 87 89	12, 20, 39, 53	0
1	B	298/300 (99%)	-0.25	2 (0%) 87 89	11, 18, 35, 59	0
1	C	297/300 (99%)	0.04	1 (0%) 93 94	13, 27, 49, 63	0
1	D	298/300 (99%)	1.12	60 (20%) 1 1	21, 41, 77, 108	0
1	E	296/300 (98%)	0.83	33 (11%) 5 6	19, 42, 76, 91	0
1	F	295/300 (98%)	3.35	231 (78%) 0 0	62, 90, 119, 145	0
All	All	1784/1800 (99%)	0.81	329 (18%) 1 1	11, 33, 99, 145	0

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	VAL	10.4
1	F	206	ILE	10.3
1	F	100	LEU	9.3
1	F	132	TYR	8.4
1	F	39	ILE	8.2
1	F	189	GLY	7.7
1	F	205	VAL	7.6
1	F	294	LEU	7.5
1	F	8	ALA	7.3
1	F	160	ILE	7.2
1	F	10	VAL	7.2
1	F	161	LYS	7.1
1	F	5	VAL	7.1
1	F	102	VAL	6.6
1	F	246	LEU	6.4
1	F	207	SER	6.4
1	F	106	TYR	6.3
1	F	76	ALA	6.3
1	F	225	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
1	F	41	LEU	6.1
1	F	40	VAL	6.1
1	F	101	VAL	6.0
1	F	6	GLY	6.0
1	F	29	TYR	5.9
1	F	9	ILE	5.8
1	F	129	ILE	5.8
1	F	42	GLY	5.8
1	F	209	VAL	5.8
1	F	187	TRP	5.7
1	F	73	ILE	5.7
1	F	43	THR	5.7
1	F	0	THR	5.5
1	F	7	THR	5.5
1	F	188	SER	5.5
1	F	18	LEU	5.4
1	F	170	ILE	5.3
1	F	201	GLY	5.2
1	F	99	VAL	5.2
1	F	131	VAL	5.2
1	F	261	LEU	5.2
1	F	163	ALA	5.2
1	F	157	VAL	5.1
1	F	281	VAL	5.1
1	F	288	LEU	5.0
1	F	74	VAL	5.0
1	F	2	PHE	5.0
1	F	16	GLY	5.0
1	F	243	MET	5.0
1	F	127	LEU	5.0
1	F	224	TYR	4.9
1	D	226	SER	4.9
1	F	291	SER	4.8
1	D	196	TYR	4.8
1	F	13	PHE	4.8
1	F	130	VAL	4.8
1	F	78	THR	4.7
1	F	38	LEU	4.7
1	F	154	LEU	4.7
1	F	158	VAL	4.7
1	F	212	VAL	4.7
1	F	105	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	204	GLY	4.6
1	F	273	LEU	4.6
1	F	219	GLU	4.6
1	F	134	VAL	4.5
1	F	31	LEU	4.5
1	F	87	LEU	4.4
1	F	180	ALA	4.4
1	F	37	ALA	4.4
1	D	235	VAL	4.4
1	F	152	ALA	4.4
1	F	258	ALA	4.3
1	F	186	VAL	4.3
1	D	223	GLU	4.3
1	F	69	LYS	4.2
1	F	279	LYS	4.2
1	F	255	VAL	4.2
1	F	15	ASN	4.2
1	F	221	CYS	4.2
1	F	11	THR	4.2
1	F	77	GLY	4.2
1	F	4	GLY	4.1
1	E	206	ILE	4.1
1	F	194	THR	4.1
1	F	121	ILE	4.1
1	D	234	GLU	4.0
1	D	222	ALA	4.0
1	F	277	SER	4.0
1	F	98	GLY	4.0
1	D	208	VAL	4.0
1	F	250	THR	4.0
1	F	210	SER	4.0
1	F	284	LEU	4.0
1	D	245	ALA	4.0
1	D	206	ILE	3.9
1	F	82	GLU	3.9
1	F	150	ILE	3.9
1	F	20	LEU	3.9
1	F	259	LEU	3.9
1	F	3	ARG	3.9
1	F	1[A]	MET	3.8
1	F	28	ARG	3.8
1	F	84	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	103	THR	3.8
1	F	21	GLU	3.8
1	D	225	PHE	3.8
1	D	232	SER	3.8
1	D	197	LEU	3.8
1	F	174	VAL	3.8
1	F	26	LEU	3.7
1	F	66	VAL	3.7
1	F	128	GLY	3.7
1	F	96	ALA	3.7
1	F	265	ILE	3.7
1	F	197	LEU	3.7
1	F	88	VAL	3.7
1	F	260	ASN	3.7
1	D	167	ILE	3.7
1	F	120	TYR	3.6
1	F	85	LEU	3.6
1	F	211	ASN	3.6
1	F	35	VAL	3.6
1	F	264	PHE	3.6
1	F	227	GLY	3.6
1	F	267	ASN	3.5
1	F	164	ASN	3.5
1	D	199	CYS	3.5
1	F	148	ALA	3.5
1	F	251	ASN	3.5
1	D	195	PHE	3.5
1	D	168	ASP	3.5
1	F	237	ALA	3.4
1	F	290	GLU	3.4
1	F	190	ASN	3.4
1	D	294	LEU	3.4
1	F	272	PRO	3.4
1	F	247	PHE	3.4
1	D	228	ASN	3.4
1	D	229	LEU	3.4
1	F	233	ALA	3.4
1	F	44	THR	3.4
1	F	271	LEU	3.4
1	D	237	ALA	3.3
1	F	45	GLY	3.3
1	F	91	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	269	LEU	3.3
1	F	151	ALA	3.3
1	F	49	THR	3.3
1	F	184	PHE	3.3
1	F	133	ASN	3.3
1	F	159	GLY	3.3
1	F	23	TYR	3.3
1	F	53	ASP	3.3
1	F	95	GLY	3.3
1	D	201	GLY	3.2
1	F	195	PHE	3.2
1	D	8	ALA	3.2
1	F	126	ASP	3.2
1	F	70	ILE	3.2
1	F	242	LEU	3.2
1	F	118	TYR	3.2
1	F	64	GLU	3.2
1	F	27	VAL	3.2
1	D	39	ILE	3.2
1	F	32	GLU	3.2
1	E	20	LEU	3.1
1	E	67	ASP	3.1
1	F	191	ASP	3.1
1	F	200	ALA	3.1
1	F	220	LEU	3.1
1	F	252	PRO	3.1
1	F	59	VAL	3.1
1	F	276	ALA	3.1
1	F	213	ALA	3.1
1	F	12	PRO	3.1
1	F	72	VAL	3.1
1	F	248	VAL	3.1
1	F	198	LEU	3.1
1	F	50	VAL	3.0
1	F	270	ARG	3.0
1	F	239	LEU	3.0
1	F	177	THR	3.0
1	F	139	GLY	3.0
1	F	217	MET	3.0
1	F	275	PRO	3.0
1	F	93	LYS	3.0
1	D	209	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	239	LEU	3.0
1	D	293	LEU	2.9
1	E	28	ARG	2.9
1	F	229	LEU	2.9
1	F	56	GLU	2.9
1	E	63	LEU	2.9
1	F	75	GLY	2.9
1	F	179	GLN	2.9
1	D	205	VAL	2.9
1	E	59	VAL	2.9
1	F	234	GLU	2.8
1	F	140	VAL	2.8
1	F	114	LEU	2.8
1	F	143	LEU	2.8
1	D	65	ILE	2.8
1	F	149	ARG	2.8
1	F	203	ASP	2.8
1	F	199	CYS	2.8
1	E	-1	PHE	2.8
1	F	94	LEU	2.8
1	E	91	ALA	2.8
1	D	9	ILE	2.8
1	F	48	PRO	2.8
1	F	181	ARG	2.8
1	F	63	LEU	2.8
1	F	54	GLU	2.8
1	D	44	THR	2.7
1	F	71	PRO	2.7
1	F	293	LEU	2.7
1	D	-3	ASP	2.7
1	D	170	ILE	2.7
1	F	147	ALA	2.7
1	E	53	ASP	2.7
1	F	58	LEU	2.7
1	F	81	THR	2.7
1	D	212	VAL	2.7
1	D	238	LYS	2.7
1	F	263	GLY	2.7
1	F	230	GLU	2.6
1	F	109	PRO	2.6
1	F	47	SER	2.6
1	F	254	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	25	ARG	2.6
1	F	34	GLY	2.6
1	F	79	ASN	2.6
1	F	60	SER	2.6
1	D	230	GLU	2.6
1	F	110	THR	2.6
1	F	183	ASP	2.6
1	D	231	LYS	2.6
1	F	185	MET	2.6
1	F	30	GLN	2.6
1	F	104	PRO	2.5
1	D	130	VAL	2.5
1	D	198	LEU	2.5
1	E	26	LEU	2.5
1	E	294	LEU	2.5
1	D	189	GLY	2.5
1	E	61	ARG	2.5
1	E	57	LYS	2.5
1	F	262	MET	2.5
1	F	62	THR	2.5
1	E	182	SER	2.5
1	B	-2	PRO	2.5
1	F	236	HIS	2.5
1	D	227	GLY	2.4
1	A	39	ILE	2.4
1	F	65	ILE	2.4
1	D	200	ALA	2.4
1	A	206	ILE	2.4
1	F	24	GLU	2.4
1	D	219	GLU	2.4
1	F	222	ALA	2.4
1	D	204	GLY	2.4
1	F	202	GLY	2.4
1	F	119	LYS	2.4
1	D	165	PRO	2.4
1	B	39	ILE	2.4
1	D	160	ILE	2.4
1	F	253	ILE	2.4
1	D	207	SER	2.3
1	E	58	LEU	2.3
1	F	123	GLU	2.3
1	E	18	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	-1	PHE	2.3
1	F	115	TYR	2.3
1	E	31	LEU	2.3
1	D	101	VAL	2.3
1	E	66	VAL	2.3
1	F	17	GLU	2.3
1	F	274	VAL	2.3
1	D	188	SER	2.3
1	E	15	ASN	2.3
1	D	194	THR	2.3
1	E	152	ALA	2.3
1	E	228[A]	ASN	2.3
1	E	290	GLU	2.3
1	F	278	GLU	2.3
1	D	43	THR	2.2
1	E	40	VAL	2.2
1	F	33	ASN	2.2
1	F	89	LYS	2.2
1	E	292	GLY	2.2
1	F	268	GLU	2.2
1	D	286	ASN	2.2
1	F	218	VAL	2.2
1	F	226[A]	SER	2.2
1	E	90	GLN	2.2
1	E	279	LYS	2.2
1	F	68	GLY	2.2
1	D	241	PRO	2.2
1	E	82	GLU	2.2
1	F	83	LYS	2.2
1	D	220	LEU	2.2
1	E	7	THR	2.2
1	E	38	LEU	2.1
1	F	61	ARG	2.1
1	F	176	LEU	2.1
1	D	289	LYS	2.1
1	E	115	TYR	2.1
1	F	97	ASN	2.1
1	E	293	LEU	2.1
1	F	266	GLU	2.1
1	F	117	HIS	2.1
1	D	76	ALA	2.1
1	C	53	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	192	ASP	2.1
1	F	162	GLU	2.1
1	E	291	SER	2.1
1	D	67	ASP	2.1
1	F	67	ASP	2.1
1	F	125	THR	2.1
1	F	142	VAL	2.1
1	D	100	LEU	2.1
1	F	116	GLN	2.0
1	D	148	ALA	2.0
1	D	28	ARG	2.0
1	E	5	VAL	2.0
1	F	52	GLU	2.0
1	F	57	LYS	2.0
1	F	138	THR	2.0
1	F	145	GLU	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 carbohydrates 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(Å ²)	Q<0.9
2	GOL	A	299	6/6	0.61	0.31	61,64,64,67	0
2	GOL	A	295	6/6	0.69	0.29	65,69,76,77	0
2	GOL	B	297	6/6	0.75	0.27	57,60,62,63	0
2	GOL	A	298	6/6	0.76	0.24	63,64,65,66	0
2	GOL	D	295	6/6	0.76	0.27	50,57,60,61	0
2	GOL	C	296	6/6	0.78	0.35	35,52,59,61	0
2	GOL	B	298	6/6	0.79	0.23	67,69,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	300	6/6	0.85	0.21	53,59,61,63	0
2	GOL	B	296	6/6	0.85	0.15	53,61,64,70	0
2	GOL	A	297	6/6	0.85	0.22	33,39,47,52	0
2	GOL	C	295	6/6	0.87	0.18	62,67,68,72	0
2	GOL	A	296	6/6	0.89	0.20	21,34,46,54	0
2	GOL	B	295	6/6	0.90	0.22	33,46,53,61	0
2	GOL	C	297	6/6	0.90	0.20	11,35,44,45	6
2	GOL	C	298	6/6	0.91	0.20	20,39,47,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.