



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:05 PM UTC

PDB ID : 3PB2 / pdb_00003pb2
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 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

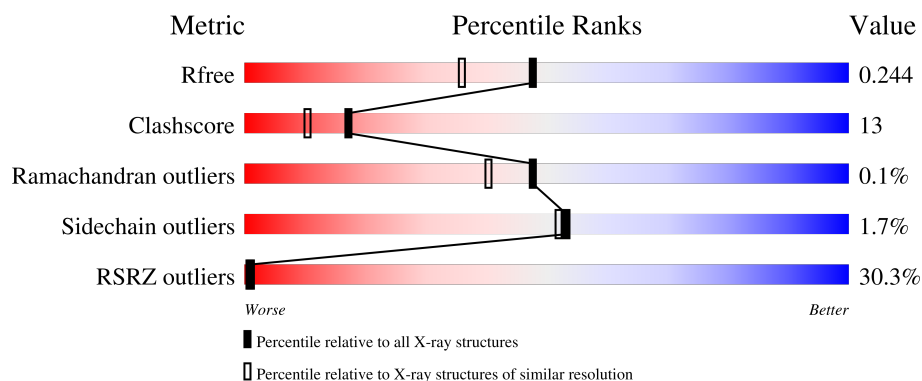
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	300	90% 10%
1	B	300	84% 15% .
1	C	300	2% 82% 17% .
1	D	300	42% 76% 22% ..
1	E	300	39% 74% 24% ..

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Mol	Chain	Length	Quality of chain
1	F	300	98% 50%45% . .

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

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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	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

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.

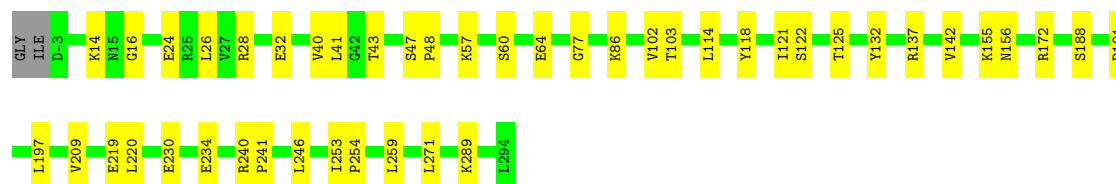
• Molecule 1: Dihydrodipicolinate synthase

Chain A: 



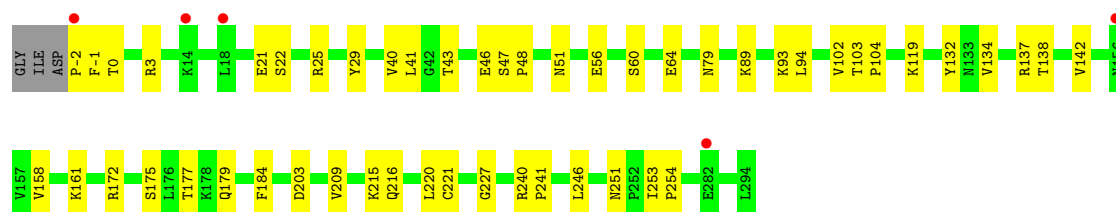
• Molecule 1: Dihydrodipicolinate synthase

Chain B: 



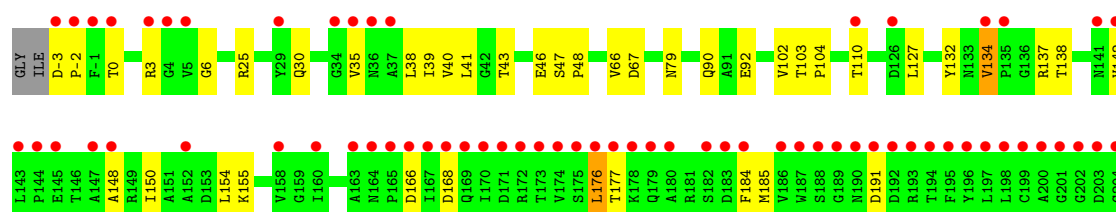
• Molecule 1: Dihydrodipicolinate synthase

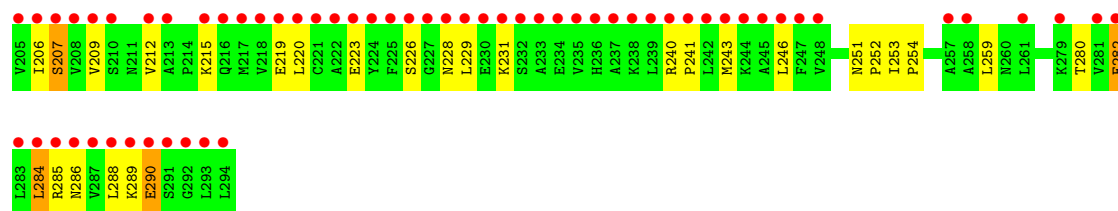
Chain C: 



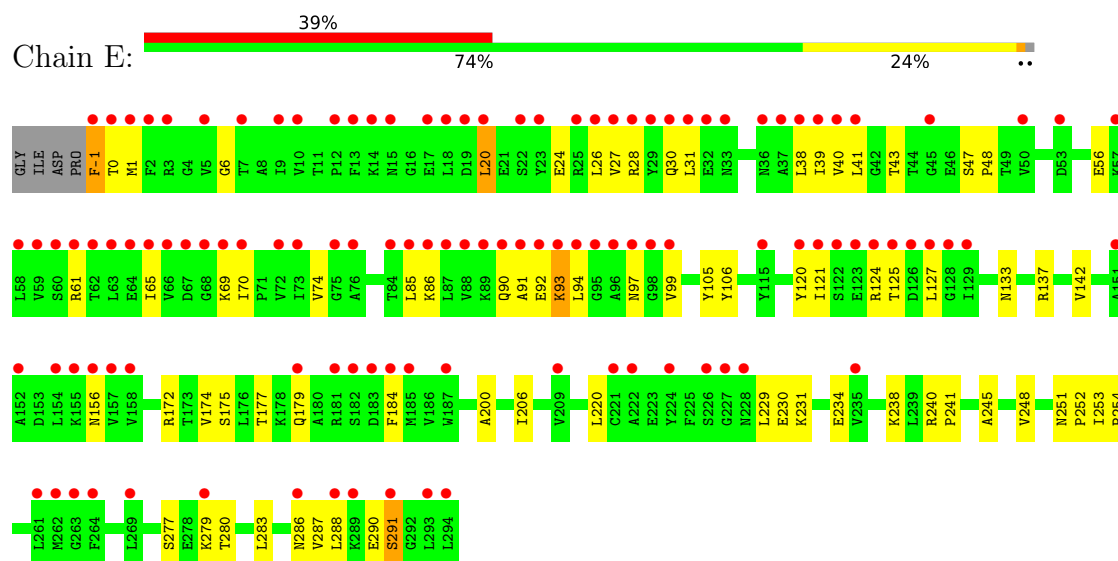
• Molecule 1: Dihydrodipicolinate synthase

Chain D: 

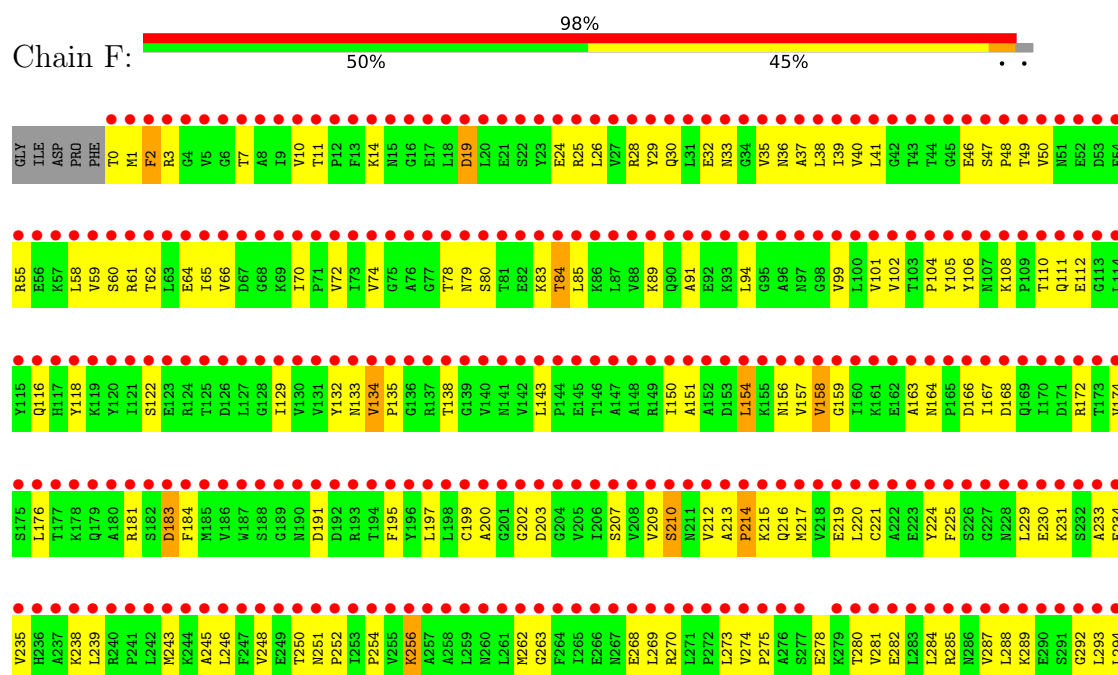




• Molecule 1: Dihydrodipicolinate synthase



• 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 33.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.19-1.90) 100.0 (33.19-1.90)	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)	0.37 , 57.8	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	0.55	0/2363	0.78	2/3207 (0.1%)
1	B	0.56	0/2348	0.77	0/3186
1	C	0.49	0/2341	0.74	0/3177
1	D	0.41	0/2331	0.75	2/3164 (0.1%)
1	E	0.41	0/2345	0.75	0/3182
1	F	0.34	0/2302	0.78	5/3126 (0.2%)
All	All	0.47	0/14030	0.76	9/19042 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	134	VAL	CA-C-N	6.30	126.50	119.32
1	D	134	VAL	C-N-CA	6.30	126.50	119.32
1	A	155	LYS	CA-C-N	6.12	129.09	120.28
1	A	155	LYS	C-N-CA	6.12	129.09	120.28
1	F	134	VAL	CA-C-N	5.77	125.24	119.24
1	F	134	VAL	C-N-CA	5.77	125.24	119.24
1	F	164	ASN	CA-C-N	5.61	125.71	119.87
1	F	164	ASN	C-N-CA	5.61	125.71	119.87
1	F	2	PHE	N-CA-C	5.33	117.60	110.35

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	31	0
1	C	2296	0	2364	39	0
1	D	2295	0	2352	57	0
1	E	2299	0	2364	61	0
1	F	2265	0	2311	145	0
2	A	36	0	48	9	1
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	7	1
3	C	227	0	0	6	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	355	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 13.

All (355) 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:HA	1:E:93:LYS:HE2	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:F:1[B]:MET:HA	1:F:1[B]:MET:HE2	1.40	1.00
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:99:VAL:HG23	1:F:129:ILE:HG13	1.45	0.95
1:F:102:VAL:HA	1:F:132:TYR:HB3	1.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:VAL:HG11	1:F:94:LEU:HD13	1.61	0.81
1:F:274:VAL:HG12	1:F:275:PRO:HD2	1.63	0.81
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:HG3	1:E:28:ARG:NH1	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:1[B]:MET:HA	1:F:1[B]:MET:CE	2.19	0.71
1:F:122:SER:OG	1:F:156:ASN:HB2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:292:GLY:C	1:F:293:LEU:HD12	2.22	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: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:F:157:VAL:HG23	1:F:157:VAL:O	1.99	0.61
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:C:21:GLU:CD	1:C:21:GLU:H	2.10	0.60
1:D:229:LEU:C	1:D:229:LEU:HD23	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:LEU:CD2	1:F:202:GLY:HA3	2.33	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:57:LYS:HZ2	2:B:298:GOL:H12	1.64	0.59
1:B:230:GLU:O	1:B:234:GLU:HG3	2.03	0.59
1:F:273:LEU:HD12	1:F:273:LEU:N	2.18	0.58
1:B:219:GLU:HG3	3:B:728:HOH:O	2.02	0.58
1:F:191:ASP:CG	1:F:209:VAL:HG12	2.28	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:HH11	1:E:28:ARG:CG	2.06	0.58
1:F:59:VAL:CG1	1:F:94:LEU:HD13	2.32	0.58
1:A:240:ARG:HB3	1:A:241:PRO:HD3	1.87	0.57
1:D:220:LEU:C	1:D:220:LEU:HD23	2.28	0.57
1:F:172:ARG:CZ	1:F:176:LEU:HD21	2.34	0.57
1:B:86:LYS:HD2	3:B:950:HOH:O	2.05	0.57
1:B:155:LYS:HD2	3:B:850:HOH:O	2.03	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:NH1	1:E:28:ARG:CG	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: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:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:VAL:HG11	1:F:72:VAL:HG21	1.89	0.54
1:E:-1:PHE:C	1:E:1:MET:H	2.16	0.54
1:E:220:LEU:C	1:E:220:LEU:HD23	2.32	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: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
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:A:228:ASN:ND2	1:A:231:LYS:HD2	2.26	0.51
1:A:240:ARG:NH2	1:E:172:ARG:HD3	2.25	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: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:70:ILE:HD12	1:F:70:ILE:C	2.36	0.51
1:F:30:GLN:OE1	1:F:35:VAL:HG21	2.11	0.51
1:F:262:MET:CE	1:F:293:LEU:HD23	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:0:THR:HB	1:F:183:ASP:OD1	2.11	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: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
1:D:282:GLU:HA	1:D:282:GLU:OE1	2.12	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:E:-1:PHE:C	1:E:1:MET:N	2.70	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:F:220:LEU:C	1:F:220:LEU:HD23	2.38	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:239:LEU:HB3	1:F:243:MET:HE3	1.95	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:33:ASN:CB	1:F:214:PRO:HB2	2.44	0.48
1:F:101:VAL:HG13	1:F:101:VAL:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLU:CD	1:C:21:GLU:N	2.71	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:25:ARG:HH11	1:F:25:ARG:HB2	1.80	0.47
1:F:39:ILE:HD12	1:F:39:ILE:N	2.30	0.47
1:F:46:GLU:C	1:F:48:PRO:HD2	2.39	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: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:D:3:ARG:HG2	1:D:185:MET:HE1	1.97	0.46
1:F:61:ARG:NH1	1:F:64:GLU:OE2	2.48	0.46
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:E:69:LYS:HA	1:E:69:LYS:HD3	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:253:ILE:HB	1:E:254:PRO:HD3	1.97	0.45
1:D:47:SER:N	1:D:48:PRO:CD	2.80	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: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:HD12	1:A:26:LEU:HA	1.85	0.45
1:D:220:LEU:HD23	1:D:220:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:THR:HG23	1:F:210:SER:HB3	1.98	0.45
1:C:220:LEU:HD23	1:C:220:LEU:C	2.42	0.44
1:F:47:SER:N	1:F:48:PRO:HD2	2.32	0.44
1:F:159:GLY:HA2	1:F:184:PHE:CZ	2.52	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:B:14:LYS:NZ	3:B:642:HOH:O	2.51	0.44
1:C:43:THR:HG21	1:C:137:ARG:CZ	2.47	0.44
1:D:38:LEU:C	1:D:39:ILE:HD12	2.43	0.44
1:F:195:PHE:CZ	1:F:233:ALA:HB2	2.52	0.44
1:F:207:SER:HB2	1:F:210:SER:CB	2.43	0.44
1:F:212:VAL:C	1:F:214:PRO:HD3	2.43	0.44
1:E:74:VAL:HG11	1:E:91:ALA:CB	2.45	0.43
1:E:105:TYR:O	1:E:106:TYR:HB3	2.18	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:79:ASN:HA	1:F:104:PRO:HB3	2.00	0.42
1:F:101:VAL:HA	3:F:411:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLU:O	1:B:28:ARG:HG3	2.18	0.42
1:D:290:GLU:HG2	1:D:290:GLU:H	1.52	0.42
1:F:245:ALA:HA	1:F:248:VAL:HG13	2.00	0.42
1:B:220:LEU:C	1:B:220:LEU:HD23	2.44	0.42
1:C:215:LYS:HE2	1:C:216:GLN:HE22	1.83	0.42
1:F:59:VAL:HG11	1:F:94:LEU:CD1	2.43	0.42
1:F:157:VAL:O	1:F:157:VAL:CG2	2.64	0.42
1:A:56:GLU:HG3	1:A:94:LEU:HD21	2.01	0.42
1:A:137:ARG:HH11	2:A:297:GOL:C1	2.32	0.42
1:B:40:VAL:HG12	1:B:41:LEU:HG	2.01	0.42
1:B:188:SER:HA	1:B:197:LEU:HD13	1.99	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
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: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:57:LYS:HZ3	2:B:298:GOL:H12	1.84	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: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:D:66:VAL:O	1:D:67:ASP:C	2.63	0.41
1:C:103:THR:HG21	1:C:142:VAL:CG2	2.50	0.41
1:C:161:LYS:NZ	3:C:931:HOH:O	2.52	0.41
1:D:46:GLU:C	1:D:48:PRO:HD2	2.46	0.41
1:D:246:LEU:HD23	1:D:246:LEU:HA	1.89	0.41
1:F:38:LEU:C	1:F:39:ILE:HD12	2.46	0.41
1:F:158:VAL:O	1:F:158:VAL:HG22	2.20	0.41
1:D:223:GLU:CD	1:D:231:LYS:HD3	2.46	0.41
1:E:229:LEU:HD23	1:E:229:LEU:C	2.46	0.41
1:F:78:THR:HG21	1:F:83:LYS:HB3	2.02	0.41
1:F:101:VAL:HG13	1:F:118:TYR:CE1	2.37	0.41
1:B:191:ASP:OD2	1:B:209:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:C	1:C:48:PRO:HD2	2.47	0.40
1:C:60:SER:O	1:C:64:GLU:HG3	2.20	0.40
1:D:229:LEU:C	1:D:229:LEU:CD2	2.92	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:C:51:ASN:OD1	1:C:51:ASN:C	2.64	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%)	36	29
All	All	1784/1800 (99%)	1750 (98%)	33 (2%)	1 (0%)	48	40

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%)	63	63
1	B	255/256 (100%)	254 (100%)	1 (0%)	84	87
1	C	255/256 (100%)	255 (100%)	0	100	100
1	D	254/256 (99%)	248 (98%)	6 (2%)	43	38
1	E	256/256 (100%)	250 (98%)	6 (2%)	44	40
1	F	249/256 (97%)	240 (96%)	9 (4%)	31	23
All	All	1527/1536 (99%)	1502 (98%)	25 (2%)	53	54

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	PRO
1	A	172	ARG
1	A	238	LYS
1	B	156	ASN
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	231	LYS
1	E	288	LEU
1	E	291	SER

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Mol	Chain	Res	Type
1	F	19	ASP
1	F	36	ASN
1	F	84	THR
1	F	108	LYS
1	F	154	LEU
1	F	158	VAL
1	F	183	ASP
1	F	210	SER
1	F	256	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	90	GLN
1	B	236	HIS
1	B	251	ASN
1	B	260	ASN
1	C	90	GLN
1	C	179	GLN
1	C	251	ASN
1	C	260	ASN
1	D	260	ASN
1	E	15	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

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	B	298	-	5,5,5	0.36	0	5,5,5	0.50	0
2	GOL	C	296	-	5,5,5	0.32	0	5,5,5	0.33	0
2	GOL	A	295	-	5,5,5	0.42	0	5,5,5	0.28	0
2	GOL	A	299	-	5,5,5	0.38	0	5,5,5	0.30	0
2	GOL	A	300	-	5,5,5	0.37	0	5,5,5	0.23	0
2	GOL	C	298	-	5,5,5	0.45	0	5,5,5	0.65	0
2	GOL	B	295	-	5,5,5	0.32	0	5,5,5	0.47	0
2	GOL	D	295	-	5,5,5	0.44	0	5,5,5	0.35	0
2	GOL	B	296	-	5,5,5	0.36	0	5,5,5	0.35	0
2	GOL	B	297	-	5,5,5	0.52	0	5,5,5	0.13	0
2	GOL	A	297	-	5,5,5	0.39	0	5,5,5	0.61	0
2	GOL	A	298	-	5,5,5	0.32	0	5,5,5	0.48	0
2	GOL	A	296	-	5,5,5	0.44	0	5,5,5	0.52	0
2	GOL	C	297	-	5,5,5	0.35	0	5,5,5	0.58	0
2	GOL	C	295	-	5,5,5	0.41	0	5,5,5	0.32	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	B	298	-	-	2/4/4/4	-
2	GOL	C	296	-	-	2/4/4/4	-
2	GOL	A	295	-	-	2/4/4/4	-
2	GOL	A	299	-	-	1/4/4/4	-
2	GOL	A	300	-	-	0/4/4/4	-
2	GOL	C	298	-	-	2/4/4/4	-
2	GOL	B	295	-	-	2/4/4/4	-
2	GOL	D	295	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	296	-	-	2/4/4/4	-
2	GOL	B	297	-	-	4/4/4/4	-
2	GOL	A	297	-	-	4/4/4/4	-
2	GOL	A	298	-	-	2/4/4/4	-
2	GOL	A	296	-	-	4/4/4/4	-
2	GOL	C	297	-	-	2/4/4/4	-
2	GOL	C	295	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	296	GOL	O1-C1-C2-O2
2	B	296	GOL	O1-C1-C2-C3
2	B	297	GOL	O1-C1-C2-C3
2	B	298	GOL	O1-C1-C2-O2
2	B	298	GOL	O1-C1-C2-C3
2	C	296	GOL	O1-C1-C2-C3
2	C	297	GOL	O1-C1-C2-C3
2	C	298	GOL	O1-C1-C2-O2
2	C	298	GOL	O1-C1-C2-C3
2	D	295	GOL	C1-C2-C3-O3
2	A	296	GOL	O1-C1-C2-O2
2	A	297	GOL	O2-C2-C3-O3
2	B	297	GOL	O1-C1-C2-O2
2	A	295	GOL	O1-C1-C2-C3
2	A	296	GOL	O1-C1-C2-C3
2	A	296	GOL	C1-C2-C3-O3
2	A	297	GOL	O1-C1-C2-C3
2	A	297	GOL	C1-C2-C3-O3
2	A	298	GOL	O1-C1-C2-C3
2	B	295	GOL	O1-C1-C2-C3
2	B	297	GOL	C1-C2-C3-O3
2	C	295	GOL	O1-C1-C2-C3
2	A	295	GOL	O1-C1-C2-O2
2	B	297	GOL	O2-C2-C3-O3
2	C	297	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	295	GOL	O2-C2-C3-O3
2	A	296	GOL	O2-C2-C3-O3
2	A	297	GOL	O1-C1-C2-O2
2	B	295	GOL	O1-C1-C2-O2
2	C	295	GOL	O1-C1-C2-O2
2	A	298	GOL	O1-C1-C2-O2
2	C	296	GOL	O1-C1-C2-O2
2	A	299	GOL	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	298	GOL	4	0
2	C	296	GOL	5	0
2	A	295	GOL	1	0
2	A	299	GOL	1	0
2	A	300	GOL	2	0
2	C	298	GOL	1	0
2	B	295	GOL	1	0
2	D	295	GOL	1	0
2	B	296	GOL	1	0
2	B	297	GOL	2	0
2	A	297	GOL	1	0
2	A	298	GOL	1	0
2	A	296	GOL	3	1
2	C	297	GOL	1	0
2	C	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%)	-0.28	0	100	100	10, 20, 39, 53	2 (0%)
1	B	298/300 (99%)	-0.37	0	100	100	11, 18, 35, 59	2 (0%)
1	C	297/300 (99%)	0.25	5 (1%)	69	72	12, 27, 49, 63	3 (1%)
1	D	298/300 (99%)	1.88	126 (42%)	0	0	21, 41, 77, 108	0
1	E	296/300 (98%)	1.66	116 (39%)	1	0	19, 42, 76, 91	4 (1%)
1	F	295/300 (98%)	4.99	294 (99%)	0	0	62, 90, 119, 145	1 (0%)
All	All	1784/1800 (99%)	1.35	541 (30%)	1	1	10, 33, 99, 145	12 (0%)

All (541) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	76	ALA	8.9
1	F	98	GLY	8.6
1	F	39	ILE	8.5
1	F	37	ALA	8.1
1	F	99	VAL	7.9
1	F	31	LEU	7.9
1	F	18	LEU	7.9
1	F	208	VAL	7.8
1	F	85	LEU	7.7
1	F	206	ILE	7.7
1	F	130	VAL	7.5
1	F	106	TYR	7.5
1	F	157	VAL	7.4
1	F	276	ALA	7.4
1	F	11	THR	7.4
1	F	10	VAL	7.3
1	F	59	VAL	7.2
1	F	212	VAL	7.2
1	F	73	ILE	7.1

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Mol	Chain	Res	Type	RSRZ
1	F	187	TRP	7.1
1	F	5	VAL	7.1
1	F	271	LEU	7.1
1	F	170	ILE	7.0
1	F	13	PHE	7.0
1	F	94	LEU	7.0
1	F	118	TYR	7.0
1	F	220	LEU	6.9
1	F	23	TYR	6.9
1	F	160	ILE	6.9
1	F	50	VAL	6.9
1	F	273	LEU	6.9
1	F	127	LEU	6.9
1	F	265	ILE	6.9
1	F	27	VAL	6.8
1	F	100	LEU	6.8
1	D	195	PHE	6.8
1	F	74	VAL	6.8
1	F	42	GLY	6.7
1	F	264	PHE	6.7
1	F	213	ALA	6.7
1	F	87	LEU	6.7
1	F	132	TYR	6.6
1	F	6	GLY	6.6
1	F	246	LEU	6.6
1	F	7	THR	6.6
1	D	222	ALA	6.6
1	F	35	VAL	6.6
1	F	131	VAL	6.6
1	F	134	VAL	6.6
1	F	84	THR	6.5
1	F	158	VAL	6.5
1	F	139	GLY	6.5
1	F	2	PHE	6.5
1	F	9	ILE	6.5
1	F	221	CYS	6.5
1	F	242	LEU	6.5
1	F	88	VAL	6.5
1	F	140	VAL	6.4
1	F	209	VAL	6.4
1	F	195	PHE	6.4
1	D	196	TYR	6.4

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Mol	Chain	Res	Type	RSRZ
1	F	63	LEU	6.4
1	F	269	LEU	6.4
1	F	150	ILE	6.4
1	F	26	LEU	6.4
1	F	40	VAL	6.4
1	F	174	VAL	6.3
1	F	247	PHE	6.2
1	F	20	LEU	6.2
1	F	41	LEU	6.2
1	F	105	TYR	6.2
1	F	8	ALA	6.2
1	F	237	ALA	6.2
1	F	78	THR	6.2
1	F	287	VAL	6.1
1	D	200	ALA	6.1
1	F	235	VAL	6.1
1	D	229	LEU	6.1
1	F	143	LEU	6.1
1	F	229	LEU	6.1
1	F	189	GLY	6.0
1	F	12	PRO	6.0
1	F	43	THR	6.0
1	F	274	VAL	6.0
1	F	225	PHE	6.0
1	F	224	TYR	6.0
1	F	72	VAL	6.0
1	F	121	ILE	6.0
1	F	258	ALA	6.0
1	F	38	LEU	5.9
1	F	261	LEU	5.9
1	F	272	PRO	5.9
1	F	243	MET	5.8
1	F	239	LEU	5.8
1	F	288	LEU	5.8
1	F	151	ALA	5.8
1	F	1[A]	MET	5.8
1	F	205	VAL	5.8
1	F	29	TYR	5.8
1	F	294	LEU	5.8
1	F	129	ILE	5.8
1	F	154	LEU	5.8
1	F	201	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	F	58	LEU	5.7
1	F	194	THR	5.7
1	F	45	GLY	5.7
1	F	101	VAL	5.7
1	F	138	THR	5.6
1	F	48	PRO	5.6
1	D	199	CYS	5.6
1	D	201	GLY	5.6
1	F	104	PRO	5.6
1	F	253	ILE	5.6
1	F	199	CYS	5.6
1	F	77	GLY	5.6
1	F	259	LEU	5.5
1	F	115	TYR	5.5
1	F	128	GLY	5.5
1	F	184	PHE	5.5
1	F	102	VAL	5.5
1	F	262	MET	5.5
1	F	114	LEU	5.4
1	D	237	ALA	5.4
1	F	186	VAL	5.4
1	F	133	ASN	5.4
1	F	65	ILE	5.4
1	F	120	TYR	5.4
1	F	198	LEU	5.4
1	F	283	LEU	5.4
1	F	293	LEU	5.4
1	F	255	VAL	5.4
1	F	4	GLY	5.3
1	E	18	LEU	5.3
1	F	218	VAL	5.3
1	F	161	LYS	5.3
1	F	200	ALA	5.3
1	F	109	PRO	5.3
1	F	252	PRO	5.3
1	D	220	LEU	5.3
1	F	49	THR	5.3
1	F	222	ALA	5.3
1	F	90	GLN	5.2
1	F	57	LYS	5.2
1	F	81	THR	5.2
1	D	167	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	44	THR	5.2
1	D	283	LEU	5.2
1	F	152	ALA	5.2
1	F	163	ALA	5.2
1	F	103	THR	5.1
1	D	233	ALA	5.1
1	E	-1	PHE	5.1
1	F	62	THR	5.1
1	F	284	LEU	5.1
1	F	177	THR	5.1
1	F	182	SER	5.0
1	D	225	PHE	5.0
1	F	142	VAL	5.0
1	F	167	ILE	5.0
1	F	148	ALA	5.0
1	F	164	ASN	5.0
1	F	245	ALA	5.0
1	F	227	GLY	4.9
1	D	245	ALA	4.9
1	F	210	SER	4.9
1	F	203	ASP	4.9
1	F	54	GLU	4.9
1	D	170	ILE	4.9
1	F	16	GLY	4.9
1	F	165	PRO	4.9
1	F	226[A]	SER	4.8
1	F	117	HIS	4.8
1	F	89	LYS	4.8
1	F	257	ALA	4.8
1	F	71	PRO	4.8
1	F	260	ASN	4.8
1	F	137	ARG	4.8
1	F	197	LEU	4.8
1	F	79	ASN	4.8
1	F	270	ARG	4.8
1	E	31	LEU	4.8
1	F	251	ASN	4.7
1	F	91	ALA	4.7
1	F	275	PRO	4.7
1	F	113	GLY	4.7
1	F	250	THR	4.7
1	F	191	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	233	ALA	4.6
1	F	181	ARG	4.6
1	F	185	MET	4.5
1	F	267	ASN	4.5
1	D	232	SER	4.5
1	F	110	THR	4.5
1	E	20	LEU	4.5
1	F	155	LYS	4.4
1	F	236	HIS	4.4
1	D	224	TYR	4.4
1	F	176	LEU	4.4
1	F	111	GLN	4.4
1	F	124	ARG	4.4
1	F	228	ASN	4.4
1	F	70	ILE	4.4
1	F	34	GLY	4.3
1	D	226	SER	4.3
1	D	231	LYS	4.3
1	F	178	LYS	4.3
1	D	198	LEU	4.3
1	D	235	VAL	4.3
1	F	66	VAL	4.3
1	F	135	PRO	4.3
1	F	173	THR	4.3
1	F	217	MET	4.3
1	F	83	LYS	4.3
1	F	28	ARG	4.3
1	F	30	GLN	4.3
1	F	147	ALA	4.3
1	D	236	HIS	4.3
1	D	165	PRO	4.3
1	D	197	LEU	4.2
1	D	176	LEU	4.2
1	F	162	GLU	4.2
1	D	287	VAL	4.2
1	E	40	VAL	4.2
1	E	59	VAL	4.2
1	F	68	GLY	4.2
1	F	196	TYR	4.2
1	F	254	PRO	4.2
1	D	212	VAL	4.1
1	F	211	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	86	LYS	4.1
1	F	19	ASP	4.1
1	F	51	ASN	4.1
1	F	107	ASN	4.1
1	F	47	SER	4.1
1	F	248	VAL	4.1
1	F	3	ARG	4.1
1	F	214	PRO	4.1
1	F	190	ASN	4.1
1	F	188	SER	4.0
1	F	281	VAL	4.0
1	E	156	ASN	4.0
1	F	97	ASN	4.0
1	F	141	ASN	4.0
1	F	75	GLY	4.0
1	F	46	GLU	4.0
1	E	57	LYS	4.0
1	F	60	SER	4.0
1	F	125	THR	3.9
1	F	61	ARG	3.9
1	F	136	GLY	3.9
1	F	207	SER	3.9
1	F	95	GLY	3.9
1	D	202	GLY	3.9
1	E	27	VAL	3.9
1	F	289	LYS	3.9
1	F	204	GLY	3.9
1	D	230	GLU	3.8
1	E	63	LEU	3.8
1	D	189	GLY	3.8
1	E	95	GLY	3.8
1	D	171	ASP	3.8
1	F	25	ARG	3.8
1	E	66	VAL	3.8
1	F	36	ASN	3.8
1	E	26	LEU	3.8
1	F	240	ARG	3.8
1	F	33	ASN	3.8
1	D	205	VAL	3.8
1	D	234	GLU	3.8
1	E	72	VAL	3.8
1	D	188	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	238	LYS	3.8
1	F	244	LYS	3.8
1	F	108	LYS	3.8
1	E	157	VAL	3.8
1	F	168	ASP	3.7
1	F	241	PRO	3.7
1	E	68	GLY	3.7
1	F	249	GLU	3.7
1	D	241	PRO	3.7
1	F	144	PRO	3.7
1	D	194	THR	3.7
1	F	80	SER	3.7
1	F	256	LYS	3.7
1	D	239	LEU	3.7
1	E	76	ALA	3.7
1	F	96	ALA	3.7
1	D	168	ASP	3.7
1	D	223	GLU	3.7
1	F	202	GLY	3.7
1	F	149	ARG	3.7
1	F	17	GLU	3.6
1	D	221	CYS	3.6
1	D	284	LEU	3.6
1	F	166	ASP	3.6
1	D	5	VAL	3.6
1	F	180	ALA	3.6
1	F	159	GLY	3.6
1	F	183	ASP	3.6
1	F	192	ASP	3.6
1	E	91	ALA	3.5
1	F	156	ASN	3.5
1	D	166	ASP	3.5
1	F	171	ASP	3.5
1	F	55	ARG	3.5
1	F	193	ARG	3.5
1	F	119	LYS	3.5
1	F	263	GLY	3.5
1	F	279	LYS	3.5
1	F	21	GLU	3.5
1	F	266	GLU	3.5
1	D	240	ARG	3.5
1	D	175	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	122	SER	3.5
1	E	94	LEU	3.5
1	E	127	LEU	3.5
1	F	238	LYS	3.5
1	F	175	SER	3.4
1	F	280	THR	3.4
1	D	209	VAL	3.4
1	D	243	MET	3.4
1	D	174	VAL	3.4
1	E	87	LEU	3.4
1	F	232	SER	3.4
1	E	23	TYR	3.4
1	E	37	ALA	3.4
1	E	38	LEU	3.4
1	D	193	ARG	3.4
1	D	179	GLN	3.3
1	F	53	ASP	3.3
1	D	218	VAL	3.3
1	E	2	PHE	3.3
1	F	146	THR	3.3
1	F	277	SER	3.3
1	E	264	PHE	3.3
1	F	169	GLN	3.3
1	F	126	ASP	3.3
1	D	227	GLY	3.3
1	D	289	LYS	3.3
1	D	186	VAL	3.3
1	E	99	VAL	3.3
1	D	246	LEU	3.3
1	D	-3	ASP	3.3
1	E	61	ARG	3.3
1	F	285	ARG	3.3
1	D	204	GLY	3.3
1	F	292	GLY	3.3
1	C	-2	PRO	3.2
1	D	172	ARG	3.2
1	E	25	ARG	3.2
1	E	128	GLY	3.2
1	E	226[A]	SER	3.2
1	E	120	TYR	3.2
1	F	56	GLU	3.2
1	D	36	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	247	PHE	3.2
1	D	292	GLY	3.2
1	F	290	GLU	3.2
1	D	228	ASN	3.1
1	D	294	LEU	3.1
1	E	60	SER	3.1
1	F	22	SER	3.1
1	E	32	GLU	3.1
1	F	32	GLU	3.1
1	D	37	ALA	3.1
1	D	293	LEU	3.1
1	F	215	LYS	3.1
1	E	12	PRO	3.1
1	D	192	ASP	3.1
1	D	291	SER	3.1
1	F	82	GLU	3.1
1	F	123	GLU	3.1
1	F	93	LYS	3.0
1	E	13	PHE	3.0
1	E	152	ALA	3.0
1	D	242	LEU	3.0
1	E	182	SER	3.0
1	E	96	ALA	3.0
1	F	234	GLU	3.0
1	D	35	VAL	3.0
1	E	0	THR	3.0
1	E	53	ASP	3.0
1	F	231	LYS	3.0
1	E	124	ARG	3.0
1	E	58	LEU	2.9
1	E	155	LYS	2.9
1	F	0	THR	2.9
1	F	230	GLU	2.9
1	E	129	ILE	2.9
1	D	248	VAL	2.9
1	E	158	VAL	2.9
1	D	0	THR	2.9
1	E	125	THR	2.9
1	E	263	GLY	2.9
1	F	268	GLU	2.9
1	E	222	ALA	2.9
1	D	187	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	160	ILE	2.9
1	D	143	LEU	2.9
1	F	112	GLU	2.9
1	D	158	VAL	2.9
1	F	286	ASN	2.9
1	F	69	LYS	2.9
1	F	291	SER	2.9
1	D	-2	PRO	2.8
1	D	216	GLN	2.8
1	E	121	ILE	2.8
1	E	235	VAL	2.8
1	F	24	GLU	2.8
1	D	288	LEU	2.8
1	E	65	ILE	2.8
1	F	67	ASP	2.8
1	D	-1	PHE	2.8
1	F	15	ASN	2.8
1	E	89	LYS	2.8
1	E	70	ILE	2.8
1	D	207	SER	2.7
1	D	164	ASN	2.7
1	E	36	ASN	2.7
1	D	219	GLU	2.7
1	D	142	VAL	2.7
1	E	294	LEU	2.7
1	D	215	LYS	2.7
1	E	93	LYS	2.7
1	D	180	ALA	2.7
1	D	213	ALA	2.7
1	E	183	ASP	2.7
1	D	177	THR	2.7
1	E	9	ILE	2.7
1	D	281	VAL	2.7
1	D	148	ALA	2.6
1	D	3	ARG	2.6
1	E	7	THR	2.6
1	E	62	THR	2.6
1	F	52	GLU	2.6
1	D	206	ILE	2.6
1	D	4	GLY	2.6
1	F	172	ARG	2.6
1	E	30	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	90	GLN	2.6
1	D	261	LEU	2.6
1	E	41	LEU	2.6
1	E	88	VAL	2.6
1	E	22	SER	2.6
1	E	73	ILE	2.6
1	F	219	GLU	2.6
1	D	152	ALA	2.6
1	D	258	ALA	2.6
1	D	217	MET	2.5
1	D	126	ASP	2.5
1	E	85	LEU	2.5
1	E	288	LEU	2.5
1	D	244	LYS	2.5
1	C	156	ASN	2.5
1	D	147	ALA	2.5
1	D	257	ALA	2.5
1	D	169	GLN	2.5
1	F	216	GLN	2.5
1	F	92	GLU	2.5
1	F	145	GLU	2.5
1	D	279	LYS	2.5
1	E	269	LEU	2.5
1	E	291	SER	2.5
1	F	116	GLN	2.5
1	E	1	MET	2.5
1	D	282	GLU	2.5
1	E	50	VAL	2.5
1	F	153	ASP	2.5
1	E	227	GLY	2.4
1	E	154	LEU	2.4
1	F	179	GLN	2.4
1	F	223	GLU	2.4
1	F	282	GLU	2.4
1	D	144	PRO	2.4
1	D	286	ASN	2.4
1	D	145	GLU	2.4
1	E	64	GLU	2.4
1	E	69	LYS	2.4
1	D	203	ASP	2.4
1	E	19	ASP	2.4
1	D	163	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	5	VAL	2.4
1	E	15	ASN	2.4
1	E	14	LYS	2.4
1	E	261	LEU	2.4
1	E	179	GLN	2.4
1	E	98	GLY	2.4
1	E	209	VAL	2.4
1	D	182	SER	2.4
1	E	67	ASP	2.3
1	D	29	TYR	2.3
1	E	29	TYR	2.3
1	C	14	LYS	2.3
1	E	10	VAL	2.3
1	E	151	ALA	2.3
1	F	14	LYS	2.3
1	D	208	VAL	2.3
1	C	18	LEU	2.3
1	D	173	THR	2.3
1	E	84	THR	2.3
1	E	228[A]	ASN	2.3
1	E	289	LYS	2.3
1	E	3	ARG	2.3
1	E	39	ILE	2.3
1	C	282	GLU	2.3
1	E	185	MET	2.3
1	E	279	LYS	2.3
1	D	135	PRO	2.2
1	E	17	GLU	2.2
1	D	191	ASP	2.2
1	E	86	LYS	2.2
1	D	110	THR	2.2
1	D	290	GLU	2.2
1	E	293	LEU	2.2
1	E	115	TYR	2.2
1	E	262	MET	2.2
1	E	187	TRP	2.2
1	E	123	GLU	2.2
1	D	210	SER	2.2
1	E	33	ASN	2.1
1	E	184	PHE	2.1
1	D	34	GLY	2.1
1	E	75	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	178	LYS	2.1
1	D	285	ARG	2.1
1	E	28	ARG	2.1
1	E	92	GLU	2.1
1	E	97	ASN	2.1
1	E	126	ASP	2.1
1	E	224	TYR	2.1
1	E	122	SER	2.1
1	F	64	GLU	2.1
1	D	134	VAL	2.1
1	D	190	ASN	2.1
1	E	221	CYS	2.1
1	D	183	ASP	2.1
1	E	45	GLY	2.0
1	D	141	ASN	2.0
1	D	184	PHE	2.0
1	E	286	ASN	2.0
1	E	181	ARG	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	298	6/6	0.70	0.15	63,64,65,66	0
2	GOL	B	297	6/6	0.70	0.19	57,60,62,63	0
2	GOL	A	299	6/6	0.73	0.21	61,64,64,67	0
2	GOL	A	295	6/6	0.75	0.27	65,69,76,77	0
2	GOL	D	295	6/6	0.75	0.18	50,57,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	295	6/6	0.79	0.14	33,46,53,61	0
2	GOL	C	296	6/6	0.80	0.17	35,52,59,61	0
2	GOL	A	300	6/6	0.80	0.15	53,59,61,63	0
2	GOL	B	296	6/6	0.82	0.16	53,61,64,70	0
2	GOL	B	298	6/6	0.82	0.17	67,69,70,70	0
2	GOL	A	297	6/6	0.86	0.12	33,39,47,52	0
2	GOL	A	296	6/6	0.87	0.16	21,34,46,54	0
2	GOL	C	295	6/6	0.87	0.17	62,67,68,72	0
2	GOL	C	298	6/6	0.89	0.14	20,39,47,67	0
2	GOL	C	297	6/6	0.91	0.14	11,35,44,45	6

6.5 Other polymers [i](#)

There are no such residues in this entry.