



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 06:16 PM EDT

PDB ID : 7JVH
Title : Crystal structure of a GH43_12 retrieved from capybara gut metagenome
Authors : Cabral, L.; Domingues, M.N.; Martins, M.P.; Persinoti, G.F.; Morais, M.A.B.;
Murakami, M.T.
Deposited on : 2020-08-21
Resolution : 2.48 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

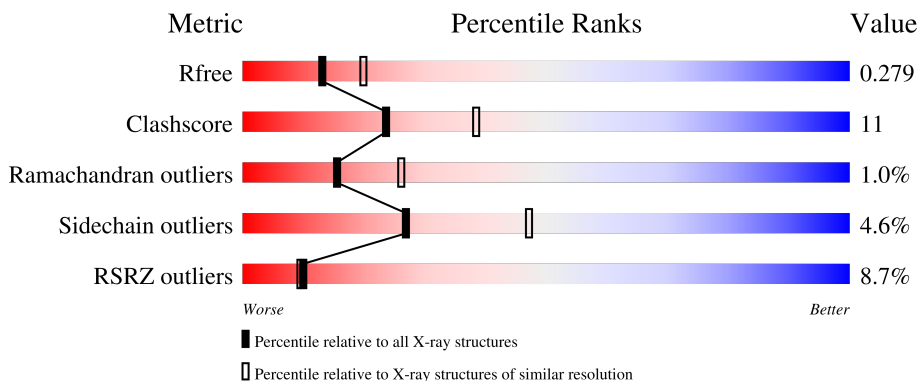
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	567	 81% 12% • 6%
1	B	567	 80% 13% • 6%
1	C	567	 2% 75% 17% • 5%
1	D	567	 2% 77% 15% •• 6%
1	E	567	 20% 63% 20% •• 12%

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Mol	Chain	Length	Quality of chain												
1	F	567	 <p>A horizontal bar chart showing the quality distribution of chain F. The bar is divided into five segments: red (23%), green (65%), yellow (18%), orange (5%), and grey (12%).</p> <table border="1"><thead><tr><th>Quality Category</th><th>Percentage</th></tr></thead><tbody><tr><td>Red</td><td>23%</td></tr><tr><td>Green</td><td>65%</td></tr><tr><td>Yellow</td><td>18%</td></tr><tr><td>Orange</td><td>5%</td></tr><tr><td>Grey</td><td>12%</td></tr></tbody></table>	Quality Category	Percentage	Red	23%	Green	65%	Yellow	18%	Orange	5%	Grey	12%
Quality Category	Percentage														
Red	23%														
Green	65%														
Yellow	18%														
Orange	5%														
Grey	12%														

2 Entry composition [i](#)

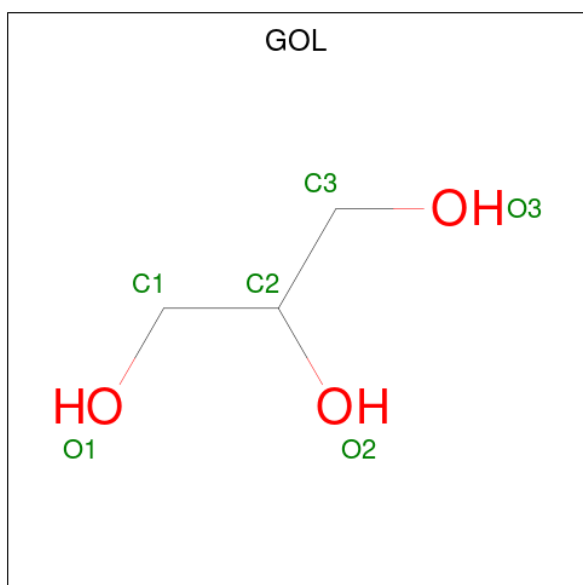
There are 3 unique types of molecules in this entry. The entry contains 25078 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoside Hydrolase Family 43_12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	535	Total 4232	C 2721	N 700	O 793	S 9	Se 9	0	0	0
1	B	535	Total 4231	C 2719	N 700	O 794	S 9	Se 9	0	0	0
1	C	536	Total 4239	C 2725	N 702	O 794	S 9	Se 9	0	0	0
1	D	534	Total 4221	C 2713	N 698	O 792	S 9	Se 9	0	0	0
1	E	497	Total 3943	C 2543	N 650	O 733	S 8	Se 9	0	0	0
1	F	499	Total 3964	C 2556	N 651	O 740	S 8	Se 9	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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


- Molecule 3 is water.

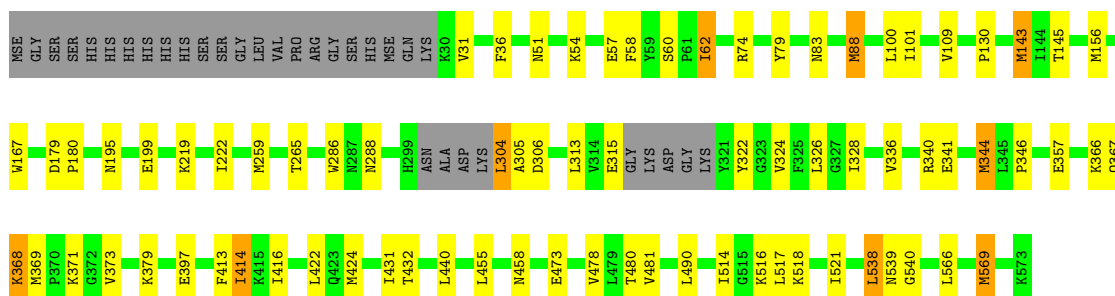
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	64	Total O 64 64	0	0
3	B	52	Total O 52 52	0	0
3	C	32	Total O 32 32	0	0
3	D	31	Total O 31 31	0	0
3	E	4	Total O 4 4	0	0
3	F	5	Total O 5 5	0	0

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.

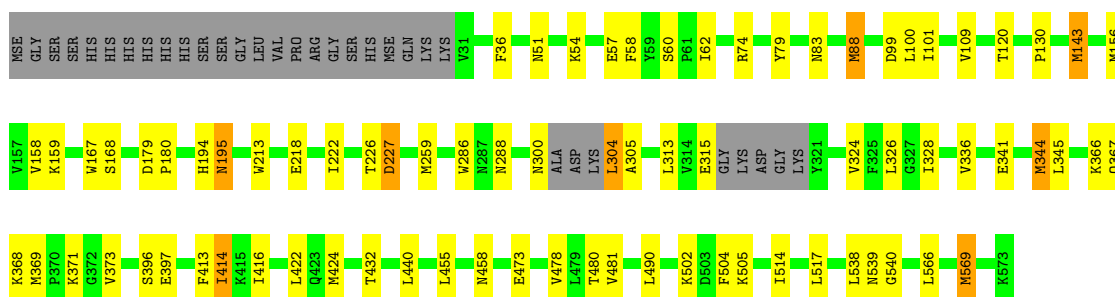
- Molecule 1: Glycoside Hydrolase Family 43_12

Chain A: 




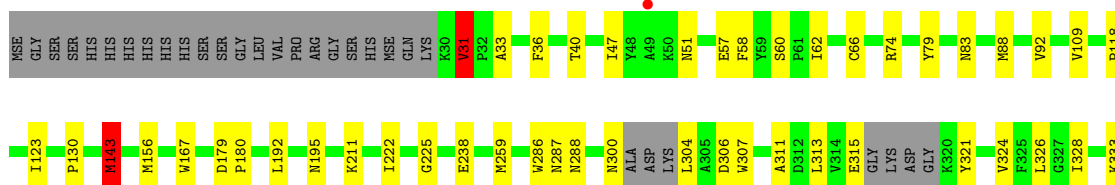
- Molecule 1: Glycoside Hydrolase Family 43_12

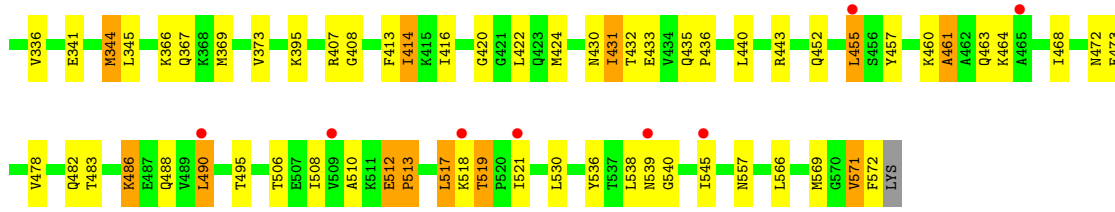
Chain B: 



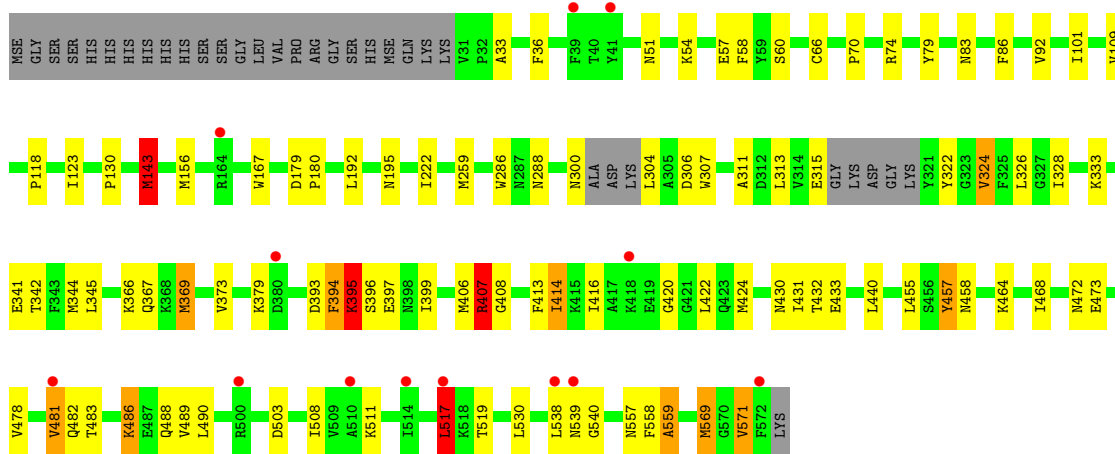
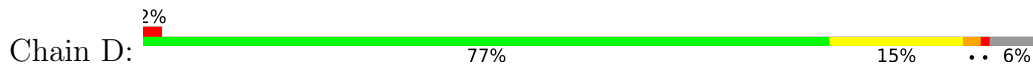
- Molecule 1: Glycoside Hydrolase Family 43_12

Chain C: 

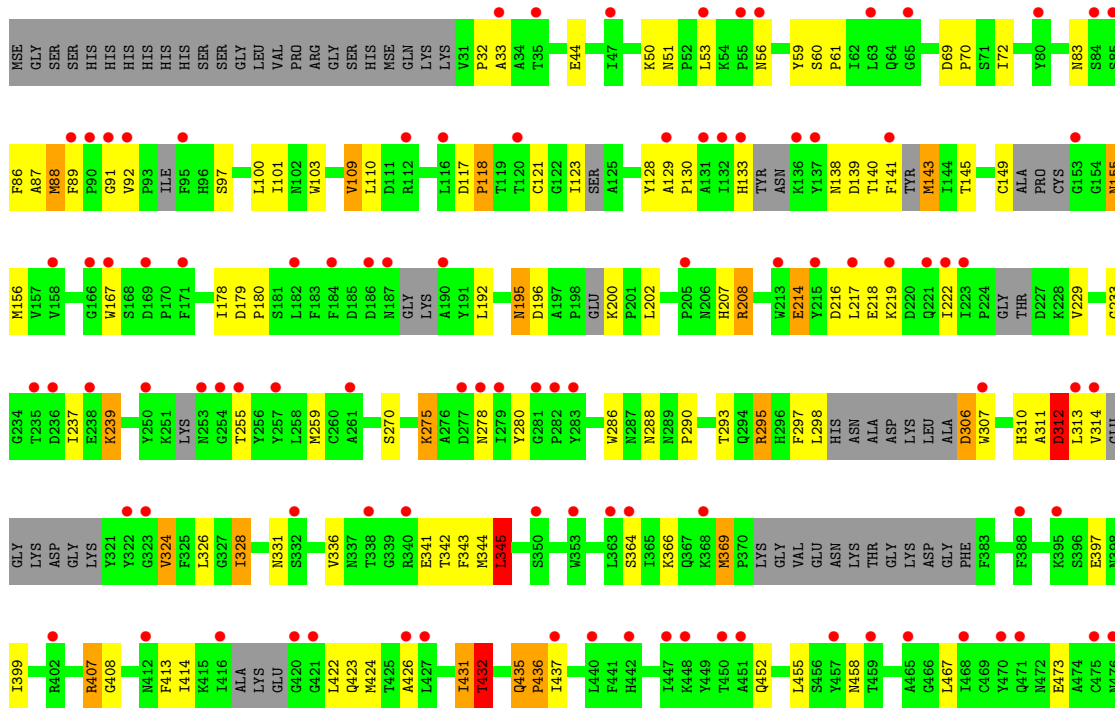


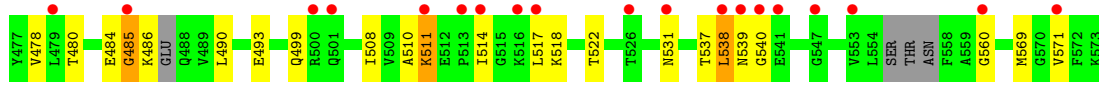


• Molecule 1: Glycoside Hydrolase Family 43_12

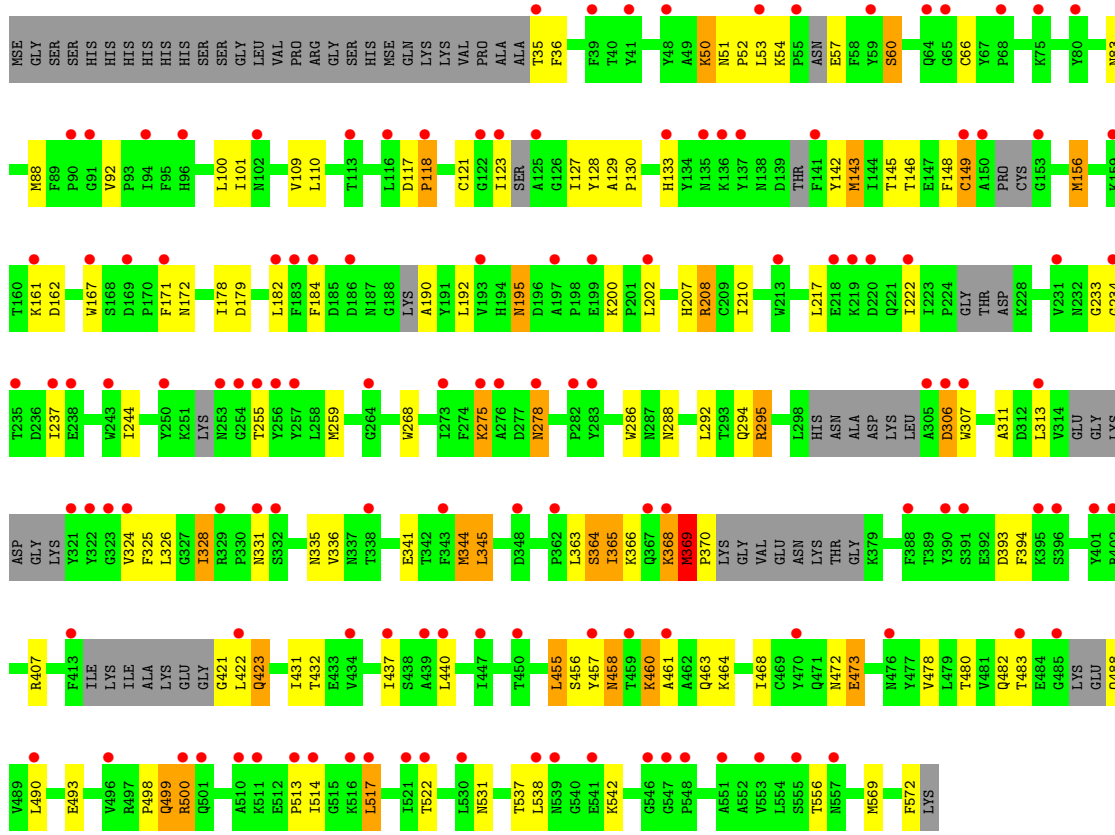


• Molecule 1: Glycoside Hydrolase Family 43_12





● Molecule 1: Glycoside Hydrolase Family 43_12



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	107.22Å 107.38Å 132.53Å 99.03° 113.38° 108.45°	Depositor
Resolution (Å)	49.20 – 2.48 49.20 – 2.48	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.20-2.48) 95.8 (49.20-2.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.8	Depositor
R, R_{free}	0.246 , 0.278 0.249 , 0.279	Depositor DCC
R_{free} test set	8303 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtrriage
Anisotropy	0.711	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.437 for k,h,-h-k-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25078	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 i

5.1 Standard geometry i

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	1/4343 (0.0%)	0.70	2/5887 (0.0%)
1	B	0.50	2/4342 (0.0%)	0.71	2/5887 (0.0%)
1	C	0.57	6/4350 (0.1%)	0.77	5/5898 (0.1%)
1	D	0.52	4/4332 (0.1%)	0.76	7/5876 (0.1%)
1	E	0.59	8/4037 (0.2%)	0.80	9/5459 (0.2%)
1	F	0.52	4/4062 (0.1%)	0.79	10/5498 (0.2%)
All	All	0.53	25/25466 (0.1%)	0.76	35/34505 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	118	PRO	N-CA	13.51	1.70	1.47
1	E	436	PRO	N-CA	13.20	1.69	1.47
1	C	513	PRO	N-CA	13.03	1.69	1.47
1	E	118	PRO	N-CA	11.76	1.67	1.47
1	C	31	VAL	C-N	9.12	1.51	1.34
1	F	345	LEU	C-N	8.93	1.51	1.34
1	D	408	GLY	C-N	8.76	1.50	1.34
1	C	408	GLY	C-N	8.75	1.50	1.34
1	E	408	GLY	C-N	8.72	1.50	1.34
1	E	345	LEU	C-N	8.62	1.50	1.34
1	D	369	MSE	C-N	8.49	1.50	1.34
1	E	89	PHE	C-N	8.44	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	345	LEU	C-N	8.42	1.50	1.34
1	B	345	LEU	C-N	8.40	1.50	1.34
1	B	60	SER	C-N	8.14	1.49	1.34
1	E	60	SER	C-N	8.05	1.49	1.34
1	D	345	LEU	C-N	8.04	1.49	1.34
1	A	60	SER	C-N	7.97	1.49	1.34
1	F	60	SER	C-N	7.92	1.49	1.34
1	C	60	SER	C-N	7.70	1.48	1.34
1	D	60	SER	C-N	7.60	1.48	1.34
1	C	512	GLU	C-N	5.75	1.45	1.34
1	F	117	ASP	C-N	5.75	1.45	1.34
1	E	435	GLN	C-N	5.74	1.45	1.34
1	E	117	ASP	C-N	5.32	1.44	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	161	LYS	N-CA-C	-9.82	84.49	111.00
1	E	431	ILE	N-CA-C	-8.60	87.78	111.00
1	C	143	MSE	CG-SE-CE	8.18	116.89	98.90
1	D	143	MSE	CG-SE-CE	8.02	116.53	98.90
1	A	344	MSE	CG-SE-CE	7.90	116.27	98.90
1	E	436	PRO	CA-N-CD	-7.51	100.98	111.50
1	E	118	PRO	CA-N-CD	-7.45	101.07	111.50
1	D	517	LEU	CA-CB-CG	7.23	131.94	115.30
1	C	513	PRO	CA-N-CD	-7.13	101.51	111.50
1	B	344	MSE	CG-SE-CE	7.12	114.57	98.90
1	F	369	MSE	CG-SE-CE	7.10	114.51	98.90
1	E	88	MSE	CG-SE-CE	7.01	114.32	98.90
1	E	432	THR	N-CA-CB	6.96	123.53	110.30
1	F	118	PRO	CA-N-CD	-6.83	101.94	111.50
1	D	457	TYR	N-CA-C	6.77	129.28	111.00
1	B	88	MSE	CG-SE-CE	6.75	113.76	98.90
1	F	364	SER	N-CA-C	6.47	128.46	111.00
1	E	510	ALA	N-CA-C	6.33	128.10	111.00
1	F	208	ARG	CG-CD-NE	6.23	124.88	111.80
1	F	278	ASN	CB-CA-C	6.21	122.83	110.40
1	A	88	MSE	CG-SE-CE	5.99	112.09	98.90
1	C	490	LEU	CA-CB-CG	5.94	128.97	115.30
1	C	344	MSE	CG-SE-CE	5.94	111.97	98.90
1	E	208	ARG	CB-CG-CD	-5.79	96.55	111.60
1	F	295	ARG	CG-CD-NE	5.73	123.83	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	406	MSE	CG-SE-CE	5.64	111.31	98.90
1	F	88	MSE	CG-SE-CE	5.46	110.91	98.90
1	E	312	ASP	CB-CA-C	5.43	121.27	110.40
1	C	88	MSE	CG-SE-CE	5.38	110.74	98.90
1	D	394	PHE	CB-CA-C	5.31	121.01	110.40
1	E	118	PRO	CA-C-O	-5.30	107.47	120.20
1	D	559	ALA	N-CA-CB	5.27	117.48	110.10
1	D	369	MSE	CG-SE-CE	5.25	110.45	98.90
1	F	278	ASN	N-CA-CB	5.25	120.05	110.60
1	F	171	PHE	N-CA-C	5.10	124.76	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	226	THR	Mainchain
1	B	227	ASP	Mainchain

5.2 Too-close contacts [i](#)

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	4232	0	4103	52	0
1	B	4231	0	4096	54	0
1	C	4239	0	4109	96	0
1	D	4221	0	4083	86	0
1	E	3943	0	3807	133	0
1	F	3964	0	3804	137	0
2	A	18	0	24	1	0
2	B	12	0	16	0	0
2	C	12	0	16	3	0
2	D	12	0	16	1	0
2	F	6	0	8	0	0
3	A	64	0	0	0	0
3	B	52	0	0	0	0
3	C	32	0	0	0	0
3	D	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	4	0	0	0	0
3	F	5	0	0	0	0
All	All	25078	0	24082	550	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 11.

All (550) 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:436:PRO:N	1:E:436:PRO:CA	1.69	1.42
1:C:513:PRO:N	1:C:513:PRO:CA	1.69	1.38
1:F:118:PRO:N	1:F:118:PRO:CA	1.70	1.34
1:F:36:PHE:CE1	1:F:455:LEU:HD13	1.69	1.25
1:E:118:PRO:HB2	1:E:407:ARG:HA	1.15	1.11
1:F:423:GLN:O	1:F:423:GLN:HG2	1.57	1.03
1:B:397:GLU:HA	1:B:416:ILE:HD12	1.42	1.00
1:A:100:LEU:HB3	1:A:344:MSE:HE1	1.44	0.99
1:D:118:PRO:O	1:D:407:ARG:HB3	1.63	0.98
1:F:36:PHE:CE1	1:F:455:LEU:CD1	2.48	0.97
1:C:130:PRO:HB3	1:C:143:MSE:HE2	1.48	0.96
1:C:490:LEU:HD23	1:C:512:GLU:O	1.64	0.96
1:E:128:TYR:CE2	1:E:178:ILE:HD12	2.00	0.96
1:F:128:TYR:CE2	1:F:178:ILE:HD12	2.00	0.96
1:F:36:PHE:HE1	1:F:455:LEU:HD13	1.27	0.96
1:D:130:PRO:HB3	1:D:143:MSE:HE2	1.48	0.95
1:E:306:ASP:O	1:E:328:ILE:HG22	1.67	0.93
1:E:101:ILE:HG13	1:E:369:MSE:HE3	1.52	0.90
1:E:214:GLU:HG3	1:E:280:TYR:OH	1.72	0.89
1:B:100:LEU:HB3	1:B:344:MSE:HE1	1.53	0.89
1:F:182:LEU:HD13	1:F:184:PHE:CE2	2.07	0.89
1:D:92:VAL:HG21	1:D:143:MSE:HE3	1.56	0.88
1:D:424:MSE:HG3	1:D:571:VAL:HG21	1.54	0.88
1:D:424:MSE:HG3	1:D:571:VAL:CG2	2.03	0.88
1:C:490:LEU:HD21	1:C:512:GLU:HB2	1.55	0.87
1:A:265:THR:HG21	1:A:340:ARG:HH11	1.36	0.87
1:E:118:PRO:O	1:E:407:ARG:HB3	1.75	0.87
1:F:92:VAL:HB	1:F:109:VAL:HG12	1.55	0.87
1:C:92:VAL:HG21	1:C:143:MSE:HE3	1.57	0.87
1:E:426:ALA:HB2	1:E:571:VAL:HG22	1.57	0.85
1:E:431:ILE:O	1:E:432:THR:HG23	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:LEU:HB3	1:F:344:MSE:HE1	1.57	0.83
1:F:331:ASN:HD21	1:F:335:ASN:HB2	1.42	0.82
1:F:182:LEU:HD13	1:F:184:PHE:CZ	2.14	0.82
1:F:364:SER:O	1:F:365:ILE:HG22	1.80	0.82
1:B:88:MSE:HE2	1:B:566:LEU:HD21	1.62	0.81
1:C:464:LYS:HG2	1:C:482:GLN:HG2	1.62	0.81
1:A:88:MSE:HE2	1:A:566:LEU:HD21	1.64	0.80
1:E:306:ASP:O	1:E:328:ILE:CG2	2.29	0.80
1:E:92:VAL:HG22	1:E:109:VAL:CG1	2.13	0.79
1:E:100:LEU:HB3	1:E:344:MSE:HE1	1.64	0.79
1:D:457:TYR:OH	1:D:483:THR:HG23	1.83	0.79
1:E:195:ASN:HD21	1:E:208:ARG:HD2	1.47	0.78
1:C:483:THR:HG22	1:C:488:GLN:HE21	1.46	0.78
1:F:101:ILE:HG13	1:F:369:MSE:HG2	1.66	0.78
1:F:498:PRO:HB2	1:F:500:ARG:HE	1.48	0.77
1:E:33:ALA:HB3	1:E:571:VAL:HG21	1.67	0.77
1:E:259:MSE:HE1	1:E:313:LEU:HD11	1.66	0.77
1:F:259:MSE:HE1	1:F:313:LEU:HD11	1.66	0.77
1:F:307:TRP:H	1:F:328:ILE:CG2	1.98	0.77
1:E:87:ALA:HB2	1:E:121:CYS:SG	2.25	0.76
1:B:259:MSE:HE1	1:B:313:LEU:HD11	1.67	0.76
1:D:130:PRO:CB	1:D:143:MSE:HE2	2.15	0.76
1:C:130:PRO:CB	1:C:143:MSE:HE2	2.16	0.76
1:E:92:VAL:CG1	1:E:109:VAL:HG13	2.16	0.75
1:D:430:ASN:OD1	1:D:433:GLU:HG3	1.87	0.74
1:D:259:MSE:HE1	1:D:313:LEU:HD11	1.70	0.74
1:D:464:LYS:HE2	1:D:482:GLN:CD	2.08	0.74
1:C:413:PHE:CD1	1:C:414:ILE:HD12	2.23	0.73
1:D:413:PHE:CD1	1:D:414:ILE:HD12	2.23	0.73
1:E:311:ALA:HA	1:E:324:VAL:O	1.88	0.73
1:F:146:THR:HG21	1:F:148:PHE:CE2	2.23	0.73
1:E:484:GLU:OE2	1:E:511:LYS:NZ	2.21	0.73
1:E:293:THR:OG1	1:E:295:ARG:HD2	1.88	0.73
1:A:259:MSE:HE1	1:A:313:LEU:HD11	1.70	0.72
1:C:259:MSE:HE1	1:C:313:LEU:HD11	1.70	0.72
1:E:306:ASP:C	1:E:328:ILE:CG2	2.57	0.72
1:D:457:TYR:CG	1:D:457:TYR:O	2.43	0.72
1:E:92:VAL:HG22	1:E:109:VAL:HG12	1.70	0.71
1:C:424:MSE:HG3	1:C:571:VAL:CG2	2.21	0.71
1:F:51:ASN:O	1:F:366:LYS:CE	2.39	0.70
1:E:92:VAL:CG2	1:E:109:VAL:CG1	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:GLN:O	1:F:423:GLN:CG	2.39	0.70
1:E:155:ASN:OD1	1:E:155:ASN:N	2.24	0.70
1:F:483:THR:HG23	1:F:488:GLN:HE21	1.56	0.70
1:D:538:LEU:O	1:D:540:GLY:N	2.25	0.70
1:C:486:LYS:HG2	1:C:486:LYS:O	1.90	0.70
1:E:522:THR:OG1	1:E:537:THR:HB	1.91	0.69
1:F:407:ARG:HH12	1:F:473:GLU:HG3	1.57	0.69
1:E:69:ASP:HA	1:E:310:HIS:ND1	2.07	0.69
1:E:51:ASN:O	1:E:366:LYS:NZ	2.22	0.69
1:C:538:LEU:O	1:C:540:GLY:N	2.25	0.69
1:E:538:LEU:O	1:E:540:GLY:N	2.25	0.69
1:B:538:LEU:O	1:B:540:GLY:N	2.26	0.69
1:E:128:TYR:CE2	1:E:179:ASP:OD1	2.45	0.69
1:E:133:HIS:NE2	1:E:312:ASP:OD2	2.26	0.69
1:F:128:TYR:CE2	1:F:179:ASP:OD1	2.45	0.69
1:E:33:ALA:CB	1:E:571:VAL:HG21	2.22	0.69
1:F:92:VAL:HB	1:F:109:VAL:CG1	2.22	0.69
1:D:369:MSE:HE2	1:D:373:VAL:HB	1.75	0.68
1:A:538:LEU:O	1:A:540:GLY:N	2.26	0.68
1:C:455:LEU:HD23	1:C:455:LEU:O	1.94	0.67
1:E:118:PRO:HB2	1:E:407:ARG:CA	2.09	0.67
1:F:118:PRO:HB2	1:F:407:ARG:HA	1.77	0.67
1:C:130:PRO:HB3	1:C:143:MSE:CE	2.24	0.67
1:C:513:PRO:N	1:C:513:PRO:C	2.47	0.67
1:C:92:VAL:HG11	1:C:143:MSE:HE3	1.77	0.67
1:E:72:ILE:HD13	1:E:314:VAL:HG11	1.76	0.67
1:F:52:PRO:O	1:F:366:LYS:NZ	2.27	0.67
1:B:369:MSE:HE2	1:B:373:VAL:HB	1.77	0.66
1:F:109:VAL:HG23	1:F:167:TRP:CD1	2.30	0.66
1:A:101:ILE:HG21	1:A:369:MSE:HE3	1.77	0.66
1:F:51:ASN:O	1:F:366:LYS:HE2	1.95	0.66
1:E:490:LEU:CD2	1:E:514:ILE:HD13	2.26	0.66
1:E:200:LYS:O	1:E:202:LEU:HD12	1.96	0.65
1:F:200:LYS:O	1:F:202:LEU:HD12	1.96	0.65
1:E:130:PRO:HB2	1:E:143:MSE:HE3	1.79	0.65
1:F:331:ASN:ND2	1:F:335:ASN:HB2	2.10	0.65
1:D:92:VAL:HG11	1:D:143:MSE:HE3	1.79	0.65
1:F:101:ILE:HG13	1:F:369:MSE:CG	2.26	0.65
1:F:311:ALA:HA	1:F:324:VAL:O	1.97	0.65
1:B:130:PRO:HB2	1:B:143:MSE:HE3	1.79	0.65
1:C:468:ILE:HD12	1:C:478:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:PRO:HB2	1:F:143:MSE:HE3	1.79	0.65
1:F:513:PRO:O	1:F:514:ILE:HD13	1.97	0.65
1:E:118:PRO:CB	1:E:407:ARG:HA	2.09	0.64
1:F:294:GLN:HB2	1:F:306:ASP:O	1.97	0.64
1:D:130:PRO:HB3	1:D:143:MSE:CE	2.25	0.64
1:D:424:MSE:HG3	1:D:571:VAL:HG22	1.80	0.64
1:D:517:LEU:HD13	1:D:519:THR:O	1.97	0.64
1:E:56:ASN:O	1:E:369:MSE:HG3	1.98	0.64
1:C:435:GLN:HB3	1:C:436:PRO:HD2	1.79	0.64
1:F:464:LYS:HG2	1:F:482:GLN:HG2	1.80	0.63
1:E:33:ALA:HB3	1:E:571:VAL:CG2	2.28	0.63
1:E:202:LEU:HD13	1:E:207:HIS:CE1	2.34	0.63
1:F:123:ILE:HG12	1:F:472:ASN:HB3	1.80	0.63
1:F:202:LEU:HD13	1:F:207:HIS:CE1	2.34	0.63
1:F:522:THR:HB	1:F:537:THR:OG1	1.98	0.63
1:E:33:ALA:CB	1:E:571:VAL:CG2	2.76	0.63
1:E:216:ASP:OD1	1:E:218:GLU:CG	2.47	0.63
1:F:234:GLY:HA2	1:F:244:ILE:HG21	1.79	0.63
1:F:490:LEU:HD23	1:F:514:ILE:HG13	1.81	0.63
1:C:430:ASN:OD1	1:C:433:GLU:HG3	1.99	0.63
1:A:130:PRO:HB2	1:A:143:MSE:HE3	1.79	0.62
1:F:35:THR:CG2	1:F:456:SER:HB2	2.29	0.62
1:F:51:ASN:HB3	1:F:366:LYS:HE3	1.80	0.62
1:C:490:LEU:HD11	1:C:536:TYR:CD1	2.34	0.62
1:E:436:PRO:N	1:E:436:PRO:C	2.52	0.62
1:B:396:SER:O	1:B:416:ILE:CD1	2.47	0.62
1:F:483:THR:HG23	1:F:488:GLN:NE2	2.14	0.62
1:C:424:MSE:HG3	1:C:571:VAL:HG21	1.81	0.62
1:D:118:PRO:HG2	1:D:407:ARG:HA	1.82	0.62
1:E:32:PRO:CD	1:F:460:LYS:HD3	2.30	0.62
1:B:120:THR:HB	2:C:602:GOL:O2	1.99	0.61
1:E:202:LEU:HD13	1:E:207:HIS:HE1	1.65	0.61
1:F:202:LEU:HD13	1:F:207:HIS:HE1	1.65	0.61
1:E:297:PHE:O	1:E:298:LEU:HB3	2.01	0.61
1:C:461:ALA:HB1	1:C:463:GLN:HG3	1.83	0.60
1:F:57:GLU:HA	1:F:368:LYS:HA	1.83	0.60
1:C:455:LEU:CD2	1:C:521:ILE:CG2	2.78	0.60
1:C:92:VAL:CG2	1:C:143:MSE:HE3	2.31	0.60
1:D:92:VAL:CG2	1:D:143:MSE:HE3	2.30	0.60
1:D:517:LEU:CD1	1:D:519:THR:O	2.48	0.60
1:C:490:LEU:CD2	1:C:512:GLU:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ASP:HB3	1:E:310:HIS:CE1	2.37	0.60
1:F:35:THR:HG22	1:F:456:SER:HB2	1.82	0.60
1:C:315:GLU:HB2	1:C:321:TYR:CE2	2.37	0.60
1:B:62:ILE:HD13	1:B:344:MSE:HB2	1.84	0.60
1:C:518:LYS:HG2	1:C:518:LYS:O	2.02	0.60
1:D:413:PHE:CE1	1:D:414:ILE:HD12	2.36	0.60
1:F:36:PHE:CD1	1:F:455:LEU:CB	2.84	0.60
1:F:130:PRO:CB	1:F:143:MSE:HE3	2.32	0.59
1:E:216:ASP:OD1	1:E:218:GLU:HG3	2.01	0.59
1:A:369:MSE:HE2	1:A:373:VAL:HB	1.84	0.59
1:E:490:LEU:HD23	1:E:514:ILE:HG21	1.83	0.59
1:B:158:VAL:CG1	1:B:168:SER:O	2.51	0.59
1:E:239:LYS:O	1:E:239:LYS:HG2	2.01	0.59
1:A:109:VAL:HG13	1:A:167:TRP:CD1	2.38	0.59
1:A:357:GLU:HG2	1:C:288:ASN:HB2	1.85	0.59
1:E:270:SER:OG	1:E:290:PRO:CB	2.51	0.59
1:E:92:VAL:HG11	1:E:110:LEU:HG	1.84	0.59
1:B:130:PRO:CB	1:B:143:MSE:HE3	2.33	0.58
1:F:133:HIS:CG	1:F:182:LEU:HD11	2.37	0.58
1:C:413:PHE:CE1	1:C:414:ILE:HD12	2.37	0.58
1:E:92:VAL:HG13	1:E:109:VAL:HG13	1.84	0.58
1:C:495:THR:HG22	1:C:506:THR:HA	1.86	0.58
1:F:133:HIS:HB2	1:F:182:LEU:HD11	1.86	0.58
1:F:146:THR:CG2	1:F:148:PHE:CE2	2.86	0.58
1:E:138:ASN:O	1:E:139:ASP:OD1	2.21	0.58
1:B:101:ILE:HG21	1:B:369:MSE:HE3	1.84	0.58
1:C:31:VAL:O	1:C:31:VAL:HG13	2.04	0.58
1:D:109:VAL:HG13	1:D:167:TRP:CD1	2.39	0.57
1:F:133:HIS:CG	1:F:182:LEU:CD1	2.86	0.57
1:C:455:LEU:CD2	1:C:521:ILE:HG22	2.34	0.57
1:E:59:TYR:CE1	1:E:366:LYS:NZ	2.72	0.57
1:C:109:VAL:HG13	1:C:167:TRP:CD1	2.39	0.57
1:B:304:LEU:HD13	1:B:305:ALA:HB2	1.85	0.57
1:E:130:PRO:CB	1:E:143:MSE:HE3	2.34	0.57
1:A:130:PRO:CB	1:A:143:MSE:HE3	2.33	0.57
1:D:457:TYR:O	1:D:457:TYR:CD1	2.57	0.57
1:F:195:ASN:OD1	1:F:208:ARG:NH1	2.37	0.57
1:F:328:ILE:HG13	1:F:336:VAL:HG21	1.86	0.57
1:A:54:LYS:NZ	1:C:238:GLU:OE2	2.34	0.57
1:F:328:ILE:CD1	1:F:336:VAL:HG21	2.34	0.57
1:A:88:MSE:CE	1:A:566:LEU:HD21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ILE:HG12	1:D:478:VAL:HG13	1.87	0.56
1:B:158:VAL:HG12	1:B:167:TRP:HB3	1.87	0.56
1:B:109:VAL:HG13	1:B:167:TRP:CD1	2.39	0.56
1:D:70:PRO:HB3	1:D:342:THR:HG23	1.87	0.56
1:F:514:ILE:O	1:F:514:ILE:HG22	2.04	0.56
1:F:133:HIS:CB	1:F:182:LEU:HD11	2.35	0.56
1:B:158:VAL:HG13	1:B:168:SER:O	2.05	0.56
1:D:101:ILE:HD12	1:D:369:MSE:HG2	1.88	0.56
1:E:432:THR:HA	1:E:473:GLU:O	2.06	0.56
1:C:36:PHE:CE1	1:C:455:LEU:HD12	2.41	0.56
1:C:424:MSE:HG3	1:C:571:VAL:HG22	1.88	0.56
1:F:36:PHE:CD1	1:F:455:LEU:HB3	2.41	0.56
1:F:109:VAL:HG23	1:F:167:TRP:CG	2.39	0.55
1:F:92:VAL:CB	1:F:109:VAL:HG12	2.31	0.55
1:C:62:ILE:HD13	1:C:344:MSE:HE3	1.88	0.55
1:C:483:THR:HG22	1:C:488:GLN:NE2	2.20	0.55
1:F:522:THR:HB	1:F:537:THR:HG1	1.72	0.55
1:E:328:ILE:CD1	1:E:336:VAL:HG21	2.37	0.55
1:F:365:ILE:HG23	1:F:366:LYS:HG2	1.89	0.55
1:D:86:PHE:HZ	2:D:601:GOL:HO3	1.55	0.55
1:E:32:PRO:HD3	1:F:460:LYS:HD3	1.88	0.54
1:A:54:LYS:HB2	1:A:57:GLU:OE1	2.07	0.54
1:E:214:GLU:N	1:E:214:GLU:OE1	2.39	0.54
1:A:304:LEU:HD13	1:A:305:ALA:HB2	1.88	0.54
1:E:397:GLU:O	1:E:399:ILE:HD12	2.07	0.54
1:C:333:LYS:HE2	1:C:530:LEU:HD12	1.89	0.54
1:C:490:LEU:HD11	1:C:536:TYR:CE1	2.43	0.54
1:A:58:PHE:CE1	1:A:367:GLN:HB2	2.42	0.54
1:F:307:TRP:H	1:F:328:ILE:HG22	1.72	0.54
1:B:88:MSE:CE	1:B:566:LEU:HD21	2.35	0.54
1:D:464:LYS:HE2	1:D:482:GLN:OE1	2.08	0.54
1:F:268:TRP:CD2	1:F:295:ARG:HD3	2.42	0.54
1:A:432:THR:HA	1:A:473:GLU:O	2.08	0.54
1:B:54:LYS:HB2	1:B:57:GLU:OE1	2.08	0.54
1:D:101:ILE:HG21	1:D:369:MSE:HE3	1.89	0.54
1:A:62:ILE:HD13	1:A:344:MSE:HB2	1.90	0.54
1:D:54:LYS:HB2	1:D:57:GLU:OE1	2.08	0.54
1:C:517:LEU:HD12	1:C:519:THR:HG23	1.90	0.53
1:F:457:TYR:OH	1:F:483:THR:OG1	2.25	0.53
1:D:311:ALA:HA	1:D:324:VAL:O	2.09	0.53
1:E:32:PRO:HD2	1:F:460:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:THR:HA	1:B:473:GLU:O	2.09	0.53
1:C:455:LEU:HD22	1:C:521:ILE:HG23	1.90	0.53
1:E:478:VAL:HG22	1:E:480:THR:HG23	1.89	0.53
1:D:558:PHE:O	1:D:558:PHE:HD1	1.92	0.53
1:F:407:ARG:HH12	1:F:473:GLU:CG	2.20	0.53
1:A:259:MSE:CE	1:A:313:LEU:HD11	2.39	0.53
1:D:92:VAL:HG21	1:D:143:MSE:CE	2.36	0.53
1:D:414:ILE:HG12	1:D:422:LEU:HD22	1.90	0.53
1:C:414:ILE:HG12	1:C:422:LEU:HD22	1.91	0.53
1:E:91:GLY:O	1:E:92:VAL:CG1	2.57	0.52
1:F:432:THR:HA	1:F:473:GLU:O	2.09	0.52
1:E:216:ASP:OD1	1:E:218:GLU:HG2	2.09	0.52
1:F:182:LEU:CD1	1:F:184:PHE:CE2	2.88	0.52
1:F:307:TRP:H	1:F:328:ILE:HG21	1.73	0.52
1:C:40:THR:OG1	1:C:452:GLN:HG3	2.09	0.52
1:C:300:ASN:HD21	1:C:304:LEU:N	2.08	0.52
1:C:432:THR:HA	1:C:473:GLU:O	2.09	0.52
1:F:500:ARG:CD	1:F:500:ARG:H	2.23	0.52
1:D:259:MSE:CE	1:D:313:LEU:HD11	2.40	0.52
1:B:130:PRO:HA	1:B:143:MSE:HE1	1.92	0.52
1:E:109:VAL:HG23	1:E:167:TRP:CD2	2.45	0.52
1:F:36:PHE:CD1	1:F:455:LEU:HB2	2.44	0.52
1:F:53:LEU:HD23	1:F:366:LYS:CD	2.39	0.52
1:F:190:ALA:HB2	1:F:217:LEU:HD21	1.91	0.52
1:D:432:THR:HA	1:D:473:GLU:O	2.09	0.52
1:F:461:ALA:HB1	1:F:463:GLN:HG3	1.91	0.52
1:A:397:GLU:HA	1:A:416:ILE:HG13	1.92	0.51
1:E:92:VAL:CG1	1:E:110:LEU:HG	2.41	0.51
1:B:109:VAL:HG13	1:B:167:TRP:CG	2.45	0.51
1:A:130:PRO:HA	1:A:143:MSE:HE1	1.91	0.51
1:C:109:VAL:HG13	1:C:167:TRP:CG	2.45	0.51
1:D:36:PHE:CE2	1:D:569:MSE:HB2	2.46	0.51
1:D:109:VAL:HG13	1:D:167:TRP:CG	2.45	0.51
1:E:297:PHE:O	1:E:298:LEU:CB	2.58	0.51
1:E:490:LEU:HD21	1:E:514:ILE:HD13	1.91	0.51
1:A:109:VAL:HG13	1:A:167:TRP:CG	2.45	0.51
1:C:468:ILE:HG23	1:C:478:VAL:HG22	1.92	0.51
1:D:413:PHE:CE1	1:D:414:ILE:CD1	2.94	0.51
1:C:369:MSE:HE2	1:C:373:VAL:HB	1.91	0.51
1:D:464:LYS:HG2	1:D:482:GLN:HG2	1.93	0.51
1:F:51:ASN:O	1:F:366:LYS:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:PRO:HA	1:F:143:MSE:HE1	1.93	0.51
1:B:36:PHE:CE2	1:B:569:MSE:HB2	2.46	0.51
1:D:300:ASN:HD21	1:D:304:LEU:N	2.08	0.51
1:D:333:LYS:HE2	1:D:530:LEU:HD12	1.92	0.50
1:A:265:THR:O	1:A:265:THR:HG22	2.10	0.50
1:E:91:GLY:O	1:E:92:VAL:HG13	2.11	0.50
1:E:233:GLY:HA3	1:E:237:ILE:CD1	2.41	0.50
1:F:50:LYS:HD3	1:F:50:LYS:N	2.27	0.50
1:F:233:GLY:HA3	1:F:237:ILE:CD1	2.42	0.50
1:C:413:PHE:CE1	1:C:414:ILE:CD1	2.94	0.50
1:E:92:VAL:HG11	1:E:109:VAL:HG13	1.92	0.50
1:E:91:GLY:C	1:E:92:VAL:HG12	2.31	0.50
1:F:328:ILE:HG13	1:F:336:VAL:CG2	2.41	0.50
1:E:130:PRO:HA	1:E:143:MSE:HE1	1.94	0.50
1:A:478:VAL:HG12	1:A:480:THR:HG23	1.93	0.50
1:C:510:ALA:HB1	1:C:545:ILE:HD11	1.92	0.50
1:E:59:TYR:HE1	1:E:366:LYS:NZ	2.10	0.50
1:E:195:ASN:OD1	1:E:208:ARG:NH1	2.44	0.50
1:F:259:MSE:CE	1:F:313:LEU:HD11	2.39	0.50
1:F:537:THR:HG22	1:F:542:LYS:CB	2.42	0.50
1:B:396:SER:O	1:B:416:ILE:HD13	2.12	0.49
1:E:328:ILE:HG13	1:E:336:VAL:CG2	2.42	0.49
1:D:431:ILE:HD11	1:D:468:ILE:HG21	1.94	0.49
1:E:431:ILE:O	1:E:431:ILE:HG22	2.10	0.49
1:A:36:PHE:CE2	1:A:569:MSE:HB2	2.47	0.49
1:D:326:LEU:HA	1:D:341:GLU:O	2.12	0.49
1:E:61:PRO:HB3	1:E:343:PHE:CD1	2.47	0.49
1:A:431:ILE:HG22	2:A:602:GOL:H32	1.94	0.49
1:E:423:GLN:CD	1:F:460:LYS:HB3	2.33	0.49
1:B:504:PHE:CE2	1:C:225:GLY:HA3	2.47	0.49
1:C:118:PRO:O	1:C:407:ARG:HB3	2.12	0.49
1:C:326:LEU:HA	1:C:341:GLU:O	2.12	0.49
1:F:54:LYS:O	1:F:57:GLU:HB2	2.13	0.49
1:C:286:TRP:CD2	1:C:288:ASN:HB3	2.48	0.49
1:D:92:VAL:HG11	1:D:143:MSE:CE	2.42	0.49
1:E:128:TYR:CG	1:E:129:ALA:N	2.79	0.49
1:B:158:VAL:CG1	1:B:167:TRP:HB3	2.42	0.49
1:C:495:THR:CG2	1:C:506:THR:OG1	2.60	0.49
1:F:478:VAL:HG13	1:F:493:GLU:HB2	1.95	0.49
1:B:286:TRP:CD2	1:B:288:ASN:HB3	2.48	0.49
1:B:478:VAL:HG12	1:B:480:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:ILE:HG13	1:E:336:VAL:HG21	1.94	0.49
1:F:123:ILE:HG12	1:F:472:ASN:CB	2.42	0.49
1:D:397:GLU:HB3	1:D:416:ILE:HD13	1.94	0.49
1:A:286:TRP:CD2	1:A:288:ASN:HB3	2.48	0.48
1:D:481:VAL:HG13	1:D:490:LEU:HD21	1.94	0.48
1:F:326:LEU:HA	1:F:341:GLU:O	2.13	0.48
1:B:300:ASN:HD21	1:B:304:LEU:N	2.11	0.48
1:E:478:VAL:CG1	1:E:493:GLU:HB2	2.43	0.48
1:F:36:PHE:HD1	1:F:455:LEU:HB3	1.78	0.48
1:C:92:VAL:HG11	1:C:143:MSE:CE	2.41	0.48
1:D:51:ASN:HB3	1:D:366:LYS:HD2	1.94	0.48
1:D:395:LYS:HG2	1:D:420:GLY:HA3	1.95	0.48
1:E:286:TRP:CD2	1:E:288:ASN:HB3	2.48	0.48
1:F:128:TYR:CG	1:F:129:ALA:N	2.79	0.48
1:C:211:LYS:NZ	2:C:602:GOL:H2	2.29	0.48
1:C:457:TYR:C	1:C:457:TYR:CD1	2.85	0.48
1:D:394:PHE:HZ	1:D:569:MSE:HE1	1.79	0.48
1:D:489:VAL:HG11	1:D:511:LYS:HE2	1.95	0.48
1:E:140:THR:O	1:E:141:PHE:HB2	2.13	0.48
1:E:233:GLY:HA3	1:E:237:ILE:HD13	1.95	0.48
1:A:328:ILE:HD12	1:A:336:VAL:HG21	1.94	0.48
1:C:47:ILE:HG13	1:C:47:ILE:O	2.13	0.48
1:E:508:ILE:N	1:E:508:ILE:HD12	2.28	0.48
1:F:537:THR:HG22	1:F:542:LYS:HB2	1.96	0.48
1:C:92:VAL:CG1	1:C:143:MSE:HE3	2.44	0.48
1:D:286:TRP:CD2	1:D:288:ASN:HB3	2.48	0.48
1:E:128:TYR:HE2	1:E:179:ASP:OD1	1.93	0.48
1:E:290:PRO:HG3	1:E:295:ARG:HH11	1.79	0.48
1:E:326:LEU:HA	1:E:341:GLU:O	2.13	0.48
1:F:128:TYR:HE2	1:F:179:ASP:OD1	1.93	0.48
1:D:508:ILE:HD12	1:D:508:ILE:N	2.29	0.48
1:A:51:ASN:HB3	1:A:366:LYS:HD2	1.96	0.48
1:F:490:LEU:HD23	1:F:514:ILE:CG1	2.42	0.48
1:E:485:GLY:O	1:E:486:LYS:C	2.53	0.48
1:F:458:ASN:C	1:F:460:LYS:H	2.17	0.48
1:D:538:LEU:HD23	1:D:538:LEU:H	1.79	0.47
1:D:483:THR:HG22	1:D:488:GLN:HE21	1.78	0.47
1:D:558:PHE:O	1:D:558:PHE:CD1	2.67	0.47
1:F:368:LYS:HB3	1:F:368:LYS:HE2	1.53	0.47
1:C:508:ILE:N	1:C:508:ILE:HD12	2.29	0.47
1:E:306:ASP:HB3	1:E:328:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:TRP:CD2	1:F:288:ASN:HB3	2.48	0.47
1:E:259:MSE:CE	1:E:313:LEU:HD11	2.38	0.47
1:F:210:ILE:HG12	1:F:244:ILE:HD12	1.96	0.47
1:F:233:GLY:HA3	1:F:237:ILE:HD13	1.96	0.47
1:A:326:LEU:HA	1:A:341:GLU:O	2.13	0.47
1:D:481:VAL:HG13	1:D:490:LEU:CD2	2.44	0.47
1:F:468:ILE:HD11	1:F:572:PHE:CE2	2.50	0.47
1:B:326:LEU:HA	1:B:341:GLU:O	2.13	0.47
1:C:259:MSE:CE	1:C:313:LEU:HD11	2.40	0.47
1:C:395:LYS:HD3	1:C:420:GLY:HA3	1.97	0.47
1:D:70:PRO:CB	1:D:342:THR:HG23	2.45	0.47
1:B:51:ASN:HB3	1:B:366:LYS:HD2	1.96	0.47
1:E:91:GLY:C	1:E:92:VAL:CG1	2.83	0.47
1:C:311:ALA:HA	1:C:324:VAL:O	2.15	0.46
1:C:443:ARG:HA	1:C:566:LEU:HD23	1.97	0.46
1:D:424:MSE:SE	1:D:571:VAL:HG22	2.64	0.46
1:B:99:ASP:HB2	1:B:373:VAL:HG11	1.97	0.46
1:C:40:THR:OG1	1:C:452:GLN:CG	2.64	0.46
1:E:311:ALA:CA	1:E:324:VAL:O	2.62	0.46
1:B:259:MSE:CE	1:B:313:LEU:HD11	2.39	0.46
1:E:70:PRO:HB3	1:E:342:THR:HG23	1.96	0.46
1:E:431:ILE:O	1:E:431:ILE:CG2	2.59	0.46
1:D:58:PHE:CD1	1:D:369:MSE:HG2	2.51	0.46
1:C:490:LEU:CD2	1:C:512:GLU:O	2.49	0.46
1:D:413:PHE:O	1:D:424:MSE:HA	2.16	0.46
1:B:328:ILE:HD12	1:B:336:VAL:HG21	1.97	0.46
1:C:62:ILE:CD1	1:C:344:MSE:HE3	2.45	0.46
1:D:33:ALA:HB3	1:D:571:VAL:HG11	1.98	0.46
1:F:36:PHE:CZ	1:F:455:LEU:HD13	2.42	0.46
1:E:326:LEU:C	1:E:326:LEU:HD12	2.36	0.46
1:B:158:VAL:HG11	1:B:168:SER:O	2.16	0.45
1:C:326:LEU:C	1:C:326:LEU:HD12	2.37	0.45
1:A:74:ARG:HD2	1:A:79:TYR:CE1	2.52	0.45
1:F:307:TRP:CE2	1:F:328:ILE:HD12	2.51	0.45
1:D:464:LYS:HE2	1:D:482:GLN:NE2	2.31	0.45
1:A:326:LEU:HD12	1:A:326:LEU:C	2.37	0.45
1:B:74:ARG:HD2	1:B:79:TYR:CE1	2.51	0.45
1:F:328:ILE:CG1	1:F:336:VAL:HG21	2.47	0.45
1:B:158:VAL:HG12	1:B:159:LYS:N	2.32	0.45
1:A:514:ILE:HD12	1:A:517:LEU:HD13	1.98	0.45
1:C:413:PHE:O	1:C:424:MSE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:TYR:CD1	1:D:344:MSE:HE3	2.51	0.45
1:D:424:MSE:CG	1:D:571:VAL:HG22	2.45	0.45
1:E:128:TYR:HE2	1:E:178:ILE:HD12	1.70	0.45
1:F:110:LEU:HD11	1:F:156:MSE:HE1	1.99	0.45
1:F:307:TRP:CD2	1:F:328:ILE:HD12	2.52	0.45
1:F:369:MSE:HB3	1:F:370:PRO:CD	2.47	0.45
1:A:324:VAL:HG12	1:A:344:MSE:HG3	1.97	0.45
1:C:58:PHE:CD1	1:C:369:MSE:HG2	2.52	0.45
1:F:326:LEU:HD12	1:F:326:LEU:C	2.36	0.45
1:C:490:LEU:CD1	1:C:536:TYR:CD1	3.00	0.45
1:D:222:ILE:O	1:D:222:ILE:HD12	2.17	0.45
1:E:413:PHE:O	1:E:424:MSE:HA	2.17	0.45
1:F:53:LEU:HD23	1:F:366:LYS:HD3	1.98	0.45
1:F:468:ILE:HD11	1:F:572:PHE:HE2	1.82	0.44
1:D:517:LEU:C	1:D:517:LEU:HD12	2.37	0.44
1:A:538:LEU:HD12	1:A:538:LEU:HA	1.82	0.44
1:B:326:LEU:C	1:B:326:LEU:HD12	2.38	0.44
1:E:53:LEU:HD23	1:E:366:LYS:HZ2	1.81	0.44
1:F:345:LEU:HD11	1:F:363:LEU:HD21	1.99	0.44
1:D:92:VAL:CG1	1:D:143:MSE:HE3	2.46	0.44
1:E:33:ALA:CB	1:E:571:VAL:HG23	2.47	0.44
1:E:97:SER:HB3	1:E:103:TRP:CZ3	2.52	0.44
1:F:92:VAL:CG1	1:F:109:VAL:HG12	2.48	0.44
1:A:222:ILE:HD12	1:A:222:ILE:O	2.17	0.44
1:D:326:LEU:HD12	1:D:326:LEU:C	2.37	0.44
1:E:478:VAL:HG13	1:E:493:GLU:HB2	1.99	0.44
1:F:422:LEU:HD11	1:F:440:LEU:HD23	1.99	0.44
1:A:413:PHE:O	1:A:424:MSE:HA	2.17	0.44
1:B:83:ASN:C	1:B:130:PRO:HG3	2.38	0.44
1:E:222:ILE:HD12	1:E:222:ILE:O	2.18	0.44
1:F:142:TYR:HB3	1:F:182:LEU:HD21	2.00	0.44
1:A:83:ASN:C	1:A:130:PRO:HG3	2.38	0.44
1:D:58:PHE:CE1	1:D:367:GLN:HB2	2.52	0.44
1:D:83:ASN:C	1:D:130:PRO:HG3	2.38	0.44
1:F:222:ILE:O	1:F:222:ILE:HD12	2.18	0.44
1:F:233:GLY:O	1:F:244:ILE:HG12	2.18	0.44
1:A:481:VAL:HG22	1:A:490:LEU:HD21	2.00	0.44
1:B:514:ILE:HD12	1:B:517:LEU:HD13	1.98	0.44
1:F:292:LEU:HD21	1:F:325:PHE:CG	2.53	0.44
1:C:495:THR:HG22	1:C:506:THR:CA	2.48	0.44
1:B:481:VAL:HG22	1:B:490:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ILE:HG13	1:C:572:PHE:CZ	2.53	0.43
1:E:97:SER:CB	1:E:103:TRP:CE3	3.01	0.43
1:A:199:GLU:HA	1:A:199:GLU:OE1	2.18	0.43
1:C:431:ILE:HG13	1:C:572:PHE:HZ	1.83	0.43
1:D:33:ALA:HB3	1:D:571:VAL:CG1	2.48	0.43
1:D:397:GLU:CB	1:D:416:ILE:HD13	2.49	0.43
1:E:214:GLU:H	1:E:214:GLU:CD	2.19	0.43
1:E:431:ILE:O	1:E:432:THR:CG2	2.58	0.43
1:E:514:ILE:HD12	1:E:517:LEU:HD13	2.00	0.43
1:F:83:ASN:C	1:F:130:PRO:HG3	2.39	0.43
1:E:83:ASN:C	1:E:130:PRO:HG3	2.39	0.43
1:E:195:ASN:ND2	1:E:208:ARG:HD2	2.23	0.43
1:E:255:THR:HG21	1:E:275:LYS:HE2	2.01	0.43
1:F:255:THR:HG21	1:F:275:LYS:HE2	2.00	0.43
1:F:345:LEU:HD11	1:F:363:LEU:CD2	2.48	0.43
1:D:394:PHE:CZ	1:D:569:MSE:HE1	2.53	0.43
1:B:413:PHE:O	1:B:424:MSE:HA	2.18	0.43
1:C:222:ILE:HD12	1:C:222:ILE:O	2.18	0.43
1:A:322:TYR:CD2	1:A:346:PRO:HA	2.53	0.43
1:C:83:ASN:C	1:C:130:PRO:HG3	2.38	0.43
1:B:58:PHE:CE1	1:B:367:GLN:HB2	2.53	0.43
1:B:222:ILE:HD12	1:B:222:ILE:O	2.18	0.43
1:C:74:ARG:HD2	1:C:79:TYR:CE1	2.54	0.43
1:C:455:LEU:CD2	1:C:521:ILE:HG23	2.48	0.43
1:E:306:ASP:C	1:E:328:ILE:HG22	2.31	0.43
1:E:109:VAL:HG23	1:E:167:TRP:CG	2.53	0.43
1:A:101:ILE:CG2	1:A:369:MSE:HE3	2.48	0.42
1:A:521:ILE:HG13	1:A:538:LEU:HD13	2.01	0.42
1:E:109:VAL:HA	1:E:167:TRP:CE3	2.54	0.42
1:F:458:ASN:HB2	1:F:460:LYS:HD2	2.01	0.42
1:F:461:ALA:CB	1:F:463:GLN:HG3	2.49	0.42
1:A:328:ILE:HD12	1:A:336:VAL:CG2	2.49	0.42
1:D:503:ASP:OD1	1:D:503:ASP:N	2.39	0.42
1:E:426:ALA:HB2	1:E:571:VAL:CG2	2.40	0.42
1:F:35:THR:HG23	1:F:35:THR:O	2.20	0.42
1:F:394:PHE:HB2	1:F:421:GLY:N	2.34	0.42
1:B:414:ILE:HG12	1:B:422:LEU:HD22	2.01	0.42
1:C:211:LYS:HZ3	2:C:602:GOL:H2	1.85	0.42
1:E:307:TRP:CD2	1:E:328:ILE:HD12	2.55	0.42
1:A:143:MSE:HE1	1:A:145:THR:HB	2.02	0.42
1:A:179:ASP:N	1:A:180:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ASP:N	1:B:180:PRO:CD	2.83	0.42
1:D:558:PHE:CD1	1:D:558:PHE:C	2.93	0.42
1:E:490:LEU:HD23	1:E:514:ILE:CG2	2.49	0.42
1:F:292:LEU:HD21	1:F:325:PHE:CD2	2.54	0.42
1:F:499:GLN:HG3	1:F:500:ARG:NE	2.34	0.42
1:C:58:PHE:CE1	1:C:367:GLN:HB2	2.55	0.42
1:D:123:ILE:HG12	1:D:472:ASN:HB3	2.00	0.42
1:E:290:PRO:HG3	1:E:295:ARG:NH1	2.35	0.42
1:F:490:LEU:HD13	1:F:490:LEU:HA	1.92	0.42
1:E:307:TRP:CE2	1:E:328:ILE:HD12	2.54	0.42
1:A:414:ILE:HG12	1:A:422:LEU:HD22	2.02	0.41
1:B:481:VAL:HG22	1:B:490:LEU:CD2	2.50	0.41
1:C:57:GLU:OE1	1:C:366:LYS:HE3	2.20	0.41
1:C:422:LEU:HD11	1:C:440:LEU:HD23	2.02	0.41
1:E:286:TRP:CE2	1:E:288:ASN:HB3	2.55	0.41
1:F:192:LEU:C	1:F:192:LEU:HD23	2.41	0.41
1:D:286:TRP:CE2	1:D:288:ASN:HB3	2.56	0.41
1:F:60:SER:O	1:F:365:ILE:HD12	2.20	0.41
1:B:213:TRP:CZ3	1:B:227:ASP:HB3	2.55	0.41
1:B:538:LEU:HA	1:B:538:LEU:HD23	1.74	0.41
1:C:33:ALA:HB3	1:C:571:VAL:HG11	2.01	0.41
1:C:179:ASP:N	1:C:180:PRO:CD	2.84	0.41
1:C:286:TRP:CE2	1:C:288:ASN:HB3	2.56	0.41
1:D:486:LYS:HD2	1:D:486:LYS:O	2.20	0.41
1:E:196:ASP:O	1:E:208:ARG:HD3	2.20	0.41
1:F:143:MSE:HE1	1:F:145:THR:HB	2.03	0.41
1:F:393:ASP:O	1:F:421:GLY:N	2.53	0.41
1:A:368:LYS:CE	1:C:287:ASN:OD1	2.69	0.41
1:A:481:VAL:HG22	1:A:490:LEU:CD2	2.50	0.41
1:D:74:ARG:HD2	1:D:79:TYR:CE1	2.56	0.41
1:D:307:TRP:CD2	1:D:328:ILE:HD13	2.56	0.41
1:D:422:LEU:HD11	1:D:440:LEU:HD23	2.01	0.41
1:E:345:LEU:HD23	1:E:345:LEU:HA	1.86	0.41
1:B:422:LEU:HD11	1:B:440:LEU:HD23	2.02	0.41
1:D:179:ASP:N	1:D:180:PRO:CD	2.84	0.41
1:E:128:TYR:CD2	1:E:179:ASP:OD1	2.74	0.41
1:E:435:GLN:HB3	1:E:436:PRO:HD2	2.02	0.41
1:F:286:TRP:CE2	1:F:288:ASN:HB3	2.55	0.41
1:A:286:TRP:CE2	1:A:288:ASN:HB3	2.56	0.41
1:B:286:TRP:CE2	1:B:288:ASN:HB3	2.56	0.41
1:B:324:VAL:HG12	1:B:344:MSE:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:VAL:HG21	1:C:143:MSE:CE	2.38	0.41
1:C:192:LEU:C	1:C:192:LEU:HD23	2.41	0.41
1:E:92:VAL:CG2	1:E:109:VAL:HG13	2.46	0.41
1:E:97:SER:HB2	1:E:103:TRP:CD2	2.56	0.41
1:C:307:TRP:CD2	1:C:328:ILE:HD13	2.56	0.41
1:C:455:LEU:HD23	1:C:455:LEU:C	2.41	0.41
1:D:192:LEU:HD23	1:D:192:LEU:C	2.41	0.41
1:E:143:MSE:HE1	1:E:145:THR:HB	2.03	0.41
1:E:192:LEU:C	1:E:192:LEU:HD23	2.41	0.41
1:F:128:TYR:HE2	1:F:178:ILE:HD12	1.71	0.41
1:A:516:LYS:O	1:A:518:LYS:HG3	2.21	0.41
1:E:100:LEU:HD22	1:E:344:MSE:HE1	2.02	0.41
1:E:499:GLN:HG2	1:E:560:GLY:CA	2.51	0.40
1:F:92:VAL:CG2	1:F:127:ILE:HG21	2.51	0.40
1:C:118:PRO:HG2	1:C:407:ARG:HA	2.04	0.40
1:D:468:ILE:HG23	1:D:478:VAL:HG22	2.02	0.40
1:E:97:SER:HB2	1:E:103:TRP:CE3	2.57	0.40
1:F:118:PRO:CB	1:F:407:ARG:HA	2.49	0.40
1:B:194:HIS:ND1	1:B:195:ASN:O	2.54	0.40
1:C:123:ILE:HG12	1:C:472:ASN:HB3	2.03	0.40
1:C:336:VAL:HG12	1:C:557:ASN:OD1	2.22	0.40
1:F:92:VAL:CG1	1:F:109:VAL:CG1	3.00	0.40
1:F:133:HIS:CG	1:F:182:LEU:HD12	2.57	0.40
1:F:478:VAL:HG22	1:F:480:THR:HG23	2.02	0.40
1:A:422:LEU:HD11	1:A:440:LEU:HD23	2.02	0.40
1:B:328:ILE:HD12	1:B:336:VAL:CG2	2.51	0.40
1:E:179:ASP:N	1:E:180:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	529/567 (93%)	498 (94%)	28 (5%)	3 (1%)	25	40
1	B	529/567 (93%)	497 (94%)	30 (6%)	2 (0%)	34	52
1	C	530/567 (94%)	500 (94%)	26 (5%)	4 (1%)	19	33
1	D	528/567 (93%)	489 (93%)	31 (6%)	8 (2%)	10	16
1	E	465/567 (82%)	425 (91%)	34 (7%)	6 (1%)	12	19
1	F	473/567 (83%)	438 (93%)	28 (6%)	7 (2%)	10	16
All	All	3054/3402 (90%)	2847 (93%)	177 (6%)	30 (1%)	15	26

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	539	ASN
1	B	539	ASN
1	C	539	ASN
1	D	395	LYS
1	D	458	ASN
1	D	539	ASN
1	E	432	THR
1	E	539	ASN
1	F	517	LEU
1	D	393	ASP
1	D	559	ALA
1	E	485	GLY
1	F	172	ASN
1	F	538	LEU
1	A	458	ASN
1	B	458	ASN
1	D	396	SER
1	E	86	PHE
1	C	31	VAL
1	D	407	ARG
1	E	458	ASN
1	F	149	CYS
1	C	66	CYS
1	C	461	ALA
1	D	66	CYS
1	E	511	LYS
1	F	162	ASP
1	F	365	ILE
1	F	66	CYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	455/470 (97%)	440 (97%)	15 (3%)	38	61
1	B	455/470 (97%)	442 (97%)	13 (3%)	42	66
1	C	456/470 (97%)	441 (97%)	15 (3%)	38	61
1	D	454/470 (97%)	436 (96%)	18 (4%)	31	53
1	E	425/470 (90%)	388 (91%)	37 (9%)	10	18
1	F	426/470 (91%)	400 (94%)	26 (6%)	18	34
All	All	2671/2820 (95%)	2547 (95%)	124 (5%)	27	47

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	143	MSE
1	A	156	MSE
1	A	195	ASN
1	A	219	LYS
1	A	304	LEU
1	A	306	ASP
1	A	315	GLU
1	A	368	LYS
1	A	371	LYS
1	A	379	LYS
1	A	414	ILE
1	A	455	LEU
1	A	538	LEU
1	A	569	MSE
1	B	143	MSE
1	B	156	MSE
1	B	195	ASN
1	B	218	GLU
1	B	304	LEU
1	B	315	GLU
1	B	368	LYS

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Mol	Chain	Res	Type
1	B	371	LYS
1	B	414	ILE
1	B	455	LEU
1	B	502	LYS
1	B	505	LYS
1	B	569	MSE
1	C	51	ASN
1	C	143	MSE
1	C	156	MSE
1	C	195	ASN
1	C	306	ASP
1	C	414	ILE
1	C	416	ILE
1	C	431	ILE
1	C	455	LEU
1	C	460	LYS
1	C	486	LYS
1	C	517	LEU
1	C	519	THR
1	C	569	MSE
1	C	571	VAL
1	D	143	MSE
1	D	156	MSE
1	D	195	ASN
1	D	306	ASP
1	D	315	GLU
1	D	324	VAL
1	D	379	LYS
1	D	395	LYS
1	D	399	ILE
1	D	407	ARG
1	D	414	ILE
1	D	455	LEU
1	D	481	VAL
1	D	486	LYS
1	D	517	LEU
1	D	557	ASN
1	D	569	MSE
1	D	571	VAL
1	E	44	GLU
1	E	50	LYS
1	E	88	MSE

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Mol	Chain	Res	Type
1	E	109	VAL
1	E	123	ILE
1	E	143	MSE
1	E	149	CYS
1	E	155	ASN
1	E	156	MSE
1	E	195	ASN
1	E	214	GLU
1	E	217	LEU
1	E	219	LYS
1	E	229	VAL
1	E	239	LYS
1	E	275	LYS
1	E	278	ASN
1	E	295	ARG
1	E	306	ASP
1	E	312	ASP
1	E	324	VAL
1	E	328	ILE
1	E	331	ASN
1	E	345	LEU
1	E	364	SER
1	E	369	MSE
1	E	407	ARG
1	E	414	ILE
1	E	422	LEU
1	E	437	ILE
1	E	452	GLN
1	E	455	LEU
1	E	467	LEU
1	E	518	LYS
1	E	531	ASN
1	E	538	LEU
1	E	569	MSE
1	F	50	LYS
1	F	121	CYS
1	F	143	MSE
1	F	149	CYS
1	F	156	MSE
1	F	195	ASN
1	F	275	LYS
1	F	278	ASN

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Mol	Chain	Res	Type
1	F	306	ASP
1	F	328	ILE
1	F	344	MSE
1	F	368	LYS
1	F	369	MSE
1	F	423	GLN
1	F	431	ILE
1	F	437	ILE
1	F	455	LEU
1	F	458	ASN
1	F	460	LYS
1	F	473	GLU
1	F	499	GLN
1	F	500	ARG
1	F	517	LEU
1	F	531	ASN
1	F	556	THR
1	F	569	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	488	GLN
1	C	488	GLN
1	D	488	GLN
1	E	488	GLN
1	F	488	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

10 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	601	-	5,5,5	0.10	0	5,5,5	0.28	0
2	GOL	D	602	-	5,5,5	0.11	0	5,5,5	0.37	0
2	GOL	F	601	-	5,5,5	0.10	0	5,5,5	0.27	0
2	GOL	B	602	-	5,5,5	0.12	0	5,5,5	0.36	0
2	GOL	A	603	-	5,5,5	0.09	0	5,5,5	0.26	0
2	GOL	D	601	-	5,5,5	0.10	0	5,5,5	0.33	0
2	GOL	B	601	-	5,5,5	0.13	0	5,5,5	0.40	0
2	GOL	C	601	-	5,5,5	0.11	0	5,5,5	0.34	0
2	GOL	A	602	-	5,5,5	0.09	0	5,5,5	0.30	0
2	GOL	C	602	-	5,5,5	0.16	0	5,5,5	0.38	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	601	-	-	1/4/4/4	-
2	GOL	D	602	-	-	3/4/4/4	-
2	GOL	F	601	-	-	0/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	A	603	-	-	3/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	C	602	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	GOL	C1-C2-C3-O3
2	D	601	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-O2
2	A	602	GOL	C1-C2-C3-O3
2	A	603	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	D	602	GOL	O1-C1-C2-C3
2	C	601	GOL	O2-C2-C3-O3
2	D	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O2-C2-C3-O3
2	B	602	GOL	O1-C1-C2-O2
2	C	602	GOL	O1-C1-C2-O2
2	D	602	GOL	O2-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
2	A	603	GOL	O1-C1-C2-O2
2	A	601	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-C3
2	A	603	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	GOL	1	0
2	A	602	GOL	1	0
2	C	602	GOL	3	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	526/567 (92%)	-0.02	0 100 100	41, 58, 83, 112	0
1	B	526/567 (92%)	-0.01	0 100 100	41, 58, 85, 115	0
1	C	527/567 (92%)	0.14	9 (1%) 70 71	45, 74, 120, 155	0
1	D	525/567 (92%)	0.08	13 (2%) 57 59	44, 75, 121, 167	0
1	E	488/567 (86%)	1.30	116 (23%) 0 0	101, 118, 147, 190	0
1	F	490/567 (86%)	1.39	130 (26%) 0 0	102, 118, 151, 178	0
All	All	3082/3402 (90%)	0.46	268 (8%) 10 9	41, 77, 136, 190	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	500	ARG	9.4
1	E	133	HIS	7.6
1	E	255	THR	7.6
1	F	539	ASN	7.5
1	E	539	ASN	6.8
1	F	553	VAL	6.5
1	F	307	TRP	6.4
1	F	137	TYR	6.2
1	E	517	LEU	6.2
1	F	440	LEU	6.1
1	F	538	LEU	6.1
1	F	557	ASN	5.9
1	E	132	ILE	5.8
1	F	517	LEU	5.8
1	F	447	ILE	5.7
1	F	305	ALA	5.5
1	F	219	LYS	5.5
1	E	421	GLY	5.4
1	F	68	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	102	ASN	5.3
1	F	323	GLY	5.2
1	F	396	SER	5.2
1	F	401	TYR	5.2
1	F	123	ILE	5.2
1	F	149	CYS	5.1
1	F	135	ASN	5.1
1	E	516	LYS	5.1
1	E	182	LEU	5.0
1	F	255	THR	5.0
1	C	521	ILE	4.9
1	F	141	PHE	4.9
1	E	447	ILE	4.8
1	E	131	ALA	4.8
1	F	332	SER	4.8
1	F	514	ILE	4.7
1	F	184	PHE	4.7
1	E	420	GLY	4.6
1	F	541	GLU	4.6
1	F	153	GLY	4.6
1	E	412	ASN	4.6
1	F	395	LYS	4.6
1	C	545	ILE	4.6
1	E	485	GLY	4.4
1	F	513	PRO	4.4
1	E	538	LEU	4.3
1	E	91	GLY	4.3
1	F	182	LEU	4.3
1	F	237	ILE	4.2
1	E	254	GLY	4.2
1	E	501	GLN	4.2
1	F	331	ASN	4.2
1	F	65	GLY	4.1
1	F	254	GLY	4.1
1	F	283	TYR	4.1
1	F	213	TRP	4.1
1	E	238	GLU	4.1
1	E	217	LEU	4.1
1	F	324	VAL	4.1
1	E	235	THR	4.0
1	F	322	TYR	4.0
1	D	510	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	522	THR	4.0
1	E	219	LYS	4.0
1	C	539	ASN	3.9
1	E	450	THR	3.9
1	F	496	VAL	3.9
1	F	243	TRP	3.9
1	E	205	PRO	3.9
1	E	368	LYS	3.9
1	D	572	PHE	3.8
1	D	380	ASP	3.8
1	E	171	PHE	3.8
1	E	279	ILE	3.8
1	E	388	PHE	3.7
1	E	84	SER	3.7
1	E	65	GLY	3.7
1	E	322	TYR	3.7
1	E	184	PHE	3.7
1	E	313	LEU	3.7
1	F	516	LYS	3.6
1	F	55	PRO	3.6
1	D	41	TYR	3.6
1	F	150	ALA	3.6
1	D	539	ASN	3.6
1	F	53	LEU	3.6
1	F	321	TYR	3.6
1	F	390	TYR	3.6
1	E	526	THR	3.6
1	E	540	GLY	3.6
1	F	39	PHE	3.5
1	E	56	ASN	3.5
1	E	323	GLY	3.5
1	F	367	GLN	3.5
1	F	257	TYR	3.5
1	E	261	ALA	3.5
1	F	250	TYR	3.5
1	E	95	PHE	3.5
1	F	276	ALA	3.5
1	E	440	LEU	3.5
1	D	500	ARG	3.5
1	E	223	ILE	3.4
1	E	222	ILE	3.4
1	F	348	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	64	GLN	3.4
1	F	171	PHE	3.4
1	E	257	TYR	3.4
1	F	238	GLU	3.4
1	F	450	THR	3.3
1	E	513	PRO	3.3
1	F	136	LYS	3.3
1	F	368	LYS	3.3
1	D	538	LEU	3.3
1	F	273	ILE	3.3
1	E	475	CYS	3.3
1	E	571	VAL	3.3
1	C	455	LEU	3.3
1	F	500	ARG	3.3
1	F	490	LEU	3.3
1	F	413	PHE	3.3
1	E	395	LYS	3.2
1	F	306	ASP	3.2
1	F	437	ILE	3.2
1	F	521	ILE	3.2
1	F	461	ALA	3.2
1	E	141	PHE	3.2
1	F	555	SER	3.2
1	E	90	PRO	3.2
1	C	518	LYS	3.2
1	E	47	ILE	3.1
1	F	388	PHE	3.1
1	F	80	TYR	3.1
1	F	35	THR	3.1
1	E	476	ASN	3.1
1	E	35	THR	3.1
1	E	332	SER	3.0
1	F	282	PRO	3.0
1	E	278	ASN	3.0
1	E	221	GLN	3.0
1	E	55	PRO	3.0
1	F	278	ASN	3.0
1	C	465	ALA	3.0
1	E	531	ASN	3.0
1	E	85	SER	3.0
1	E	80	TYR	3.0
1	E	153	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	53	LEU	2.9
1	F	91	GLY	2.9
1	E	511	LYS	2.9
1	E	92	VAL	2.9
1	E	120	THR	2.9
1	F	343	PHE	2.9
1	C	509	VAL	2.9
1	F	547	GLY	2.9
1	E	465	ALA	2.9
1	E	448	LYS	2.9
1	F	530	LEU	2.9
1	E	166	GLY	2.8
1	E	553	VAL	2.8
1	E	89	PHE	2.8
1	F	133	HIS	2.8
1	E	136	LYS	2.8
1	F	548	PRO	2.8
1	F	218	GLU	2.8
1	F	459	THR	2.8
1	E	363	LEU	2.8
1	F	313	LEU	2.7
1	E	236	ASP	2.7
1	D	164	ARG	2.7
1	E	215	TYR	2.7
1	F	402	ARG	2.7
1	E	426	ALA	2.7
1	E	283	TYR	2.7
1	F	434	VAL	2.6
1	F	439	ALA	2.6
1	C	490	LEU	2.6
1	E	137	TYR	2.6
1	E	277	ASP	2.6
1	E	112	ARG	2.6
1	F	329	ARG	2.6
1	F	183	PHE	2.6
1	E	187	ASN	2.6
1	E	547	GLY	2.6
1	F	90	PRO	2.5
1	F	116	LEU	2.5
1	F	231	VAL	2.5
1	F	546	GLY	2.5
1	E	167	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	48	TYR	2.5
1	F	457	TYR	2.5
1	E	282	PRO	2.5
1	E	442	HIS	2.5
1	E	560	GLY	2.5
1	E	479	LEU	2.5
1	F	59	TYR	2.5
1	E	186	ASP	2.4
1	F	362	PRO	2.4
1	C	49	ALA	2.4
1	F	483	THR	2.4
1	F	41	TYR	2.4
1	E	307	TRP	2.4
1	F	161	LYS	2.4
1	E	338	THR	2.4
1	E	402	ARG	2.4
1	F	118	PRO	2.4
1	F	338	THR	2.4
1	F	186	ASP	2.4
1	E	281	GLY	2.4
1	F	96	HIS	2.4
1	F	199	GLU	2.4
1	E	190	ALA	2.4
1	F	511	LYS	2.4
1	F	94	ILE	2.4
1	F	125	ALA	2.4
1	E	116	LEU	2.4
1	F	264	GLY	2.3
1	F	485	GLY	2.3
1	F	169	ASP	2.3
1	F	510	ALA	2.3
1	F	476	ASN	2.3
1	E	353	TRP	2.3
1	F	167	TRP	2.3
1	D	481	VAL	2.3
1	D	39	PHE	2.3
1	E	129	ALA	2.3
1	E	250	TYR	2.3
1	E	364	SER	2.3
1	F	422	LEU	2.3
1	E	158	VAL	2.3
1	E	350	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	197	ALA	2.3
1	F	391	SER	2.3
1	E	169	ASP	2.3
1	F	470	TYR	2.3
1	E	427	LEU	2.3
1	F	202	LEU	2.3
1	D	418	LYS	2.2
1	F	193	VAL	2.2
1	F	275	LYS	2.2
1	F	122	GLY	2.2
1	F	159	LYS	2.2
1	F	113	THR	2.2
1	E	213	TRP	2.2
1	E	541	GLU	2.2
1	E	457	TYR	2.2
1	E	470	TYR	2.2
1	E	451	ALA	2.2
1	D	517	LEU	2.2
1	E	253	ASN	2.2
1	D	514	ILE	2.2
1	F	222	ILE	2.2
1	F	235	THR	2.2
1	E	314	VAL	2.2
1	F	220	ASP	2.2
1	E	340	ARG	2.2
1	E	459	THR	2.1
1	F	234	GLY	2.1
1	E	514	ILE	2.1
1	E	63	LEU	2.1
1	E	437	ILE	2.1
1	F	253	ASN	2.1
1	F	256	TYR	2.1
1	E	471	GLN	2.1
1	F	551	ALA	2.1
1	E	33	ALA	2.0
1	F	75	LYS	2.0
1	F	501	GLN	2.0
1	E	468	ILE	2.0
1	E	416	ILE	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 monosaccharides 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	F	601	6/6	0.82	0.12	74,86,91,92	0
2	GOL	B	602	6/6	0.90	0.14	71,75,80,82	0
2	GOL	B	601	6/6	0.90	0.24	51,61,64,69	0
2	GOL	A	602	6/6	0.91	0.17	71,79,86,91	0
2	GOL	C	602	6/6	0.92	0.16	50,52,63,68	0
2	GOL	A	603	6/6	0.93	0.18	59,70,74,74	0
2	GOL	D	601	6/6	0.94	0.20	51,57,61,68	0
2	GOL	C	601	6/6	0.94	0.21	59,62,66,75	0
2	GOL	D	602	6/6	0.95	0.18	40,52,58,60	0
2	GOL	A	601	6/6	0.97	0.13	45,51,55,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.