



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:56 AM UTC

PDB ID : 1RU3 / pdb_00001ru3
Title : Crystal Structure of the monomeric acetyl-CoA synthase from *Carboxydothermus hydrogenoformans*
Authors : Svetlitchnyi, V.; Dobbek, H.; Meyer-Klaucke, W.; Meins, T.; Thiele, B.; Rmer, P.; Huber, R.; Meyer, O.
Deposited on : 2003-12-11
Resolution : 2.20 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

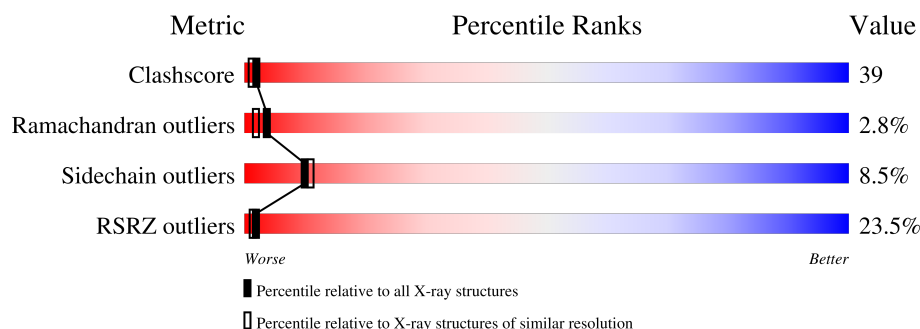
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	732	

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
4	GOL	A	959	-	X	-	-
4	GOL	A	960	-	X	-	-
4	GOL	A	961	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	962	-	X	-	-
4	GOL	A	963	-	X	-	-
4	GOL	A	964	-	X	-	-
4	GOL	A	965	-	X	-	-
4	GOL	A	966	-	X	-	-
4	GOL	A	967	-	X	-	-
4	GOL	A	968	-	X	-	-
4	GOL	A	969	-	X	-	-
4	GOL	A	970	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6064 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.

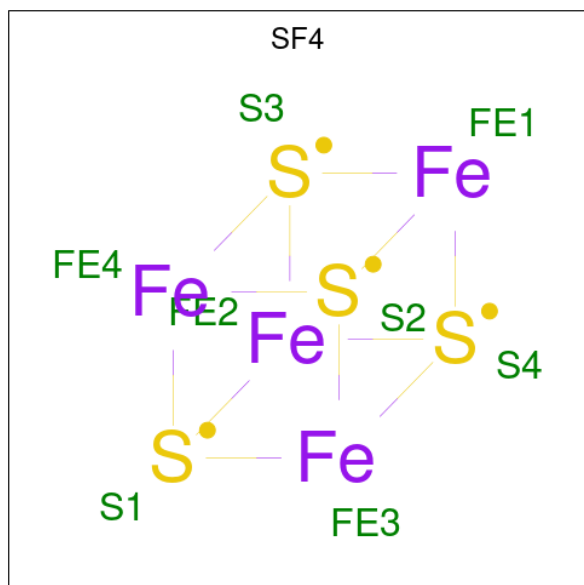
- Molecule 1 is a protein called Acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5759	3697	964	1069	29			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ni	0	0
			2	2		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

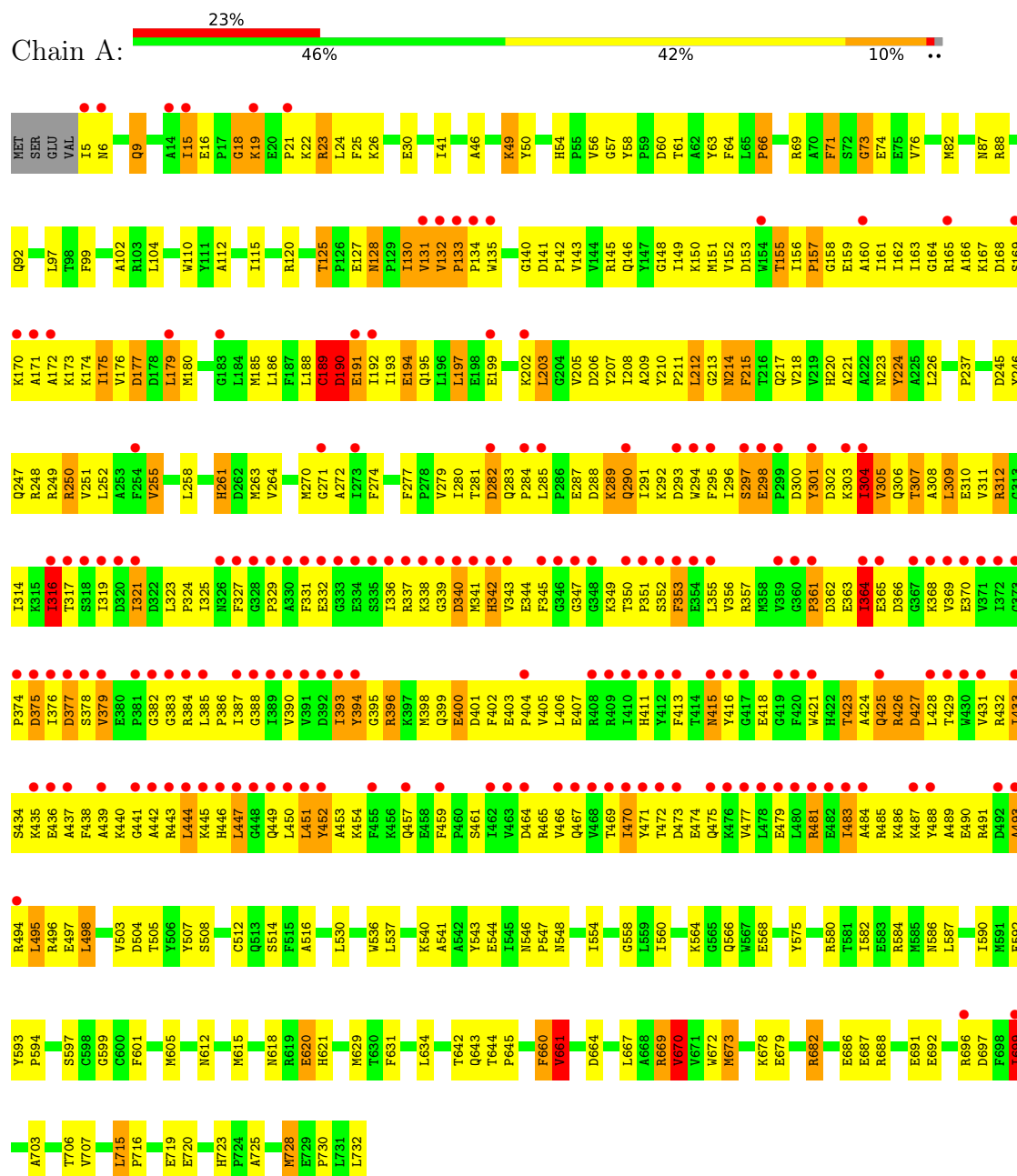
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total 223	O 223	0	0

3 Residue-property plots [i](#)

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: Acetyl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	200.31 Å 200.31 Å 169.41 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.20) 98.7 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.19 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.274 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: NI, SF4, 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	1.00	12/5893 (0.2%)	1.35	71/7978 (0.9%)

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	A	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	728	MET	SD-CE	-10.10	1.54	1.79
1	A	190	ASP	CA-C	-9.29	1.40	1.52
1	A	189	CYS	CA-C	-8.15	1.43	1.52
1	A	41	ILE	CA-CB	8.08	1.64	1.54
1	A	673	MET	SD-CE	-7.12	1.61	1.79
1	A	190	ASP	CA-CB	6.52	1.64	1.53
1	A	593	TYR	CA-C	-6.09	1.49	1.53
1	A	593	TYR	CA-CB	5.92	1.57	1.52
1	A	593	TYR	C-O	-5.58	1.21	1.23
1	A	670	VAL	CA-CB	5.37	1.60	1.54
1	A	516	ALA	CA-CB	5.19	1.60	1.53
1	A	112	ALA	CA-CB	5.13	1.61	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	CYS	CA-C-N	10.77	142.11	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	CYS	C-N-CA	10.77	142.11	121.54
1	A	214	ASN	N-CA-C	10.74	126.86	114.62
1	A	189	CYS	O-C-N	10.74	136.25	123.36
1	A	156	ILE	CA-C-N	9.44	129.19	119.56
1	A	156	ILE	C-N-CA	9.44	129.19	119.56
1	A	289	LYS	N-CA-C	-8.94	99.72	110.44
1	A	73	GLY	N-CA-C	8.85	125.61	115.08
1	A	63	TYR	N-CA-C	8.84	122.56	112.57
1	A	140	GLY	N-CA-C	8.81	122.02	112.33
1	A	490	GLU	N-CA-C	-8.54	102.99	113.50
1	A	191	GLU	N-CA-C	8.48	120.52	111.28
1	A	179	LEU	N-CA-C	-7.92	101.60	111.11
1	A	155	THR	N-CA-C	-7.56	102.73	110.97
1	A	481	ARG	N-CA-C	-7.39	104.11	113.72
1	A	281	THR	N-CA-C	7.13	121.66	110.17
1	A	516	ALA	CA-C-N	6.97	127.27	119.32
1	A	516	ALA	C-N-CA	6.97	127.27	119.32
1	A	190	ASP	N-CA-C	6.91	125.51	110.80
1	A	224	TYR	N-CA-C	-6.88	103.00	111.40
1	A	128	ASN	CA-C-N	6.87	126.84	119.76
1	A	128	ASN	C-N-CA	6.87	126.84	119.76
1	A	379	VAL	N-CA-C	6.83	117.30	107.88
1	A	661	VAL	N-CA-CB	-6.82	99.97	111.23
1	A	157	PRO	N-CA-C	6.72	122.58	113.84
1	A	697	ASP	N-CA-C	6.65	120.38	112.93
1	A	214	ASN	CA-C-N	-6.54	109.04	121.54
1	A	214	ASN	C-N-CA	-6.54	109.04	121.54
1	A	400	GLU	N-CA-C	-6.48	104.22	111.28
1	A	340	ASP	N-CA-C	-6.31	107.42	114.62
1	A	615	MET	N-CA-C	-6.29	99.96	109.95
1	A	312	ARG	N-CA-C	-6.28	104.06	111.03
1	A	382	GLY	N-CA-C	-6.25	104.13	114.76
1	A	125	THR	N-CA-C	-6.21	101.04	108.25
1	A	707	VAL	N-CA-C	-6.19	104.81	110.82
1	A	221	ALA	N-CA-C	-6.19	103.85	112.45
1	A	342	HIS	N-CA-C	-6.18	103.26	111.24
1	A	250	ARG	CA-C-N	-6.09	114.95	122.93
1	A	250	ARG	C-N-CA	-6.09	114.95	122.93
1	A	146	GLN	N-CA-C	6.08	117.58	111.07
1	A	363	GLU	N-CA-C	6.04	119.70	112.93
1	A	130	ILE	N-CA-C	5.97	117.00	111.45
1	A	447	LEU	N-CA-C	-5.96	104.91	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	CYS	N-CA-C	5.94	117.82	107.49
1	A	261	HIS	N-CA-C	5.91	118.76	109.96
1	A	218	VAL	N-CA-C	-5.91	104.29	112.50
1	A	290	GLN	N-CA-C	5.88	118.05	108.76
1	A	190	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	669	ARG	CA-C-N	-5.79	115.14	122.37
1	A	669	ARG	C-N-CA	-5.79	115.14	122.37
1	A	485	ARG	N-CA-C	-5.75	105.37	112.38
1	A	175	ILE	N-CA-C	5.65	115.84	110.42
1	A	284	PRO	N-CA-C	-5.63	101.38	110.55
1	A	699	ILE	CB-CA-C	-5.62	103.84	112.05
1	A	49	LYS	N-CA-C	5.57	118.55	111.69
1	A	210	TYR	N-CA-C	5.46	119.29	108.59
1	A	156	ILE	N-CA-C	-5.46	97.09	108.88
1	A	271	GLY	N-CA-C	-5.41	106.13	113.37
1	A	58	TYR	CA-C-N	-5.38	113.73	120.51
1	A	58	TYR	C-N-CA	-5.38	113.73	120.51
1	A	316	ILE	N-CA-C	5.30	114.84	108.06
1	A	71	PHE	N-CA-C	5.20	117.86	111.82
1	A	543	TYR	N-CA-C	-5.16	105.56	111.14
1	A	215	PHE	N-CA-C	-5.16	99.81	110.80
1	A	593	TYR	CB-CA-C	-5.16	105.86	110.71
1	A	493	ALA	N-CA-C	-5.13	105.33	111.03
1	A	46	ALA	N-CA-C	-5.13	105.69	111.28
1	A	66	PRO	N-CA-C	5.09	122.95	112.47
1	A	214	ASN	CB-CA-C	-5.07	102.53	109.28
1	A	706	THR	N-CA-C	-5.05	106.63	112.89
1	A	364	ILE	N-CA-C	5.03	115.51	108.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	CYS	Mainchain
1	A	394	TYR	Sidechain

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	5759	0	5735	445	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	72	0	48	8	0
5	A	223	0	0	6	0
All	All	6064	0	5783	448	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 39.

All (448) 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)
4:A:966:GOL:C1	4:A:966:GOL:O1	1.65	1.42
1:A:351:PRO:HG2	1:A:386:PRO:HB3	1.23	1.19
1:A:22:LYS:HE2	1:A:97:LEU:HD12	1.34	1.09
1:A:725:ALA:HA	1:A:728:MET:HE3	1.35	1.08
1:A:163:ILE:HA	1:A:189:CYS:O	1.58	1.03
1:A:385:LEU:HD12	1:A:386:PRO:HD2	1.38	1.01
1:A:132:VAL:HG22	1:A:133:PRO:HD2	1.45	0.99
1:A:723:HIS:HD2	1:A:725:ALA:H	1.11	0.94
1:A:566:GLN:HE22	1:A:584:ARG:HE	1.17	0.91
1:A:173:LYS:O	1:A:177:ASP:HB2	1.70	0.91
1:A:151:MET:HE1	1:A:224:TYR:CE1	2.06	0.91
1:A:192:ILE:HD11	1:A:258:LEU:HD12	1.52	0.90
1:A:102:ALA:HB1	1:A:270:MET:HE2	1.53	0.90
1:A:22:LYS:CE	1:A:97:LEU:HD12	2.02	0.89
1:A:151:MET:HE1	1:A:224:TYR:HE1	1.37	0.89
1:A:386:PRO:O	1:A:472:THR:HA	1.71	0.88
1:A:356:VAL:HG13	1:A:393:ILE:HD11	1.56	0.87
1:A:444:LEU:HD12	1:A:470:ILE:HG21	1.54	0.87
1:A:350:THR:HG21	1:A:384:ARG:HB3	1.57	0.87
1:A:723:HIS:CD2	1:A:725:ALA:H	1.93	0.85
1:A:247:GLN:O	1:A:251:VAL:HG22	1.77	0.84
1:A:321:ILE:CG2	1:A:453:ALA:HB2	2.07	0.83
1:A:134:PRO:HD2	1:A:135:TRP:CE3	2.14	0.83
1:A:331:PHE:HB2	1:A:416:TYR:O	1.77	0.82
1:A:351:PRO:CG	1:A:386:PRO:HB3	2.06	0.82
1:A:351:PRO:HG2	1:A:386:PRO:CB	2.07	0.82
1:A:165:ARG:HB3	1:A:191:GLU:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:HB3	5:A:886:HOH:O	1.80	0.81
1:A:179:LEU:HD22	1:A:186:LEU:HD21	1.62	0.81
1:A:376:ILE:HG21	1:A:442:ALA:O	1.81	0.80
1:A:171:ALA:HB1	1:A:301:TYR:CE2	2.18	0.79
1:A:483:ILE:O	1:A:486:LYS:HB3	1.83	0.79
1:A:171:ALA:HB1	1:A:301:TYR:CD2	2.18	0.78
1:A:376:ILE:HG22	1:A:443:ARG:HD3	1.66	0.78
1:A:120:ARG:HH22	1:A:217:GLN:NE2	1.81	0.77
1:A:280:ILE:HD13	1:A:308:ALA:HA	1.66	0.77
1:A:424:ALA:HB3	1:A:429:THR:HA	1.65	0.77
1:A:205:VAL:HG23	1:A:206:ASP:H	1.49	0.77
1:A:446:HIS:O	1:A:450:LEU:HD13	1.86	0.75
1:A:150:LYS:HD2	1:A:155:THR:HG21	1.69	0.74
1:A:203:LEU:HB2	1:A:209:ALA:HB3	1.69	0.74
1:A:350:THR:CG2	1:A:384:ARG:HB3	2.16	0.74
1:A:321:ILE:HD13	1:A:321:ILE:H	1.52	0.74
1:A:723:HIS:HD2	1:A:725:ALA:N	1.86	0.74
1:A:102:ALA:CB	1:A:270:MET:HE2	2.18	0.73
1:A:22:LYS:HE2	1:A:97:LEU:CD1	2.17	0.72
1:A:664:ASP:O	1:A:669:ARG:HD3	1.87	0.72
1:A:443:ARG:H	1:A:446:HIS:HD2	1.35	0.72
1:A:321:ILE:HG21	1:A:449:GLN:O	1.89	0.72
1:A:426:ARG:C	1:A:428:LEU:H	1.98	0.72
1:A:296:ILE:HG13	1:A:298:GLU:OE1	1.90	0.72
1:A:321:ILE:HG21	1:A:453:ALA:HB2	1.70	0.72
1:A:369:VAL:HG11	1:A:449:GLN:NE2	2.04	0.71
1:A:385:LEU:HG	1:A:472:THR:HB	1.71	0.71
1:A:331:PHE:CD1	1:A:418:GLU:HB2	2.25	0.70
1:A:386:PRO:HB2	1:A:477:VAL:HG21	1.74	0.70
1:A:387:ILE:HA	1:A:471:TYR:O	1.92	0.70
1:A:166:ALA:HB3	1:A:172:ALA:HB2	1.73	0.70
1:A:247:GLN:OE1	1:A:251:VAL:HG21	1.91	0.70
1:A:398:MET:HE1	1:A:406:LEU:HD11	1.74	0.70
1:A:151:MET:CE	1:A:224:TYR:HE1	2.04	0.70
1:A:340:ASP:O	1:A:435:LYS:HG3	1.92	0.69
1:A:158:GLY:HA2	1:A:252:LEU:HB2	1.73	0.69
1:A:132:VAL:HG22	1:A:133:PRO:CD	2.20	0.69
1:A:725:ALA:CA	1:A:728:MET:HE3	2.19	0.69
1:A:324:PRO:HG3	1:A:441:GLY:O	1.92	0.69
1:A:376:ILE:CG2	1:A:443:ARG:HD3	2.22	0.69
1:A:688:ARG:NH2	1:A:692:GLU:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASP:OD2	1:A:444:LEU:HB2	1.92	0.68
1:A:494:ARG:O	1:A:497:GLU:HG2	1.93	0.68
1:A:280:ILE:CD1	1:A:308:ALA:HA	2.23	0.68
1:A:120:ARG:HH21	1:A:131:VAL:CG2	2.07	0.68
1:A:404:PRO:HG3	1:A:491:ARG:HD3	1.76	0.68
1:A:444:LEU:CD1	1:A:470:ILE:HG21	2.24	0.67
1:A:307:THR:O	1:A:311:VAL:HG13	1.95	0.67
1:A:205:VAL:HG23	1:A:206:ASP:N	2.10	0.67
1:A:298:GLU:O	1:A:304:ILE:HD11	1.94	0.67
1:A:208:ILE:O	1:A:208:ILE:HG13	1.95	0.66
1:A:503:VAL:HG12	1:A:505:THR:H	1.60	0.66
1:A:71:PHE:CE2	1:A:226:LEU:HD11	2.30	0.66
1:A:332:GLU:HG3	1:A:415:ASN:HB3	1.76	0.66
1:A:134:PRO:HD2	1:A:135:TRP:CZ3	2.30	0.66
1:A:166:ALA:HB3	1:A:195:GLN:HE22	1.61	0.66
1:A:343:VAL:HG13	1:A:383:GLY:O	1.96	0.65
1:A:421:TRP:CE3	1:A:432:ARG:HB2	2.32	0.65
1:A:292:LYS:O	1:A:293:ASP:HB2	1.96	0.65
1:A:321:ILE:HG23	1:A:453:ALA:HB2	1.77	0.65
1:A:403:GLU:HB2	1:A:404:PRO:HD3	1.77	0.65
1:A:316:ILE:N	1:A:316:ILE:HD13	2.11	0.65
1:A:393:ILE:HD12	1:A:393:ILE:N	2.10	0.65
1:A:425:GLN:CG	1:A:426:ARG:H	2.10	0.65
1:A:151:MET:HG3	1:A:159:GLU:OE2	1.97	0.64
1:A:304:ILE:HG22	1:A:305:VAL:N	2.13	0.64
1:A:560:ILE:HD11	1:A:568:GLU:HG2	1.79	0.64
1:A:319:ILE:HG12	1:A:453:ALA:CA	2.28	0.64
1:A:621:HIS:HD2	5:A:790:HOH:O	1.80	0.64
1:A:191:GLU:O	1:A:194:GLU:HG2	1.98	0.64
1:A:489:ALA:O	1:A:493:ALA:HB2	1.98	0.64
1:A:298:GLU:OE2	1:A:307:THR:CG2	2.46	0.64
1:A:167:LYS:HG2	1:A:171:ALA:CB	2.29	0.63
1:A:192:ILE:CD1	1:A:258:LEU:HD12	2.29	0.63
1:A:263:MET:HE2	5:A:896:HOH:O	1.98	0.63
1:A:169:SER:HB3	1:A:199:GLU:CD	2.24	0.62
1:A:317:THR:HA	5:A:822:HOH:O	1.98	0.62
1:A:385:LEU:CG	1:A:472:THR:HB	2.29	0.62
1:A:167:LYS:HG3	1:A:168:ASP:OD1	1.99	0.62
1:A:558:GLY:O	1:A:568:GLU:HG3	1.99	0.62
1:A:369:VAL:HG11	1:A:449:GLN:HE21	1.64	0.62
4:A:966:GOL:C1	4:A:966:GOL:HO1	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HB2	1:A:209:ALA:CB	2.29	0.62
1:A:321:ILE:HG12	1:A:321:ILE:O	2.00	0.62
1:A:399:GLN:HE21	1:A:401:ASP:HB2	1.65	0.62
1:A:314:ILE:HG22	1:A:316:ILE:HD12	1.82	0.62
1:A:30:GLU:OE2	1:A:263:MET:HE1	1.99	0.61
1:A:342:HIS:HB3	1:A:433:ILE:HD11	1.83	0.61
1:A:386:PRO:HG2	1:A:472:THR:O	1.99	0.61
1:A:245:ASP:OD2	1:A:249:ARG:NH1	2.34	0.61
1:A:402:PHE:O	1:A:406:LEU:HG	2.00	0.61
1:A:6:ASN:HD21	1:A:9:GLN:HB2	1.66	0.61
1:A:306:GLN:O	1:A:310:GLU:HG3	2.01	0.61
1:A:197:LEU:HD11	1:A:203:LEU:HD21	1.82	0.61
1:A:407:GLU:OE1	1:A:491:ARG:NH1	2.26	0.61
1:A:163:ILE:HG13	1:A:163:ILE:O	2.00	0.61
1:A:290:GLN:HG2	1:A:291:ILE:N	2.15	0.61
1:A:300:ASP:OD2	1:A:302:ASP:HB2	2.01	0.61
1:A:352:SER:O	1:A:353:PHE:HB3	2.00	0.60
1:A:66:PRO:HB2	1:A:223:ASN:HB2	1.83	0.60
4:A:966:GOL:H11	4:A:967:GOL:O3	2.00	0.60
1:A:442:ALA:O	1:A:443:ARG:NH1	2.34	0.60
1:A:165:ARG:HB3	1:A:191:GLU:CB	2.30	0.60
1:A:298:GLU:O	1:A:304:ILE:CD1	2.50	0.60
1:A:350:THR:HB	1:A:351:PRO:HD2	1.84	0.59
1:A:477:VAL:O	1:A:481:ARG:HB2	2.02	0.59
1:A:413:PHE:CE1	1:A:454:LYS:HB3	2.36	0.59
1:A:361:PRO:HG2	1:A:362:ASP:H	1.68	0.59
1:A:494:ARG:HA	1:A:497:GLU:CD	2.27	0.59
1:A:329:PRO:HA	1:A:416:TYR:CD1	2.38	0.59
1:A:376:ILE:N	1:A:444:LEU:HD23	2.18	0.59
1:A:507:TYR:CZ	1:A:540:LYS:HG3	2.37	0.59
1:A:566:GLN:HB2	1:A:586:ASN:ND2	2.16	0.59
1:A:176:VAL:O	1:A:180:MET:CB	2.50	0.59
1:A:356:VAL:HG13	1:A:393:ILE:CD1	2.29	0.59
1:A:174:LYS:NZ	1:A:301:TYR:O	2.28	0.58
1:A:375:ASP:CG	1:A:444:LEU:HB2	2.28	0.58
1:A:390:VAL:HG23	1:A:390:VAL:O	2.02	0.58
1:A:398:MET:HE3	1:A:399:GLN:O	2.03	0.58
1:A:454:LYS:HZ2	1:A:457:GLN:CD	2.12	0.58
1:A:303:LYS:O	1:A:304:ILE:C	2.47	0.58
1:A:483:ILE:HG13	1:A:484:ALA:N	2.17	0.58
1:A:345:PHE:HB2	1:A:431:VAL:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LYS:NZ	1:A:592:GLU:OE2	2.37	0.58
1:A:629:MET:HE3	1:A:634:LEU:HD21	1.86	0.58
1:A:261:HIS:HE1	1:A:285:LEU:HD21	1.67	0.58
1:A:176:VAL:O	1:A:180:MET:HB2	2.03	0.57
1:A:384:ARG:O	1:A:385:LEU:HB2	2.04	0.57
1:A:349:LYS:HD3	1:A:384:ARG:CZ	2.34	0.57
1:A:300:ASP:C	1:A:302:ASP:H	2.13	0.57
1:A:120:ARG:NH2	1:A:131:VAL:CG1	2.68	0.56
1:A:336:ILE:O	1:A:432:ARG:HD3	2.05	0.56
1:A:491:ARG:C	1:A:493:ALA:N	2.61	0.56
1:A:566:GLN:HE22	1:A:584:ARG:NE	1.97	0.56
1:A:452:TYR:CD1	1:A:452:TYR:C	2.84	0.56
1:A:157:PRO:O	1:A:252:LEU:HD12	2.05	0.56
1:A:120:ARG:NH2	1:A:131:VAL:HG11	2.19	0.56
1:A:251:VAL:O	1:A:312:ARG:NH2	2.39	0.56
1:A:202:LYS:HD2	1:A:207:TYR:OH	2.06	0.55
1:A:376:ILE:O	1:A:379:VAL:HG12	2.06	0.55
1:A:491:ARG:C	1:A:493:ALA:H	2.11	0.55
1:A:620:GLU:H	1:A:620:GLU:CD	2.14	0.55
1:A:30:GLU:CD	1:A:263:MET:HE1	2.31	0.55
1:A:160:ALA:HB3	1:A:186:LEU:CD2	2.37	0.55
1:A:323:LEU:HB3	1:A:324:PRO:HD2	1.89	0.55
1:A:324:PRO:HG2	1:A:325:ILE:HG23	1.89	0.55
1:A:161:ILE:O	1:A:255:VAL:HG23	2.07	0.55
1:A:163:ILE:CA	1:A:189:CYS:O	2.46	0.54
1:A:319:ILE:HG12	1:A:453:ALA:HA	1.89	0.54
1:A:120:ARG:HE	1:A:130:ILE:HD12	1.72	0.54
1:A:160:ALA:HB3	1:A:186:LEU:HD22	1.88	0.54
1:A:323:LEU:HD23	1:A:446:HIS:ND1	2.23	0.54
1:A:427:ASP:C	1:A:428:LEU:HD12	2.33	0.54
1:A:169:SER:HB3	1:A:199:GLU:OE2	2.08	0.54
1:A:423:THR:HG23	1:A:424:ALA:N	2.22	0.54
1:A:189:CYS:C	1:A:190:ASP:OD2	2.51	0.53
1:A:282:ASP:OD1	1:A:301:TYR:CE1	2.62	0.53
1:A:426:ARG:HB3	1:A:488:TYR:CE2	2.43	0.53
1:A:151:MET:CE	1:A:224:TYR:CE1	2.85	0.53
1:A:540:LYS:HE2	1:A:544:GLU:OE2	2.09	0.53
1:A:148:GLY:O	1:A:151:MET:HB3	2.08	0.53
1:A:667:LEU:O	1:A:670:VAL:HG13	2.08	0.53
1:A:251:VAL:HG23	1:A:277:PHE:CE1	2.44	0.53
1:A:174:LYS:NZ	1:A:302:ASP:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLN:HB2	1:A:586:ASN:HD22	1.73	0.53
1:A:120:ARG:NH2	1:A:217:GLN:NE2	2.56	0.53
1:A:454:LYS:NZ	1:A:457:GLN:NE2	2.57	0.53
1:A:349:LYS:HB3	1:A:384:ARG:HD3	1.89	0.53
1:A:110:TRP:CZ2	1:A:272:ALA:HA	2.43	0.52
1:A:23:ARG:HB2	1:A:288:ASP:O	2.08	0.52
1:A:425:GLN:O	1:A:429:THR:CG2	2.57	0.52
1:A:400:GLU:HG3	1:A:403:GLU:OE2	2.08	0.52
1:A:64:PHE:HA	4:A:962:GOL:C3	2.40	0.52
1:A:283:GLN:O	1:A:297:SER:HB3	2.09	0.52
1:A:386:PRO:HG2	1:A:472:THR:C	2.33	0.52
1:A:351:PRO:O	1:A:477:VAL:HG11	2.10	0.52
1:A:445:LYS:O	1:A:445:LYS:HG2	2.09	0.52
1:A:338:LYS:HG3	1:A:341:MET:HE1	1.90	0.52
1:A:365:GLU:HG3	1:A:368:LYS:CD	2.39	0.52
1:A:394:TYR:C	1:A:394:TYR:CD2	2.87	0.52
1:A:19:LYS:O	1:A:19:LYS:HG2	2.09	0.52
1:A:169:SER:O	1:A:199:GLU:OE2	2.28	0.52
1:A:263:MET:HG3	1:A:264:VAL:N	2.24	0.52
1:A:207:TYR:O	1:A:208:ILE:HG12	2.09	0.52
1:A:438:PHE:HA	1:A:442:ALA:HB3	1.91	0.52
1:A:507:TYR:OH	1:A:540:LYS:HG3	2.10	0.52
1:A:261:HIS:CE1	1:A:285:LEU:HD21	2.45	0.51
1:A:428:LEU:HD12	1:A:428:LEU:N	2.26	0.51
1:A:261:HIS:ND1	1:A:289:LYS:NZ	2.57	0.51
1:A:421:TRP:HE3	1:A:432:ARG:HB2	1.74	0.51
1:A:292:LYS:HE2	5:A:818:HOH:O	2.09	0.51
1:A:245:ASP:CG	1:A:249:ARG:HH11	2.18	0.51
1:A:316:ILE:HD13	1:A:316:ILE:H	1.76	0.51
1:A:160:ALA:HB2	1:A:179:LEU:HD21	1.91	0.51
1:A:452:TYR:HD2	1:A:466:VAL:O	1.94	0.51
1:A:730:PRO:HB2	1:A:732:LEU:CD1	2.41	0.51
1:A:24:LEU:HB2	1:A:289:LYS:HA	1.92	0.51
1:A:135:TRP:HA	1:A:211:PRO:HG2	1.93	0.51
1:A:341:MET:SD	1:A:344:GLU:HB2	2.51	0.51
1:A:365:GLU:HB2	1:A:368:LYS:CB	2.41	0.50
1:A:450:LEU:O	1:A:454:LYS:HG2	2.11	0.50
1:A:715:LEU:HB3	1:A:716:PRO:HD3	1.93	0.50
1:A:166:ALA:CB	1:A:172:ALA:HB2	2.40	0.50
1:A:130:ILE:HG13	1:A:131:VAL:N	2.27	0.50
1:A:158:GLY:HA3	1:A:314:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASP:OD1	4:A:965:GOL:H11	2.11	0.50
1:A:298:GLU:OE2	1:A:307:THR:HB	2.11	0.50
1:A:174:LYS:HZ3	1:A:302:ASP:HA	1.75	0.50
1:A:368:LYS:O	1:A:467:GLN:HG3	2.11	0.50
1:A:99:PHE:O	1:A:99:PHE:CD1	2.65	0.50
1:A:342:HIS:HB3	1:A:433:ILE:CD1	2.42	0.50
1:A:282:ASP:OD1	1:A:301:TYR:HE1	1.95	0.49
1:A:323:LEU:HD11	1:A:450:LEU:HD12	1.94	0.49
1:A:375:ASP:CG	1:A:376:ILE:H	2.19	0.49
1:A:387:ILE:HD12	1:A:387:ILE:C	2.37	0.49
1:A:426:ARG:HD3	1:A:488:TYR:CD1	2.46	0.49
1:A:168:ASP:OD2	1:A:170:LYS:HB2	2.11	0.49
1:A:120:ARG:HH21	1:A:131:VAL:HG22	1.77	0.49
1:A:194:GLU:O	1:A:195:GLN:C	2.54	0.49
1:A:214:ASN:N	1:A:217:GLN:OE1	2.38	0.49
1:A:393:ILE:HG22	1:A:394:TYR:N	2.27	0.49
1:A:149:ILE:HG23	1:A:150:LYS:N	2.28	0.49
1:A:337:ARG:HG2	1:A:337:ARG:HH11	1.77	0.49
1:A:406:LEU:HD23	1:A:459:PHE:CZ	2.47	0.49
1:A:176:VAL:O	1:A:180:MET:HB3	2.13	0.49
1:A:732:LEU:HD12	5:A:799:HOH:O	2.12	0.49
1:A:365:GLU:HB2	1:A:368:LYS:HB2	1.95	0.48
1:A:245:ASP:CG	1:A:249:ARG:NH1	2.71	0.48
1:A:426:ARG:O	1:A:428:LEU:N	2.45	0.48
1:A:484:ALA:O	1:A:487:LYS:N	2.46	0.48
1:A:290:GLN:HG2	1:A:291:ILE:H	1.78	0.48
1:A:546:ASN:C	1:A:546:ASN:ND2	2.71	0.48
1:A:300:ASP:O	1:A:302:ASP:N	2.46	0.48
1:A:405:VAL:HG21	1:A:541:ALA:HB3	1.94	0.48
1:A:426:ARG:HD2	1:A:488:TYR:CG	2.47	0.48
1:A:353:PHE:CE2	1:A:388:GLY:HA3	2.49	0.48
1:A:423:THR:CG2	1:A:424:ALA:N	2.75	0.48
1:A:424:ALA:CB	1:A:428:LEU:O	2.61	0.48
1:A:473:ASP:OD1	1:A:475:GLN:HB2	2.14	0.48
1:A:365:GLU:HG3	1:A:368:LYS:HD3	1.96	0.48
1:A:190:ASP:OD1	1:A:214:ASN:O	2.32	0.48
1:A:247:GLN:C	1:A:251:VAL:HG22	2.38	0.48
1:A:255:VAL:HG13	1:A:279:VAL:HA	1.94	0.48
1:A:130:ILE:HG13	1:A:131:VAL:H	1.78	0.48
1:A:546:ASN:O	1:A:548:ASN:N	2.47	0.48
1:A:339:GLY:C	1:A:340:ASP:OD1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:O	1:A:393:ILE:CD1	2.62	0.47
1:A:377:ASP:OD1	1:A:377:ASP:N	2.41	0.47
1:A:426:ARG:O	1:A:429:THR:HG23	2.14	0.47
1:A:16:GLU:C	1:A:18:GLY:H	2.23	0.47
1:A:338:LYS:O	1:A:338:LYS:HG2	2.13	0.47
1:A:343:VAL:CG1	1:A:383:GLY:O	2.62	0.47
1:A:388:GLY:O	1:A:471:TYR:HD2	1.97	0.47
1:A:686:GLU:OE2	1:A:699:ILE:HD11	2.14	0.47
1:A:120:ARG:HH22	1:A:131:VAL:HG11	1.79	0.47
1:A:261:HIS:CG	1:A:289:LYS:HZ3	2.30	0.47
1:A:133:PRO:HA	1:A:134:PRO:C	2.39	0.47
1:A:323:LEU:HD22	1:A:446:HIS:HB3	1.97	0.47
1:A:395:GLY:HA2	1:A:464:ASP:OD2	2.15	0.47
1:A:74:GLU:OE2	1:A:88:ARG:NH2	2.44	0.47
1:A:425:GLN:HG3	1:A:426:ARG:H	1.78	0.47
1:A:679:GLU:OE2	1:A:682:ARG:HD2	2.13	0.47
1:A:699:ILE:H	1:A:699:ILE:HG13	1.33	0.47
1:A:176:VAL:O	1:A:176:VAL:CG1	2.61	0.47
1:A:25:PHE:HD2	1:A:97:LEU:O	1.97	0.47
1:A:385:LEU:CD1	1:A:386:PRO:HD2	2.27	0.47
1:A:508:SER:HB3	1:A:554:ILE:HD11	1.97	0.47
1:A:316:ILE:N	1:A:316:ILE:CD1	2.76	0.47
1:A:152:VAL:HG11	1:A:246:TYR:OH	2.15	0.46
1:A:176:VAL:O	1:A:176:VAL:HG12	2.15	0.46
1:A:425:GLN:O	1:A:429:THR:HG22	2.15	0.46
1:A:385:LEU:CD2	1:A:472:THR:HB	2.46	0.46
1:A:605:MET:HE1	1:A:661:VAL:HG21	1.96	0.46
1:A:179:LEU:HD22	1:A:186:LEU:CD2	2.38	0.46
1:A:280:ILE:HD11	1:A:311:VAL:HG21	1.98	0.46
1:A:426:ARG:CD	1:A:488:TYR:CD1	2.98	0.46
1:A:454:LYS:NZ	1:A:457:GLN:CD	2.74	0.46
1:A:672:TRP:HA	1:A:703:ALA:O	2.15	0.46
1:A:57:GLY:HA3	4:A:962:GOL:C3	2.45	0.46
1:A:99:PHE:O	1:A:99:PHE:HD1	1.99	0.46
1:A:153:ASP:C	1:A:153:ASP:OD1	2.59	0.46
1:A:406:LEU:HD23	1:A:459:PHE:CE1	2.51	0.46
1:A:696:ARG:H	1:A:696:ARG:HG3	1.35	0.46
1:A:347:GLY:C	1:A:349:LYS:H	2.23	0.46
1:A:287:GLU:O	1:A:287:GLU:HG2	2.15	0.46
1:A:484:ALA:C	1:A:486:LYS:N	2.69	0.46
1:A:590:ILE:HA	1:A:594:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:CE1	1:A:270:MET:HE1	2.51	0.46
1:A:205:VAL:CG2	1:A:206:ASP:H	2.25	0.45
1:A:213:GLY:HA3	1:A:217:GLN:CD	2.41	0.45
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.60	0.45
1:A:308:ALA:O	1:A:311:VAL:HG22	2.15	0.45
1:A:355:LEU:HD11	1:A:487:LYS:HD3	1.97	0.45
1:A:280:ILE:HD13	1:A:308:ALA:CA	2.42	0.45
1:A:319:ILE:HG12	1:A:453:ALA:HB1	1.99	0.45
1:A:660:PHE:O	1:A:661:VAL:C	2.59	0.45
1:A:366:ASP:OD1	1:A:452:TYR:HE2	2.00	0.45
1:A:436:GLU:O	1:A:439:ALA:HB3	2.16	0.45
1:A:390:VAL:O	1:A:390:VAL:CG2	2.64	0.45
1:A:152:VAL:HB	1:A:250:ARG:HD2	1.99	0.45
1:A:64:PHE:O	1:A:66:PRO:HD3	2.17	0.45
1:A:245:ASP:O	1:A:249:ARG:HG3	2.17	0.45
1:A:298:GLU:OE2	1:A:307:THR:HG21	2.16	0.45
1:A:324:PRO:HB2	1:A:440:LYS:O	2.17	0.45
1:A:69:ARG:O	1:A:73:GLY:HA2	2.17	0.45
1:A:291:ILE:HG21	1:A:294:TRP:HB2	1.98	0.45
1:A:280:ILE:HD11	1:A:311:VAL:CG2	2.46	0.44
1:A:434:SER:O	1:A:437:ALA:HB3	2.17	0.44
1:A:447:LEU:O	1:A:451:LEU:HB2	2.17	0.44
1:A:212:LEU:HG	1:A:220:HIS:HB2	1.98	0.44
1:A:403:GLU:CB	1:A:404:PRO:HD3	2.45	0.44
1:A:495:LEU:CD2	1:A:537:LEU:HD12	2.46	0.44
1:A:338:LYS:HA	1:A:341:MET:HE2	1.99	0.44
1:A:345:PHE:HB3	1:A:387:ILE:HG12	1.98	0.44
1:A:445:LYS:O	1:A:449:GLN:HG2	2.17	0.44
1:A:481:ARG:O	1:A:481:ARG:HG2	2.16	0.44
1:A:193:ILE:O	1:A:197:LEU:HD22	2.18	0.44
1:A:374:PRO:HB2	1:A:378:SER:HB2	1.98	0.44
1:A:546:ASN:ND2	1:A:548:ASN:H	2.16	0.44
1:A:215:PHE:HE2	1:A:264:VAL:HG21	1.83	0.44
1:A:498:LEU:HD21	1:A:537:LEU:HD21	1.98	0.44
1:A:6:ASN:O	1:A:6:ASN:CG	2.61	0.44
1:A:300:ASP:C	1:A:302:ASP:N	2.76	0.44
1:A:644:THR:O	1:A:645:PRO:C	2.59	0.44
1:A:76:VAL:O	4:A:962:GOL:O2	2.36	0.44
1:A:327:PHE:CD1	1:A:327:PHE:C	2.95	0.44
1:A:344:GLU:OE1	1:A:349:LYS:HD2	2.17	0.44
1:A:245:ASP:OD1	1:A:249:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASP:OD2	1:A:301:TYR:OH	2.26	0.44
1:A:546:ASN:C	1:A:546:ASN:HD22	2.24	0.44
1:A:251:VAL:O	1:A:251:VAL:HG23	2.18	0.44
1:A:336:ILE:O	1:A:432:ARG:NH1	2.51	0.44
1:A:451:LEU:O	1:A:452:TYR:C	2.61	0.44
1:A:629:MET:HE3	1:A:634:LEU:CD2	2.46	0.44
1:A:175:ILE:HG13	1:A:176:VAL:N	2.33	0.43
1:A:6:ASN:HD21	1:A:9:GLN:CB	2.28	0.43
1:A:329:PRO:HG3	1:A:416:TYR:CE1	2.53	0.43
1:A:370:GLU:HB2	1:A:469:THR:HG23	2.01	0.43
1:A:387:ILE:HD12	1:A:387:ILE:O	2.18	0.43
1:A:411:HIS:O	1:A:415:ASN:HB2	2.18	0.43
1:A:479:GLU:O	1:A:483:ILE:HG23	2.18	0.43
1:A:291:ILE:CG2	1:A:294:TRP:HB2	2.48	0.43
1:A:425:GLN:CG	1:A:426:ARG:N	2.77	0.43
1:A:120:ARG:HH21	1:A:131:VAL:HG21	1.82	0.43
1:A:426:ARG:HB3	1:A:488:TYR:CZ	2.53	0.43
1:A:49:LYS:HE2	1:A:50:TYR:CZ	2.54	0.43
1:A:61:THR:HA	1:A:141:ASP:CG	2.44	0.43
1:A:452:TYR:CD2	1:A:466:VAL:HB	2.53	0.43
1:A:575:TYR:HA	1:A:582:ILE:O	2.19	0.43
1:A:687:GLU:O	1:A:691:GLU:HG3	2.17	0.43
1:A:21:PRO:HG3	1:A:290:GLN:O	2.19	0.43
1:A:353:PHE:HA	1:A:427:ASP:HA	2.00	0.43
1:A:484:ALA:C	1:A:486:LYS:H	2.27	0.43
1:A:503:VAL:HG11	1:A:536:TRP:CZ2	2.53	0.43
1:A:71:PHE:CE2	1:A:226:LEU:CD1	3.01	0.43
1:A:398:MET:HE1	1:A:406:LEU:CD1	2.47	0.43
1:A:188:LEU:O	1:A:212:LEU:HB2	2.18	0.42
1:A:251:VAL:HG23	1:A:277:PHE:CZ	2.54	0.42
1:A:474:GLU:O	1:A:474:GLU:CG	2.66	0.42
1:A:131:VAL:HG11	1:A:217:GLN:HE22	1.82	0.42
1:A:164:GLY:N	1:A:189:CYS:O	2.52	0.42
1:A:197:LEU:CD1	1:A:203:LEU:HD21	2.48	0.42
1:A:251:VAL:CG2	1:A:277:PHE:CZ	3.03	0.42
1:A:319:ILE:HG12	1:A:453:ALA:C	2.44	0.42
1:A:364:ILE:HG13	1:A:467:GLN:HE21	1.84	0.42
1:A:82:MET:HE2	1:A:115:ILE:HG23	2.02	0.42
1:A:251:VAL:HG21	1:A:277:PHE:HZ	1.84	0.42
1:A:426:ARG:C	1:A:428:LEU:N	2.64	0.42
1:A:323:LEU:CD1	1:A:450:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:H	1:A:446:HIS:CD2	2.25	0.42
1:A:319:ILE:HG12	1:A:453:ALA:CB	2.50	0.42
1:A:575:TYR:O	1:A:580:ARG:HA	2.19	0.42
1:A:120:ARG:HH21	1:A:131:VAL:CG1	2.32	0.42
1:A:298:GLU:OE2	1:A:307:THR:CB	2.67	0.42
1:A:361:PRO:CG	1:A:362:ASP:H	2.32	0.42
1:A:426:ARG:NH1	1:A:488:TYR:HB3	2.35	0.42
1:A:618:ASN:H	1:A:618:ASN:ND2	2.18	0.42
1:A:15:ILE:HD12	1:A:21:PRO:HD2	2.02	0.42
1:A:148:GLY:HA2	1:A:151:MET:HE3	2.02	0.42
1:A:6:ASN:ND2	1:A:9:GLN:CB	2.83	0.41
1:A:162:ILE:HD12	1:A:188:LEU:CD2	2.51	0.41
1:A:169:SER:C	1:A:199:GLU:OE2	2.63	0.41
1:A:247:GLN:O	1:A:251:VAL:CG2	2.60	0.41
1:A:364:ILE:HD13	1:A:465:ARG:CB	2.51	0.41
1:A:503:VAL:HG13	4:A:965:GOL:H12	2.01	0.41
1:A:71:PHE:CZ	1:A:226:LEU:HD11	2.55	0.41
1:A:356:VAL:HG21	1:A:407:GLU:HA	2.01	0.41
1:A:396:ARG:HG3	1:A:464:ASP:OD2	2.21	0.41
1:A:564:LYS:NZ	1:A:592:GLU:CD	2.79	0.41
1:A:437:ALA:C	1:A:439:ALA:N	2.77	0.41
1:A:185:MET:HA	1:A:208:ILE:HG13	2.03	0.41
1:A:192:ILE:O	1:A:193:ILE:C	2.63	0.41
1:A:425:GLN:HE21	1:A:425:GLN:HB3	1.66	0.41
1:A:445:LYS:HE2	1:A:449:GLN:NE2	2.36	0.41
1:A:719:GLU:O	1:A:720:GLU:C	2.63	0.41
1:A:60:ASP:OD2	1:A:142:PRO:HD2	2.21	0.41
1:A:279:VAL:HG11	1:A:295:PHE:CE1	2.55	0.41
1:A:357:ARG:O	1:A:393:ILE:HD13	2.20	0.41
1:A:365:GLU:HG3	1:A:368:LYS:HD2	2.02	0.41
1:A:512:CYS:C	1:A:514:SER:N	2.78	0.41
1:A:24:LEU:HD22	1:A:295:PHE:CD2	2.56	0.41
1:A:26:LYS:HE3	1:A:97:LEU:HD11	2.02	0.41
1:A:308:ALA:O	1:A:309:LEU:C	2.63	0.41
1:A:351:PRO:HB2	1:A:477:VAL:HG11	2.02	0.41
1:A:405:VAL:HG21	1:A:541:ALA:CB	2.51	0.41
1:A:454:LYS:O	1:A:457:GLN:N	2.54	0.41
1:A:597:SER:HB3	1:A:601:PHE:CD2	2.56	0.41
1:A:620:GLU:CD	1:A:620:GLU:N	2.78	0.41
1:A:125:THR:OG1	1:A:128:ASN:HB2	2.20	0.40
1:A:24:LEU:CD2	1:A:295:PHE:CD2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLU:O	1:A:474:GLU:HG3	2.20	0.40
1:A:50:TYR:HB3	1:A:54:HIS:CG	2.56	0.40
1:A:56:VAL:HG22	1:A:57:GLY:N	2.35	0.40
1:A:337:ARG:HG2	1:A:337:ARG:NH1	2.36	0.40
1:A:584:ARG:HH11	1:A:584:ARG:HD2	1.73	0.40
1:A:673:MET:HG3	1:A:678:LYS:HB2	2.01	0.40
1:A:261:HIS:CB	1:A:289:LYS:HZ3	2.34	0.40
1:A:631:PHE:CD1	1:A:631:PHE:C	2.99	0.40
1:A:454:LYS:NZ	1:A:457:GLN:HE22	2.19	0.40
1:A:597:SER:HB3	1:A:601:PHE:HD2	1.87	0.40
1:A:715:LEU:N	1:A:716: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	726/732 (99%)	639 (88%)	67 (9%)	20 (3%)	4 2

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASP
1	A	301	TYR
1	A	304	ILE
1	A	375	ASP
1	A	353	PHE
1	A	444	LEU
1	A	461	SER
1	A	18	GLY
1	A	133	PRO
1	A	427	ASP

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Mol	Chain	Res	Type
1	A	599	GLY
1	A	19	LYS
1	A	396	ARG
1	A	426	ARG
1	A	495	LEU
1	A	660	PHE
1	A	305	VAL
1	A	496	ARG
1	A	547	PRO
1	A	361	PRO

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	610/614 (99%)	558 (92%)	52 (8%)	10	11

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	9	GLN
1	A	15	ILE
1	A	23	ARG
1	A	92	GLN
1	A	104	LEU
1	A	127	GLU
1	A	131	VAL
1	A	132	VAL
1	A	143	VAL
1	A	145	ARG
1	A	177	ASP
1	A	190	ASP
1	A	194	GLU
1	A	197	LEU
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	212	LEU
1	A	237	PRO
1	A	248	ARG
1	A	255	VAL
1	A	274	PHE
1	A	282	ASP
1	A	297	SER
1	A	298	GLU
1	A	304	ILE
1	A	307	THR
1	A	309	LEU
1	A	316	ILE
1	A	321	ILE
1	A	364	ILE
1	A	377	ASP
1	A	393	ILE
1	A	415	ASN
1	A	423	THR
1	A	425	GLN
1	A	433	ILE
1	A	451	LEU
1	A	452	TYR
1	A	470	ILE
1	A	483	ILE
1	A	498	LEU
1	A	530	LEU
1	A	587	LEU
1	A	612	ASN
1	A	620	GLU
1	A	642	THR
1	A	643	GLN
1	A	661	VAL
1	A	670	VAL
1	A	682	ARG
1	A	699	ILE
1	A	715	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	GLN

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Mol	Chain	Res	Type
1	A	87	ASN
1	A	146	GLN
1	A	195	GLN
1	A	243	HIS
1	A	306	GLN
1	A	399	GLN
1	A	411	HIS
1	A	425	GLN
1	A	446	HIS
1	A	449	GLN
1	A	467	GLN
1	A	475	GLN
1	A	513	GLN
1	A	546	ASN
1	A	551	ASN
1	A	552	GLN
1	A	566	GLN
1	A	571	ASN
1	A	577	ASN
1	A	579	GLN
1	A	586	ASN
1	A	612	ASN
1	A	680	GLN
1	A	723	HIS

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 ⓘ

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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
4	GOL	A	962	-	5,5,5	5.27	5 (100%)	5,5,5	5.92	3 (60%)
4	GOL	A	970	-	5,5,5	4.76	5 (100%)	5,5,5	6.14	3 (60%)
4	GOL	A	969	-	5,5,5	4.42	5 (100%)	5,5,5	5.82	3 (60%)
4	GOL	A	965	-	5,5,5	4.69	5 (100%)	5,5,5	6.11	3 (60%)
4	GOL	A	967	-	5,5,5	4.88	5 (100%)	5,5,5	5.91	3 (60%)
4	GOL	A	960	-	5,5,5	4.89	5 (100%)	5,5,5	6.16	3 (60%)
4	GOL	A	963	-	5,5,5	4.68	5 (100%)	5,5,5	6.06	3 (60%)
4	GOL	A	961	-	5,5,5	4.77	5 (100%)	5,5,5	6.07	3 (60%)
4	GOL	A	968	-	5,5,5	4.59	5 (100%)	5,5,5	6.08	3 (60%)
3	SF4	A	733	1	0,12,12	-	-	-	-	-
4	GOL	A	959	-	5,5,5	4.87	5 (100%)	5,5,5	6.07	3 (60%)
4	GOL	A	964	-	5,5,5	4.69	5 (100%)	5,5,5	6.23	3 (60%)
4	GOL	A	966	-	5,5,5	4.75	5 (100%)	5,5,5	6.26	3 (60%)

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
4	GOL	A	962	-	-	2/4/4/4	-
4	GOL	A	970	-	-	2/4/4/4	-
4	GOL	A	969	-	-	2/4/4/4	-
4	GOL	A	965	-	-	2/4/4/4	-
4	GOL	A	967	-	-	2/4/4/4	-
4	GOL	A	963	-	-	3/4/4/4	-
4	GOL	A	960	-	-	3/4/4/4	-
4	GOL	A	961	-	-	3/4/4/4	-
4	GOL	A	968	-	-	3/4/4/4	-
3	SF4	A	733	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	959	-	-	3/4/4/4	-
4	GOL	A	964	-	-	2/4/4/4	-
4	GOL	A	966	-	-	2/4/4/4	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	962	GOL	C3-C2	-8.73	1.18	1.51
4	A	959	GOL	C3-C2	-8.46	1.19	1.51
4	A	967	GOL	C3-C2	-8.28	1.20	1.51
4	A	960	GOL	C3-C2	-8.10	1.20	1.51
4	A	963	GOL	C3-C2	-7.98	1.21	1.51
4	A	961	GOL	C3-C2	-7.97	1.21	1.51
4	A	964	GOL	C3-C2	-7.86	1.21	1.51
4	A	970	GOL	C3-C2	-7.80	1.22	1.51
4	A	965	GOL	C3-C2	-7.79	1.22	1.51
4	A	968	GOL	C3-C2	-7.46	1.23	1.51
4	A	966	GOL	C3-C2	-7.35	1.23	1.51
4	A	969	GOL	C3-C2	-7.23	1.24	1.51
4	A	966	GOL	O1-C1	5.47	1.65	1.42
4	A	962	GOL	O2-C2	-5.27	1.28	1.43
4	A	968	GOL	O1-C1	5.01	1.63	1.42
4	A	965	GOL	O1-C1	4.85	1.62	1.42
4	A	964	GOL	O1-C1	4.80	1.62	1.42
4	A	962	GOL	O1-C1	4.71	1.62	1.42
4	A	959	GOL	O1-C1	4.68	1.62	1.42
4	A	960	GOL	O1-C1	4.63	1.61	1.42
4	A	967	GOL	O1-C1	4.58	1.61	1.42
4	A	963	GOL	O1-C1	4.56	1.61	1.42
4	A	970	GOL	O1-C1	4.55	1.61	1.42
4	A	961	GOL	O1-C1	4.43	1.61	1.42
4	A	969	GOL	O1-C1	4.07	1.59	1.42
4	A	970	GOL	O3-C3	3.79	1.58	1.42
4	A	966	GOL	O3-C3	3.78	1.58	1.42
4	A	969	GOL	O3-C3	3.63	1.57	1.42
4	A	968	GOL	O3-C3	3.56	1.57	1.42
4	A	965	GOL	O3-C3	3.47	1.57	1.42
4	A	964	GOL	O3-C3	3.44	1.56	1.42
4	A	960	GOL	O3-C3	3.44	1.56	1.42
4	A	967	GOL	O3-C3	3.44	1.56	1.42
4	A	961	GOL	O3-C3	3.43	1.56	1.42
4	A	960	GOL	O2-C2	-3.38	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	963	GOL	O3-C3	3.22	1.55	1.42
4	A	961	GOL	C1-C2	-3.15	1.39	1.51
4	A	970	GOL	C1-C2	-3.06	1.40	1.51
4	A	959	GOL	O3-C3	3.06	1.55	1.42
4	A	967	GOL	O2-C2	-3.01	1.34	1.43
4	A	960	GOL	C1-C2	-3.01	1.40	1.51
4	A	969	GOL	O2-C2	-3.00	1.34	1.43
4	A	961	GOL	O2-C2	-2.99	1.34	1.43
4	A	967	GOL	C1-C2	-2.93	1.40	1.51
4	A	966	GOL	O2-C2	-2.86	1.35	1.43
4	A	959	GOL	C1-C2	-2.85	1.40	1.51
4	A	970	GOL	O2-C2	-2.84	1.35	1.43
4	A	964	GOL	O2-C2	-2.75	1.35	1.43
4	A	959	GOL	O2-C2	-2.75	1.35	1.43
4	A	963	GOL	C1-C2	-2.72	1.41	1.51
4	A	965	GOL	C1-C2	-2.71	1.41	1.51
4	A	963	GOL	O2-C2	-2.67	1.35	1.43
4	A	962	GOL	O3-C3	2.67	1.53	1.42
4	A	969	GOL	C1-C2	-2.59	1.41	1.51
4	A	968	GOL	O2-C2	-2.58	1.35	1.43
4	A	966	GOL	C1-C2	-2.53	1.42	1.51
4	A	965	GOL	O2-C2	-2.51	1.36	1.43
4	A	964	GOL	C1-C2	-2.40	1.42	1.51
4	A	962	GOL	C1-C2	-2.31	1.43	1.51
4	A	968	GOL	C1-C2	-2.28	1.43	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	966	GOL	O3-C3-C2	11.35	161.47	110.38
4	A	964	GOL	O3-C3-C2	11.32	161.33	110.38
4	A	960	GOL	O3-C3-C2	11.24	160.98	110.38
4	A	961	GOL	O3-C3-C2	11.09	160.30	110.38
4	A	970	GOL	O3-C3-C2	11.03	160.01	110.38
4	A	965	GOL	O3-C3-C2	10.99	159.86	110.38
4	A	968	GOL	O3-C3-C2	10.97	159.77	110.38
4	A	959	GOL	O3-C3-C2	10.93	159.60	110.38
4	A	963	GOL	O3-C3-C2	10.90	159.47	110.38
4	A	967	GOL	O3-C3-C2	10.65	158.34	110.38
4	A	962	GOL	O3-C3-C2	10.63	158.25	110.38
4	A	969	GOL	O3-C3-C2	10.61	158.15	110.38
4	A	970	GOL	O2-C2-C3	7.34	139.58	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	966	GOL	O2-C2-C3	7.34	139.55	109.18
4	A	959	GOL	O2-C2-C3	7.20	139.00	109.18
4	A	964	GOL	O2-C2-C3	7.19	138.95	109.18
4	A	963	GOL	O2-C2-C3	7.17	138.85	109.18
4	A	965	GOL	O2-C2-C3	7.15	138.78	109.18
4	A	961	GOL	O2-C2-C3	7.11	138.60	109.18
4	A	968	GOL	O2-C2-C3	7.08	138.50	109.18
4	A	960	GOL	O2-C2-C3	7.08	138.50	109.18
4	A	962	GOL	O2-C2-C3	7.01	138.19	109.18
4	A	967	GOL	O2-C2-C3	6.84	137.52	109.18
4	A	969	GOL	O2-C2-C3	6.78	137.24	109.18
4	A	965	GOL	O1-C1-C2	3.74	127.22	110.38
4	A	968	GOL	O1-C1-C2	3.73	127.17	110.38
4	A	967	GOL	O1-C1-C2	3.70	127.05	110.38
4	A	966	GOL	O1-C1-C2	3.62	126.68	110.38
4	A	964	GOL	O1-C1-C2	3.62	126.67	110.38
4	A	960	GOL	O1-C1-C2	3.60	126.60	110.38
4	A	963	GOL	O1-C1-C2	3.54	126.30	110.38
4	A	962	GOL	O1-C1-C2	3.53	126.26	110.38
4	A	970	GOL	O1-C1-C2	3.48	126.06	110.38
4	A	959	GOL	O1-C1-C2	3.42	125.76	110.38
4	A	969	GOL	O1-C1-C2	3.22	124.87	110.38
4	A	961	GOL	O1-C1-C2	3.19	124.76	110.38

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	959	GOL	C1-C2-C3-O3
4	A	960	GOL	C1-C2-C3-O3
4	A	961	GOL	O1-C1-C2-C3
4	A	961	GOL	C1-C2-C3-O3
4	A	962	GOL	O1-C1-C2-C3
4	A	962	GOL	C1-C2-C3-O3
4	A	963	GOL	C1-C2-C3-O3
4	A	964	GOL	O1-C1-C2-C3
4	A	964	GOL	C1-C2-C3-O3
4	A	965	GOL	O1-C1-C2-C3
4	A	965	GOL	C1-C2-C3-O3
4	A	966	GOL	C1-C2-C3-O3
4	A	967	GOL	C1-C2-C3-O3
4	A	968	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	968	GOL	C1-C2-C3-O3
4	A	969	GOL	O1-C1-C2-C3
4	A	969	GOL	C1-C2-C3-O3
4	A	970	GOL	O1-C1-C2-C3
4	A	970	GOL	C1-C2-C3-O3
4	A	959	GOL	O1-C1-C2-C3
4	A	960	GOL	O1-C1-C2-C3
4	A	963	GOL	O1-C1-C2-C3
4	A	960	GOL	O1-C1-C2-O2
4	A	963	GOL	O1-C1-C2-O2
4	A	966	GOL	O1-C1-C2-O2
4	A	967	GOL	O1-C1-C2-O2
4	A	959	GOL	O1-C1-C2-O2
4	A	968	GOL	O1-C1-C2-O2
4	A	961	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	962	GOL	3	0
4	A	965	GOL	2	0
4	A	967	GOL	1	0
4	A	966	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	728/732 (99%)	1.04	171 (23%) 2 1	31, 62, 134, 162	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	TRP	10.7
1	A	364	ILE	6.4
1	A	433	ILE	6.3
1	A	477	VAL	6.1
1	A	298	GLU	5.7
1	A	389	ILE	5.5
1	A	444	LEU	5.4
1	A	478	LEU	5.2
1	A	334	GLU	5.2
1	A	359	VAL	5.1
1	A	179	LEU	5.1
1	A	448	GLY	4.9
1	A	327	PHE	4.8
1	A	304	ILE	4.8
1	A	430	TRP	4.8
1	A	468	VAL	4.7
1	A	135	TRP	4.6
1	A	428	LEU	4.5
1	A	369	VAL	4.5
1	A	488	TYR	4.4
1	A	319	ILE	4.4
1	A	372	ILE	4.4
1	A	382	GLY	4.4
1	A	415	ASN	4.4
1	A	360	GLY	4.3
1	A	484	ALA	4.3
1	A	347	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	132	VAL	4.2
1	A	374	PRO	4.2
1	A	420	PHE	4.1
1	A	413	PHE	4.1
1	A	421	TRP	4.0
1	A	417	GLY	4.0
1	A	171	ALA	3.9
1	A	377	ASP	3.8
1	A	361	PRO	3.8
1	A	387	ILE	3.8
1	A	343	VAL	3.8
1	A	172	ALA	3.8
1	A	350	THR	3.8
1	A	493	ALA	3.8
1	A	494	ARG	3.8
1	A	429	THR	3.7
1	A	5	ILE	3.7
1	A	451	LEU	3.7
1	A	285	LEU	3.7
1	A	371	VAL	3.7
1	A	449	GLN	3.6
1	A	450	LEU	3.6
1	A	381	PRO	3.6
1	A	353	PHE	3.6
1	A	437	ALA	3.6
1	A	388	GLY	3.6
1	A	476	LYS	3.6
1	A	133	PRO	3.6
1	A	333	GLY	3.5
1	A	385	LEU	3.5
1	A	463	VAL	3.5
1	A	352	SER	3.5
1	A	466	VAL	3.5
1	A	390	VAL	3.4
1	A	411	HIS	3.4
1	A	321	ILE	3.4
1	A	379	VAL	3.4
1	A	431	VAL	3.4
1	A	442	ALA	3.4
1	A	303	LYS	3.4
1	A	342	HIS	3.4
1	A	473	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	480	LEU	3.3
1	A	408	ARG	3.3
1	A	481	ARG	3.3
1	A	394	TYR	3.3
1	A	131	VAL	3.3
1	A	328	GLY	3.3
1	A	15	ILE	3.3
1	A	367	GLY	3.2
1	A	317	THR	3.2
1	A	165	ARG	3.2
1	A	271	GLY	3.2
1	A	462	ILE	3.2
1	A	459	PHE	3.2
1	A	326	ASN	3.2
1	A	419	GLY	3.1
1	A	346	GLY	3.1
1	A	336	ILE	3.1
1	A	169	SER	3.1
1	A	492	ASP	3.1
1	A	19	LYS	3.1
1	A	183	GLY	3.1
1	A	170	LYS	3.1
1	A	316	ILE	3.0
1	A	393	ILE	3.0
1	A	297	SER	3.0
1	A	447	LEU	3.0
1	A	160	ALA	3.0
1	A	335	SER	3.0
1	A	282	ASP	3.0
1	A	455	PHE	2.9
1	A	409	ARG	2.9
1	A	412	TYR	2.9
1	A	471	TYR	2.9
1	A	392	ASP	2.9
1	A	329	PRO	2.9
1	A	338	LYS	2.9
1	A	345	PHE	2.9
1	A	318	SER	2.8
1	A	365	GLU	2.8
1	A	348	GLY	2.8
1	A	299	PRO	2.8
1	A	452	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	330	ALA	2.8
1	A	446	HIS	2.8
1	A	301	TYR	2.8
1	A	416	TYR	2.8
1	A	6	ASN	2.7
1	A	320	ASP	2.6
1	A	332	GLU	2.6
1	A	134	PRO	2.6
1	A	351	PRO	2.6
1	A	483	ILE	2.6
1	A	445	LYS	2.6
1	A	384	ARG	2.6
1	A	469	THR	2.6
1	A	290	GLN	2.6
1	A	331	PHE	2.6
1	A	341	MET	2.6
1	A	370	GLU	2.6
1	A	373	GLY	2.6
1	A	383	GLY	2.6
1	A	199	GLU	2.5
1	A	375	ASP	2.5
1	A	410	ILE	2.5
1	A	391	VAL	2.5
1	A	441	GLY	2.5
1	A	354	GLU	2.5
1	A	435	LYS	2.5
1	A	487	LYS	2.5
1	A	340	ASP	2.4
1	A	464	ASP	2.4
1	A	404	PRO	2.4
1	A	191	GLU	2.4
1	A	202	LYS	2.4
1	A	337	ARG	2.4
1	A	475	GLN	2.4
1	A	376	ILE	2.4
1	A	14	ALA	2.3
1	A	457	GLN	2.3
1	A	436	GLU	2.3
1	A	467	GLN	2.3
1	A	696	ARG	2.3
1	A	355	LEU	2.2
1	A	699	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	425	GLN	2.2
1	A	470	ILE	2.2
1	A	295	PHE	2.2
1	A	284	PRO	2.2
1	A	378	SER	2.2
1	A	443	ARG	2.1
1	A	192	ILE	2.1
1	A	154	TRP	2.1
1	A	254	PHE	2.1
1	A	273	ILE	2.1
1	A	368	LYS	2.1
1	A	479	GLU	2.1
1	A	339	GLY	2.1
1	A	472	THR	2.1
1	A	439	ALA	2.1
1	A	482	GLU	2.1
1	A	293	ASP	2.1
1	A	21	PRO	2.1

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(Å ²)	Q<0.9
4	GOL	A	964	6/6	0.58	0.18	90,106,110,114	0
4	GOL	A	968	6/6	0.62	0.13	79,83,92,94	0
4	GOL	A	961	6/6	0.69	0.18	94,104,108,113	0
4	GOL	A	963	6/6	0.70	0.14	108,119,123,125	0
4	GOL	A	966	6/6	0.76	0.18	63,84,90,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	960	6/6	0.77	0.14	88,101,102,103	0
4	GOL	A	970	6/6	0.79	0.12	95,107,113,115	0
4	GOL	A	969	6/6	0.83	0.13	63,70,84,87	0
4	GOL	A	965	6/6	0.87	0.13	74,96,108,109	0
4	GOL	A	962	6/6	0.87	0.25	48,59,66,71	0
4	GOL	A	967	6/6	0.87	0.11	85,95,101,101	0
4	GOL	A	959	6/6	0.89	0.16	85,98,102,107	0
3	SF4	A	733	8/8	0.96	0.10	44,47,48,48	0
2	NI	A	734	1/1	0.99	0.04	53,53,53,53	0
2	NI	A	735	1/1	1.00	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.