Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:02 PM GMT

PDB ID	:	1RU3
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

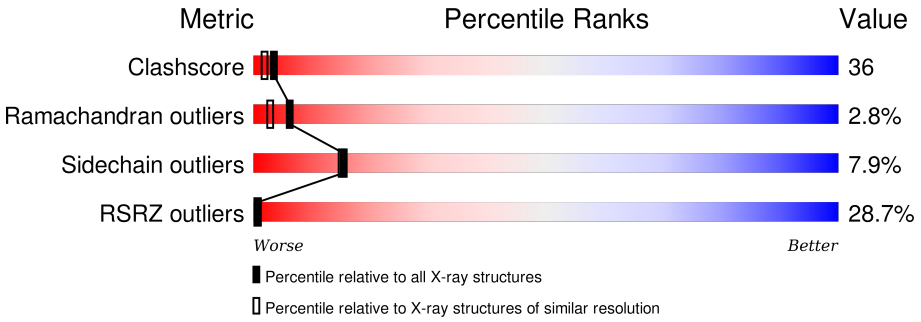
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	29% 52% 40% 7% ••

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	-	-
4	GOL	A	962	-	X	-	X

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

2 Entry composition

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.

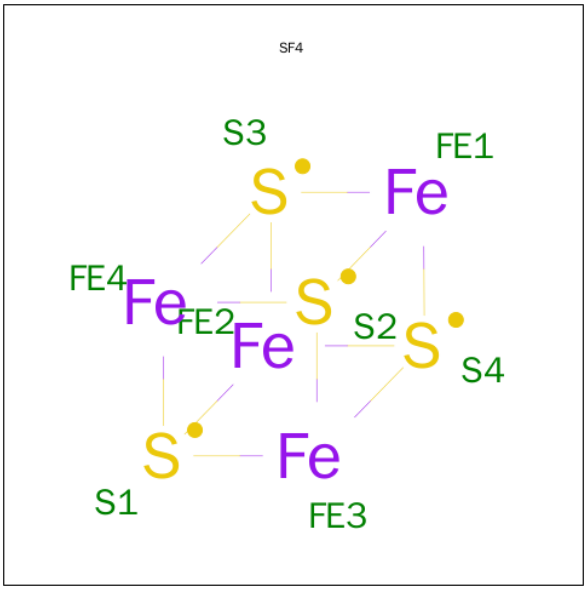
- Molecule 1 is a protein called Acetyl-CoA synthase.

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

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

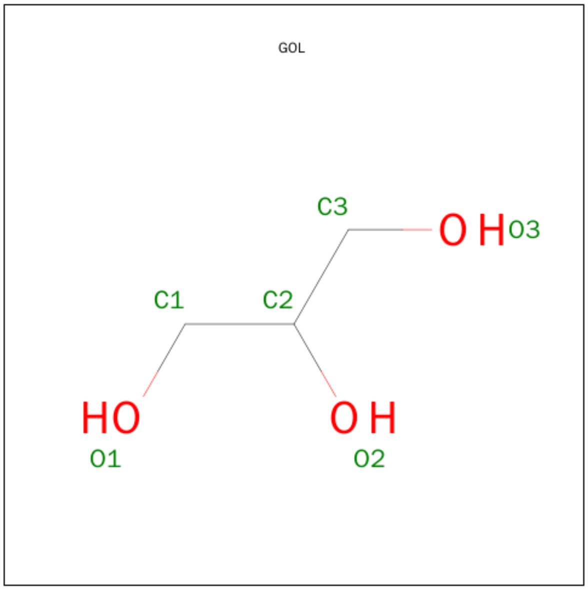
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	A	2	2	2	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

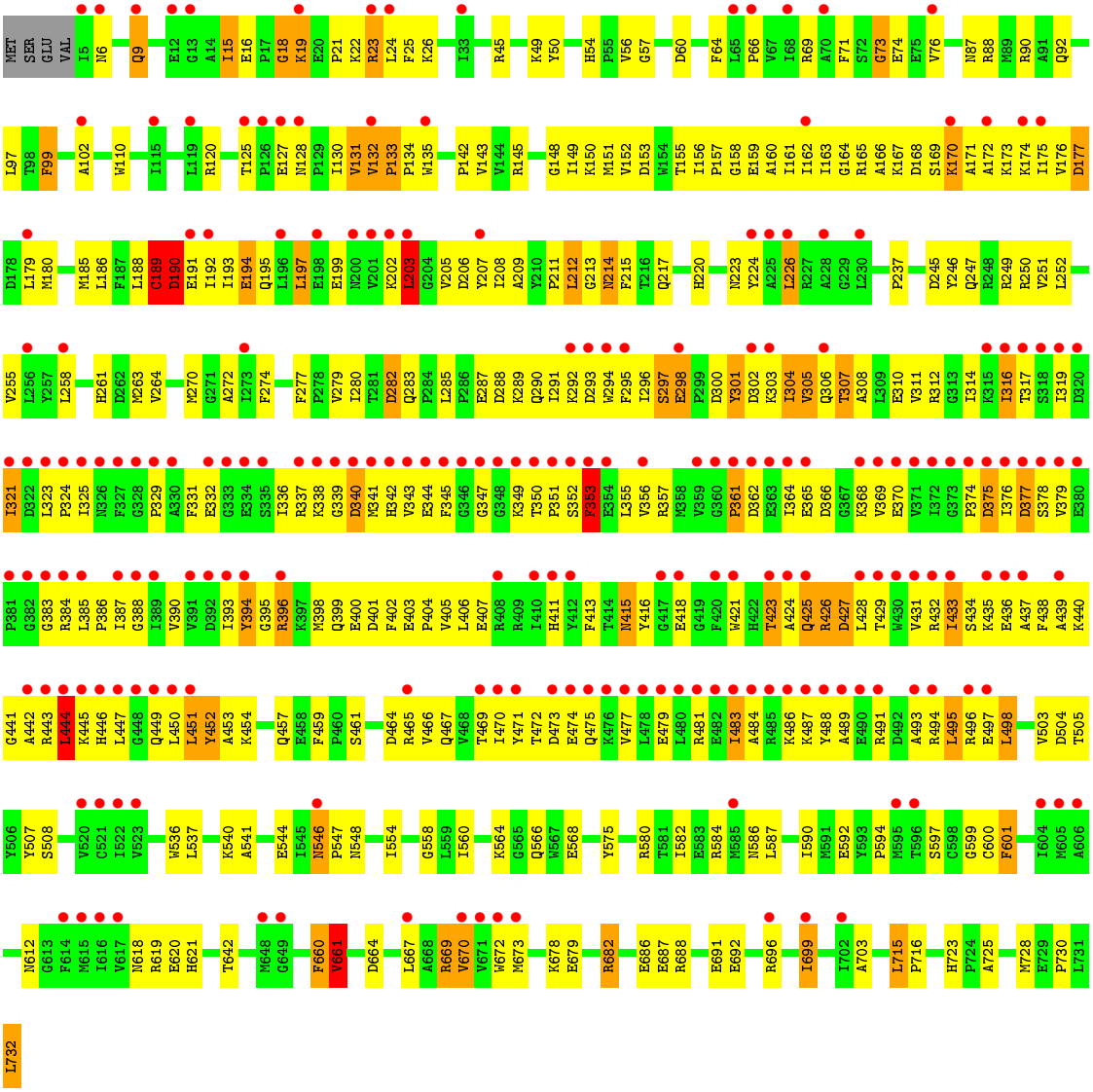
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	200.31Å 200.31Å 169.41Å 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) 98.9 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.274 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 65068 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SF4, NI

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	0.77	1/5893 (0.0%)	0.96	18/7978 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	661	VAL	CB-CG1	-5.46	1.41	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	CYS	CA-C-N	-11.37	92.19	117.20
1	A	669	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	189	CYS	O-C-N	8.47	136.25	122.70
1	A	189	CYS	C-N-CA	8.16	142.11	121.70
1	A	600	CYS	CA-CB-SG	-6.15	102.93	114.00
1	A	669	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	90	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	444	LEU	CA-CB-CG	5.99	129.09	115.30
1	A	214	ASN	N-CA-C	5.88	126.86	111.00
1	A	190	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	A	226	LEU	CA-CB-CG	-5.44	102.79	115.30
1	A	190	ASP	N-CA-C	5.37	125.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	661	VAL	N-CA-CB	-5.24	99.97	111.50
1	A	156	ILE	N-CA-C	-5.15	97.09	111.00
1	A	732	LEU	CA-CB-CG	-5.07	103.65	115.30
1	A	214	ASN	C-N-CA	-5.06	109.04	121.70
1	A	73	GLY	N-CA-C	5.01	125.61	113.10

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 (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	5759	0	5735	419	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	422	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 36.

All (422) 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:O1	4:A:966:GOL:C1	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:163:ILE:HA	1:A:189:CYS:O	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:192:ILE:HD11	1:A:258:LEU:HD12	1.52	0.90
1:A:22:LYS:CE	1:A:97:LEU:HD12	2.02	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
1:A:179:LEU:HD22	1:A:186:LEU:HD21	1.62	0.81
1:A:87:ASN:HB3	5:A:886:HOH:O	1.80	0.81
1:A:376:ILE:HG21	1:A:442:ALA:O	1.81	0.80
1:A:151:MET:HE1	1:A:224:TYR:CE1	2.18	0.79
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:H	1:A:321:ILE:HD13	1.52	0.74
1:A:723:HIS:HD2	1:A:725:ALA:N	1.86	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:247:GLN:OE1	1:A:251:VAL:HG21	1.91	0.70
1:A:166:ALA:HB3	1:A:172:ALA:HB2	1.73	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: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
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:151:MET:HE1	1:A:224:TYR:HE1	1.58	0.68
1:A:444:LEU:CD1	1:A:470:ILE:HG21	2.24	0.67
1:A:426:ARG:C	1:A:428:LEU:H	1.98	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:421:TRP:CE3	1:A:432:ARG:HB2	2.32	0.65
1:A:343:VAL:HG13	1:A:383:GLY:O	1.96	0.65
1:A:292:LYS:O	1:A:293:ASP:HB2	1.96	0.65
1:A:403:GLU:HB2	1:A:404:PRO:HD3	1.77	0.65
1:A:321:ILE:HG23	1:A:453:ALA:HB2	1.77	0.65
1:A:393:ILE:HD12	1:A:393:ILE:N	2.10	0.65
1:A:316:ILE:N	1:A:316:ILE:HD13	2.11	0.65
1:A:425:GLN:CG	1:A:426:ARG:H	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:LEU:CG	1:A:472:THR:HB	2.29	0.62
1:A:317:THR:HA	5:A:822:HOH:O	1.98	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
1:A:321:ILE:O	1:A:321:ILE:HG12	2.00	0.62
1:A:203:LEU:HB2	1:A:209:ALA:CB	2.29	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:386:PRO:HG2	1:A:472:THR:O	1.99	0.61
1:A:342:HIS:HB3	1:A:433:ILE:HD11	1.83	0.61
1:A:102:ALA:HB1	1:A:270:MET:HE2	1.82	0.61
1:A:402:PHE:O	1:A:406:LEU:HG	2.00	0.61
1:A:245:ASP:OD2	1:A:249:ARG:NH1	2.34	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:O	1:A:163:ILE:HG13	2.00	0.61
1:A:300:ASP:OD2	1:A:302:ASP:HB2	2.01	0.61
1:A:290:GLN:HG2	1:A:291:ILE:N	2.15	0.61
1:A:352:SER:O	1:A:353:PHE:HB3	2.00	0.60
4:A:966:GOL:H11	4:A:967:GOL:O3	2.00	0.60
1:A:66:PRO:HB2	1:A:223:ASN:HB2	1.83	0.60
1:A:442:ALA:O	1:A:443:ARG:NH1	2.34	0.60
1:A:725:ALA:HA	1:A:728:MET:CE	2.32	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:725:ALA:HA	1:A:728:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:PHE:CE1	1:A:454:LYS:HB3	2.36	0.59
1:A:102:ALA:CB	1:A:270:MET:HE2	2.33	0.59
1:A:361:PRO:HG2	1:A:362:ASP:H	1.68	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:566:GLN:HB2	1:A:586:ASN:ND2	2.16	0.59
1:A:507:TYR:CZ	1:A:540:LYS:HG3	2.37	0.59
1:A:356:VAL:HG13	1:A:393:ILE:CD1	2.29	0.59
1:A:176:VAL:O	1:A:180:MET:CB	2.50	0.59
1:A:174:LYS:NZ	1:A:301:TYR:O	2.28	0.58
1:A:390:VAL:HG23	1:A:390:VAL:O	2.02	0.58
1:A:483:ILE:HG13	1:A:484:ALA:N	2.17	0.58
1:A:169:SER:HB3	1:A:199:GLU:CD	2.24	0.58
1:A:345:PHE:HB2	1:A:431:VAL:HB	1.86	0.58
1:A:564:LYS:NZ	1:A:592:GLU:OE2	2.37	0.58
1:A:261:HIS:HE1	1:A:285:LEU:HD21	1.67	0.58
1:A:384:ARG:O	1:A:385:LEU:HB2	2.04	0.57
1:A:176:VAL:O	1:A:180:MET:HB2	2.03	0.57
1:A:338:LYS:HA	1:A:341:MET:HE2	1.87	0.57
1:A:349:LYS:HD3	1:A:384:ARG:CZ	2.34	0.57
1:A:120:ARG:NH2	1:A:131:VAL:CG1	2.68	0.56
1:A:566:GLN:HE22	1:A:584:ARG:NE	1.97	0.56
1:A:336:ILE:O	1:A:432:ARG:HD3	2.05	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: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:494:ARG:HA	1:A:497:GLU:CD	2.27	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
4:A:966:GOL:C1	4:A:966:GOL:HO1	2.09	0.54
1:A:319:ILE:HG12	1:A:453:ALA:HA	1.89	0.54
1:A:491:ARG:C	1:A:493:ALA:N	2.61	0.54
1:A:120:ARG:HE	1:A:130:ILE:HD12	1.72	0.54
1:A:323:LEU:HD23	1:A:446:HIS:ND1	2.23	0.54
1:A:160:ALA:HB3	1:A:186:LEU:HD22	1.88	0.54
1:A:375:ASP:CG	1:A:444:LEU:HB2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LYS:HZ2	1:A:457:GLN:CD	2.12	0.54
1:A:423:THR:HG23	1:A:424:ALA:N	2.22	0.54
1:A:169:SER:HB3	1:A:199:GLU:OE2	2.08	0.54
1:A:282:ASP:OD1	1:A:301:TYR:CE1	2.62	0.53
1:A:303:LYS:O	1:A:304:ILE:C	2.47	0.53
1:A:426:ARG:HB3	1:A:488:TYR:CE2	2.43	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:566:GLN:HB2	1:A:586:ASN:HD22	1.73	0.53
1:A:174:LYS:NZ	1:A:302:ASP:HA	2.23	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:425:GLN:O	1:A:429:THR:CG2	2.57	0.52
1:A:23:ARG:HB2	1:A:288:ASP:O	2.08	0.52
1:A:491:ARG:C	1:A:493:ALA:H	2.11	0.52
1:A:400:GLU:HG3	1:A:403:GLU:OE2	2.08	0.52
1:A:300:ASP:C	1:A:302:ASP:H	2.13	0.52
1:A:19:LYS:HG2	1:A:19:LYS:O	2.09	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: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:365:GLU:HG3	1:A:368:LYS:CD	2.39	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:438:PHE:HA	1:A:442:ALA:HB3	1.91	0.52
1:A:207:TYR:O	1:A:208:ILE:HG12	2.09	0.52
1:A:507:TYR:OH	1:A:540:LYS:HG3	2.10	0.52
1:A:452:TYR:CD1	1:A:452:TYR:C	2.84	0.52
1:A:261:HIS:CE1	1:A:285:LEU:HD21	2.45	0.51
1:A:428:LEU:N	1:A:428:LEU:HD12	2.26	0.51
1:A:421:TRP:HE3	1:A:432:ARG:HB2	1.74	0.51
1:A:261:HIS:ND1	1:A:289:LYS:NZ	2.57	0.51
1:A:292:LYS:HE2	5:A:818:HOH:O	2.09	0.51
1:A:316:ILE:H	1:A:316:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:PRO:HB2	1:A:732:LEU:CD1	2.41	0.51
1:A:341:MET:SD	1:A:344:GLU:HB2	2.51	0.51
1:A:135:TRP:HA	1:A:211:PRO:HG2	1.93	0.51
1:A:24:LEU:HB2	1:A:289:LYS:HA	1.92	0.51
1:A:620:GLU:CD	1:A:620:GLU:H	2.14	0.51
1:A:450:LEU:O	1:A:454:LYS:HG2	2.11	0.50
1:A:365:GLU:HB2	1:A:368:LYS:CB	2.41	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
1:A:504:ASP:OD1	4:A:965:GOL:H11	2.11	0.50
1:A:174:LYS:HZ1	1:A:302:ASP:HA	1.75	0.50
1:A:298:GLU:OE2	1:A:307:THR:HB	2.11	0.50
1:A:368:LYS:O	1:A:467:GLN:HG3	2.11	0.50
1:A:342:HIS:HB3	1:A:433:ILE:CD1	2.42	0.50
1:A:99:PHE:CD1	1:A:99:PHE:O	2.65	0.50
1:A:323:LEU:HD11	1:A:450:LEU:HD12	1.94	0.49
1:A:282:ASP:OD1	1:A:301:TYR:HE1	1.95	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: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:427:ASP:C	1:A:428:LEU:HD12	2.33	0.49
1:A:189:CYS:C	1:A:190:ASP:OD2	2.51	0.49
1:A:426:ARG:C	1:A:428:LEU:N	2.64	0.49
1:A:149:ILE:HG23	1:A:150:LYS:N	2.28	0.49
1:A:406:LEU:HD23	1:A:459:PHE:CZ	2.47	0.49
1:A:337:ARG:HG2	1:A:337:ARG:HH11	1.77	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:423:THR:CG2	1:A:424:ALA:N	2.75	0.48
1:A:365:GLU:HB2	1:A:368:LYS:HB2	1.95	0.48
1:A:484:ALA:O	1:A:487:LYS:N	2.46	0.48
1:A:426:ARG:O	1:A:428:LEU:N	2.45	0.48
1:A:290:GLN:HG2	1:A:291:ILE:H	1.78	0.48
1:A:300:ASP:O	1:A:302:ASP:N	2.46	0.48
1:A:426:ARG:HD2	1:A:488:TYR:CG	2.47	0.48
1:A:176:VAL:O	1:A:176:VAL:CG1	2.61	0.48
1:A:405:VAL:HG21	1:A:541:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PHE:CE2	1:A:388:GLY:HA3	2.49	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: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:357:ARG:O	1:A:393:ILE:CD1	2.62	0.47
1:A:426:ARG:O	1:A:429:THR:HG23	2.14	0.47
1:A:377:ASP:N	1:A:377:ASP:OD1	2.41	0.47
1:A:338:LYS:O	1:A:338:LYS:HG2	2.13	0.47
1:A:386:PRO:HG2	1:A:472:THR:C	2.33	0.47
1:A:388:GLY:O	1:A:471:TYR:HD2	1.97	0.47
1:A:343:VAL:CG1	1:A:383:GLY:O	2.62	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:394:TYR:C	1:A:394:TYR:CD2	2.87	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:425:GLN:CG	1:A:426:ARG:N	2.77	0.47
1:A:425:GLN:HG3	1:A:426:ARG:H	1.78	0.47
1:A:699:ILE:H	1:A:699:ILE:HG13	1.33	0.47
1:A:74:GLU:OE2	1:A:88:ARG:NH2	2.44	0.47
1:A:679:GLU:OE2	1:A:682:ARG:HD2	2.13	0.47
1:A:385:LEU:CD1	1:A:386:PRO:HD2	2.27	0.47
1:A:25:PHE:HD2	1:A:97:LEU:O	1.97	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:263:MET:HE2	5:A:896:HOH:O	2.15	0.47
1:A:176:VAL:O	1:A:176:VAL:HG12	2.15	0.46
1:A:152:VAL:HG11	1:A:246:TYR:OH	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:245:ASP:CG	1:A:249:ARG:HH11	2.18	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:102:ALA:HB1	1:A:270:MET:CE	2.46	0.46
1:A:672:TRP:HA	1:A:703:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:HD23	1:A:459:PHE:CE1	2.51	0.46
1:A:57:GLY:HA3	4:A:962:GOL:C3	2.45	0.46
1:A:99:PHE:HD1	1:A:99:PHE:O	1.99	0.46
1:A:696:ARG:HG3	1:A:696:ARG:H	1.35	0.46
1:A:287:GLU:HG2	1:A:287:GLU:O	2.15	0.46
1:A:590:ILE:HA	1:A:594:PRO:HB3	1.97	0.46
1:A:205:VAL:CG2	1:A:206:ASP:H	2.25	0.45
1:A:355:LEU:HD11	1:A:487:LYS:HD3	1.97	0.45
1:A:484:ALA:C	1:A:486:LYS:N	2.69	0.45
1:A:308:ALA:O	1:A:311:VAL:HG22	2.15	0.45
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.60	0.45
1:A:319:ILE:HG12	1:A:453:ALA:HB1	1.99	0.45
1:A:280:ILE:HD13	1:A:308:ALA:CA	2.42	0.45
1:A:151:MET:CE	1:A:224:TYR:CE1	2.85	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:387:ILE:C	1:A:387:ILE:HD12	2.37	0.45
1:A:390:VAL:CG2	1:A:390:VAL:O	2.64	0.45
1:A:375:ASP:CG	1:A:376:ILE:H	2.19	0.45
1:A:152:VAL:HB	1:A:250:ARG:HD2	1.99	0.45
1:A:324:PRO:HB2	1:A:440:LYS:O	2.17	0.45
1:A:298:GLU:OE2	1:A:307:THR:HG21	2.16	0.45
1:A:245:ASP:O	1:A:249:ARG:HG3	2.17	0.45
1:A:64:PHE:O	1:A:66:PRO:HD3	2.17	0.45
1:A:291:ILE:HG21	1:A:294:TRP:HB2	1.98	0.45
1:A:69:ARG:O	1:A:73:GLY:HA2	2.17	0.45
1:A:194:GLU:O	1:A:195:GLN:C	2.54	0.44
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:403:GLU:CB	1:A:404:PRO:HD3	2.45	0.44
1:A:245:ASP:CG	1:A:249:ARG:NH1	2.71	0.44
1:A:212:LEU:HG	1:A:220:HIS:HB2	1.98	0.44
1:A:495:LEU:CD2	1:A:537:LEU:HD12	2.46	0.44
1:A:481:ARG:O	1:A:481:ARG:HG2	2.16	0.44
1:A:445:LYS:O	1:A:449:GLN:HG2	2.17	0.44
1:A:345:PHE:HB3	1:A:387:ILE:HG12	1.98	0.44
1:A:193:ILE:O	1:A:197:LEU:HD22	2.18	0.44
1:A:546:ASN:ND2	1:A:548:ASN:H	2.16	0.44
1:A:374:PRO:HB2	1:A:378:SER:HB2	1.98	0.44
1:A:215:PHE:HE2	1:A:264:VAL:HG21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LEU:HD21	1:A:537:LEU:HD21	1.98	0.44
1:A:344:GLU:OE1	1:A:349:LYS:HD2	2.17	0.44
1:A:76:VAL:O	4:A:962:GOL:O2	2.36	0.44
1:A:151:MET:HE2	1:A:151:MET:HB2	1.84	0.44
1:A:245:ASP:OD1	1:A:249:ARG:NH1	2.50	0.44
1:A:251:VAL:HG23	1:A:251:VAL:O	2.18	0.44
1:A:336:ILE:O	1:A:432:ARG:NH1	2.51	0.44
1:A:546:ASN:ND2	1:A:546:ASN:C	2.71	0.44
1:A:175:ILE:HG13	1:A:176:VAL:N	2.33	0.43
1:A:329:PRO:HG3	1:A:416:TYR:CE1	2.53	0.43
1:A:102:ALA:CB	1:A:270:MET:CE	2.95	0.43
1:A:6:ASN:HD21	1:A:9:GLN:CB	2.28	0.43
1:A:370:GLU:HB2	1:A:469:THR:HG23	2.01	0.43
1:A:479:GLU:O	1:A:483:ILE:HG23	2.18	0.43
1:A:387:ILE:O	1:A:387:ILE:HD12	2.18	0.43
1:A:411:HIS:O	1:A:415:ASN:HB2	2.18	0.43
1:A:291:ILE:CG2	1:A:294:TRP:HB2	2.48	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:452:TYR:CD2	1:A:466:VAL:HB	2.53	0.43
1:A:687:GLU:O	1:A:691:GLU:HG3	2.17	0.43
1:A:49:LYS:HE2	1:A:50:TYR:CZ	2.54	0.43
1:A:575:TYR:HA	1:A:582:ILE:O	2.19	0.43
1:A:247:GLN:C	1:A:251:VAL:HG22	2.38	0.43
1:A:339:GLY:C	1:A:340:ASP:OD1	2.57	0.43
1:A:353:PHE:HA	1:A:427:ASP:HA	2.00	0.43
1:A:503:VAL:HG11	1:A:536:TRP:CZ2	2.53	0.43
1:A:21:PRO:HG3	1:A:290:GLN:O	2.19	0.43
1:A:71:PHE:CE2	1:A:226:LEU:CD1	3.01	0.43
1:A:16:GLU:C	1:A:18:GLY:H	2.23	0.43
1:A:251:VAL:HG23	1:A:277:PHE:CZ	2.54	0.42
1:A:398:MET:HE1	1:A:402:PHE:HB2	1.99	0.42
1:A:188:LEU:O	1:A:212:LEU:HB2	2.18	0.42
1:A:474:GLU:CG	1:A:474:GLU:O	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:133:PRO:HA	1:A:134:PRO:C	2.39	0.42
1:A:251:VAL:CG2	1:A:277:PHE:CZ	3.03	0.42
1:A:197:LEU:CD1	1:A:203:LEU:HD21	2.48	0.42
1:A:364:ILE:HG13	1:A:467:GLN:HE21	1.84	0.42
1:A:251:VAL:HG21	1:A:277:PHE:HZ	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LEU:CD1	1:A:450:LEU:HD12	2.49	0.42
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:426:ARG:NH1	1:A:488:TYR:HB3	2.35	0.42
1:A:361:PRO:CG	1:A:362:ASP:H	2.32	0.42
1:A:618:ASN:ND2	1:A:618:ASN:H	2.18	0.42
1:A:15:ILE:HD12	1:A:21:PRO:HD2	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:454:LYS:NZ	1:A:457:GLN:CD	2.74	0.41
1:A:153:ASP:OD1	1:A:153:ASP:C	2.59	0.41
1:A:247:GLN:O	1:A:251:VAL:CG2	2.60	0.41
1:A:503:VAL:HG13	4:A:965:GOL:H12	2.01	0.41
1:A:364:ILE:HD13	1:A:465:ARG:CB	2.51	0.41
1:A:356:VAL:HG21	1:A:407:GLU:HA	2.01	0.41
1:A:71:PHE:CZ	1:A:226:LEU:HD11	2.55	0.41
1:A:396:ARG:HG3	1:A:464:ASP:OD2	2.21	0.41
1:A:445:LYS:HE2	1:A:449:GLN:NE2	2.36	0.41
1:A:425:GLN:HB3	1:A:425:GLN:HE21	1.66	0.41
1:A:185:MET:HA	1:A:208:ILE:HG13	2.03	0.41
1:A:213:GLY:HA3	1:A:217:GLN:CD	2.41	0.41
1:A:357:ARG:O	1:A:393:ILE:HD13	2.20	0.41
1:A:279:VAL:HG11	1:A:295:PHE:CE1	2.55	0.41
1:A:365:GLU:HG3	1:A:368:LYS:HD2	2.02	0.41
1:A:60:ASP:OD2	1:A:142:PRO:HD2	2.21	0.41
1:A:351:PRO:HB2	1:A:477:VAL:HG11	2.02	0.41
1:A:26:LYS:HE3	1:A:97:LEU:HD11	2.02	0.41
1:A:454:LYS:O	1:A:457:GLN:N	2.54	0.41
1:A:24:LEU:HD22	1:A:295:PHE:CD2	2.56	0.41
1:A:405:VAL:HG21	1:A:541:ALA:CB	2.51	0.41
1:A:597:SER:HB3	1:A:601:PHE:CD2	2.56	0.41
1:A:125:THR:OG1	1:A:128:ASN:HB2	2.20	0.40
1:A:660:PHE:O	1:A:661:VAL:C	2.59	0.40
1:A:347:GLY:C	1:A:349:LYS:H	2.23	0.40
1:A:24:LEU:CD2	1:A:295:PHE:CD2	3.04	0.40
1:A:546:ASN:HD22	1:A:546:ASN:C	2.24	0.40
1:A:474:GLU:O	1:A:474:GLU:HG3	2.20	0.40
1:A:584:ARG:HD2	1:A:584:ARG:HH11	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:TYR:HB3	1:A:54:HIS:CG	2.56	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:454:LYS:NZ	1:A:457:GLN:HE22	2.19	0.40
1:A:715:LEU:N	1:A:716:PRO:CD	2.84	0.40
1:A:597:SER:HB3	1:A:601:PHE:HD2	1.87	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%)	6 3

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
1	A	599	GLY
1	A	19	LYS
1	A	396	ARG

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Mol	Chain	Res	Type
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

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%)	562 (92%)	48 (8%)	15 15

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	15	ILE
1	A	23	ARG
1	A	45	ARG
1	A	92	GLN
1	A	99	PHE
1	A	127	GLU
1	A	131	VAL
1	A	132	VAL
1	A	143	VAL
1	A	145	ARG
1	A	170	LYS
1	A	177	ASP
1	A	190	ASP
1	A	194	GLU
1	A	197	LEU
1	A	203	LEU
1	A	212	LEU
1	A	237	PRO

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Mol	Chain	Res	Type
1	A	274	PHE
1	A	282	ASP
1	A	297	SER
1	A	298	GLU
1	A	307	THR
1	A	316	ILE
1	A	321	ILE
1	A	340	ASP
1	A	353	PHE
1	A	377	ASP
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	483	ILE
1	A	498	LEU
1	A	546	ASN
1	A	587	LEU
1	A	601	PHE
1	A	612	ASN
1	A	619	ARG
1	A	642	THR
1	A	661	VAL
1	A	670	VAL
1	A	682	ARG
1	A	699	ILE
1	A	715	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	GLN
1	A	92	GLN
1	A	146	GLN
1	A	195	GLN
1	A	306	GLN
1	A	399	GLN
1	A	411	HIS
1	A	425	GLN

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Mol	Chain	Res	Type
1	A	446	HIS
1	A	449	GLN
1	A	467	GLN
1	A	513	GLN
1	A	546	ASN
1	A	552	GLN
1	A	566	GLN
1	A	571	ASN
1	A	579	GLN
1	A	586	ASN
1	A	612	ASN
1	A	618	ASN
1	A	643	GLN
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 carbohydrates 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	$\#\|Z\|>2$
3	SF4	A	733	1	0,12,12	0.00	-	0,24,24	0.00	-
4	GOL	A	959	-	5,5,5	4.89	5 (100%)	5,5,5	5.64	3 (60%)
4	GOL	A	960	-	5,5,5	4.91	5 (100%)	5,5,5	5.72	3 (60%)
4	GOL	A	961	-	5,5,5	4.79	5 (100%)	5,5,5	5.64	3 (60%)
4	GOL	A	962	-	5,5,5	5.27	5 (100%)	5,5,5	5.50	3 (60%)
4	GOL	A	963	-	5,5,5	4.70	5 (100%)	5,5,5	5.63	3 (60%)
4	GOL	A	964	-	5,5,5	4.71	5 (100%)	5,5,5	5.78	3 (60%)
4	GOL	A	965	-	5,5,5	4.71	5 (100%)	5,5,5	5.68	3 (60%)
4	GOL	A	966	-	5,5,5	4.76	5 (100%)	5,5,5	5.81	3 (60%)
4	GOL	A	967	-	5,5,5	4.90	5 (100%)	5,5,5	5.49	3 (60%)
4	GOL	A	968	-	5,5,5	4.60	5 (100%)	5,5,5	5.65	3 (60%)
4	GOL	A	969	-	5,5,5	4.44	5 (100%)	5,5,5	5.41	3 (60%)
4	GOL	A	970	-	5,5,5	4.78	5 (100%)	5,5,5	5.70	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
3	SF4	A	733	1	-	0/0/48/48	0/6/5/5
4	GOL	A	959	-	-	0/4/4/4	0/0/0/0
4	GOL	A	960	-	-	0/4/4/4	0/0/0/0
4	GOL	A	961	-	-	0/4/4/4	0/0/0/0
4	GOL	A	962	-	-	0/4/4/4	0/0/0/0
4	GOL	A	963	-	-	0/4/4/4	0/0/0/0
4	GOL	A	964	-	-	0/4/4/4	0/0/0/0
4	GOL	A	965	-	-	0/4/4/4	0/0/0/0
4	GOL	A	966	-	-	0/4/4/4	0/0/0/0
4	GOL	A	967	-	-	0/4/4/4	0/0/0/0
4	GOL	A	968	-	-	0/4/4/4	0/0/0/0
4	GOL	A	969	-	-	0/4/4/4	0/0/0/0
4	GOL	A	970	-	-	0/4/4/4	0/0/0/0

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	962	GOL	C3-C2	-8.85	1.18	1.52
4	A	959	GOL	C3-C2	-8.59	1.19	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	967	GOL	C3-C2	-8.41	1.20	1.52
4	A	960	GOL	C3-C2	-8.22	1.20	1.52
4	A	963	GOL	C3-C2	-8.10	1.21	1.52
4	A	961	GOL	C3-C2	-8.09	1.21	1.52
4	A	964	GOL	C3-C2	-7.99	1.21	1.52
4	A	970	GOL	C3-C2	-7.92	1.22	1.52
4	A	965	GOL	C3-C2	-7.92	1.22	1.52
4	A	968	GOL	C3-C2	-7.59	1.23	1.52
4	A	966	GOL	C3-C2	-7.48	1.23	1.52
4	A	969	GOL	C3-C2	-7.35	1.24	1.52
4	A	962	GOL	O2-C2	-5.16	1.28	1.43
4	A	960	GOL	O2-C2	-3.33	1.33	1.43
4	A	961	GOL	C1-C2	-3.28	1.39	1.52
4	A	970	GOL	C1-C2	-3.19	1.40	1.52
4	A	960	GOL	C1-C2	-3.14	1.40	1.52
4	A	967	GOL	C1-C2	-3.06	1.40	1.52
4	A	959	GOL	C1-C2	-2.98	1.40	1.52
4	A	967	GOL	O2-C2	-2.97	1.34	1.43
4	A	969	GOL	O2-C2	-2.96	1.34	1.43
4	A	961	GOL	O2-C2	-2.94	1.34	1.43
4	A	963	GOL	C1-C2	-2.86	1.41	1.52
4	A	965	GOL	C1-C2	-2.85	1.41	1.52
4	A	966	GOL	O2-C2	-2.82	1.35	1.43
4	A	970	GOL	O2-C2	-2.80	1.35	1.43
4	A	969	GOL	C1-C2	-2.72	1.41	1.52
4	A	964	GOL	O2-C2	-2.72	1.35	1.43
4	A	959	GOL	O2-C2	-2.71	1.35	1.43
4	A	966	GOL	C1-C2	-2.66	1.42	1.52
4	A	963	GOL	O2-C2	-2.64	1.35	1.43
4	A	968	GOL	O2-C2	-2.55	1.35	1.43
4	A	964	GOL	C1-C2	-2.53	1.42	1.52
4	A	965	GOL	O2-C2	-2.48	1.36	1.43
4	A	962	GOL	C1-C2	-2.45	1.43	1.52
4	A	968	GOL	C1-C2	-2.41	1.43	1.52
4	A	962	GOL	O3-C3	2.61	1.53	1.42
4	A	959	GOL	O3-C3	2.99	1.55	1.42
4	A	963	GOL	O3-C3	3.15	1.55	1.42
4	A	961	GOL	O3-C3	3.36	1.56	1.42
4	A	967	GOL	O3-C3	3.36	1.56	1.42
4	A	960	GOL	O3-C3	3.37	1.56	1.42
4	A	964	GOL	O3-C3	3.37	1.56	1.42
4	A	965	GOL	O3-C3	3.39	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	968	GOL	O3-C3	3.48	1.57	1.42
4	A	969	GOL	O3-C3	3.55	1.57	1.42
4	A	966	GOL	O3-C3	3.69	1.58	1.42
4	A	970	GOL	O3-C3	3.70	1.58	1.42
4	A	969	GOL	O1-C1	3.98	1.59	1.42
4	A	961	GOL	O1-C1	4.33	1.61	1.42
4	A	970	GOL	O1-C1	4.44	1.61	1.42
4	A	963	GOL	O1-C1	4.46	1.61	1.42
4	A	967	GOL	O1-C1	4.47	1.61	1.42
4	A	960	GOL	O1-C1	4.52	1.61	1.42
4	A	959	GOL	O1-C1	4.57	1.62	1.42
4	A	962	GOL	O1-C1	4.60	1.62	1.42
4	A	964	GOL	O1-C1	4.69	1.62	1.42
4	A	965	GOL	O1-C1	4.74	1.62	1.42
4	A	968	GOL	O1-C1	4.89	1.63	1.42
4	A	966	GOL	O1-C1	5.34	1.65	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	961	GOL	O1-C1-C2	3.01	124.76	110.18
4	A	969	GOL	O1-C1-C2	3.03	124.87	110.18
4	A	959	GOL	O1-C1-C2	3.21	125.76	110.18
4	A	970	GOL	O1-C1-C2	3.27	126.06	110.18
4	A	962	GOL	O1-C1-C2	3.32	126.26	110.18
4	A	963	GOL	O1-C1-C2	3.32	126.30	110.18
4	A	960	GOL	O1-C1-C2	3.39	126.60	110.18
4	A	964	GOL	O1-C1-C2	3.40	126.67	110.18
4	A	966	GOL	O1-C1-C2	3.40	126.68	110.18
4	A	967	GOL	O1-C1-C2	3.48	127.05	110.18
4	A	968	GOL	O1-C1-C2	3.50	127.17	110.18
4	A	965	GOL	O1-C1-C2	3.51	127.22	110.18
4	A	969	GOL	O2-C2-C3	6.24	137.24	108.65
4	A	967	GOL	O2-C2-C3	6.30	137.52	108.65
4	A	962	GOL	O2-C2-C3	6.44	138.19	108.65
4	A	960	GOL	O2-C2-C3	6.51	138.50	108.65
4	A	968	GOL	O2-C2-C3	6.51	138.50	108.65
4	A	961	GOL	O2-C2-C3	6.53	138.60	108.65
4	A	965	GOL	O2-C2-C3	6.57	138.78	108.65
4	A	963	GOL	O2-C2-C3	6.59	138.85	108.65
4	A	964	GOL	O2-C2-C3	6.61	138.95	108.65
4	A	959	GOL	O2-C2-C3	6.62	139.00	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	966	GOL	O2-C2-C3	6.74	139.55	108.65
4	A	970	GOL	O2-C2-C3	6.74	139.58	108.65
4	A	969	GOL	O3-C3-C2	9.89	158.15	110.18
4	A	962	GOL	O3-C3-C2	9.91	158.25	110.18
4	A	967	GOL	O3-C3-C2	9.93	158.34	110.18
4	A	963	GOL	O3-C3-C2	10.16	159.47	110.18
4	A	959	GOL	O3-C3-C2	10.19	159.60	110.18
4	A	968	GOL	O3-C3-C2	10.23	159.77	110.18
4	A	965	GOL	O3-C3-C2	10.24	159.86	110.18
4	A	970	GOL	O3-C3-C2	10.27	160.01	110.18
4	A	961	GOL	O3-C3-C2	10.33	160.30	110.18
4	A	960	GOL	O3-C3-C2	10.47	160.98	110.18
4	A	964	GOL	O3-C3-C2	10.55	161.33	110.18
4	A	966	GOL	O3-C3-C2	10.58	161.47	110.18

There are no chirality outliers.

There are no torsion outliers.

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	966	GOL	3	0
4	A	967	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	1.49	209 (28%) 1 1	31, 62, 134, 162	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	PHE	12.8
1	A	369	VAL	11.9
1	A	430	TRP	11.4
1	A	294	TRP	10.8
1	A	321	ILE	9.8
1	A	319	ILE	9.6
1	A	389	ILE	9.5
1	A	337	ARG	9.1
1	A	364	ILE	8.7
1	A	339	GLY	8.4
1	A	484	ALA	8.3
1	A	382	GLY	8.1
1	A	374	PRO	7.9
1	A	377	ASP	7.8
1	A	420	PHE	7.7
1	A	325	ILE	7.2
1	A	298	GLU	6.7
1	A	316	ILE	6.7
1	A	317	THR	6.6
1	A	370	GLU	6.6
1	A	477	VAL	6.6
1	A	360	GLY	6.6
1	A	132	VAL	6.5
1	A	348	GLY	6.5
1	A	361	PRO	6.4
1	A	479	GLU	6.2
1	A	439	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	347	GLY	6.1
1	A	433	ILE	6.1
1	A	476	LYS	6.1
1	A	482	GLU	6.1
1	A	475	GLN	6.0
1	A	345	PHE	6.0
1	A	496	ARG	5.9
1	A	363	GLU	5.9
1	A	362	ASP	5.9
1	A	450	LEU	5.9
1	A	428	LEU	5.8
1	A	379	VAL	5.8
1	A	320	ASP	5.8
1	A	341	MET	5.7
1	A	381	PRO	5.7
1	A	444	LEU	5.7
1	A	431	VAL	5.7
1	A	338	LYS	5.6
1	A	340	ASP	5.6
1	A	342	HIS	5.5
1	A	380	GLU	5.5
1	A	372	ILE	5.5
1	A	350	THR	5.4
1	A	437	ALA	5.4
1	A	486	LYS	5.3
1	A	489	ALA	5.3
1	A	493	ALA	5.3
1	A	435	LYS	5.3
1	A	424	ALA	5.2
1	A	333	GLY	5.2
1	A	373	GLY	5.2
1	A	126	PRO	5.2
1	A	346	GLY	5.2
1	A	412	TYR	5.2
1	A	349	LYS	5.1
1	A	451	LEU	5.1
1	A	696	ARG	5.1
1	A	368	LYS	5.0
1	A	471	TYR	5.0
1	A	473	ASP	5.0
1	A	481	ARG	4.9
1	A	494	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	522	ILE	4.9
1	A	326	ASN	4.8
1	A	478	LEU	4.7
1	A	408	ARG	4.7
1	A	447	LEU	4.7
1	A	520	VAL	4.7
1	A	135	TRP	4.5
1	A	485	ARG	4.5
1	A	375	ASP	4.5
1	A	391	VAL	4.3
1	A	324	PRO	4.2
1	A	365	GLU	4.2
1	A	328	GLY	4.2
1	A	172	ALA	4.2
1	A	318	SER	4.1
1	A	306	GLN	4.1
1	A	125	THR	4.0
1	A	344	GLU	4.0
1	A	198	GLU	4.0
1	A	387	ILE	4.0
1	A	604	ILE	3.9
1	A	445	LYS	3.9
1	A	446	HIS	3.9
1	A	483	ILE	3.9
1	A	670	VAL	3.9
1	A	170	LYS	3.8
1	A	388	GLY	3.8
1	A	354	GLU	3.8
1	A	421	TRP	3.8
1	A	330	ALA	3.8
1	A	343	VAL	3.7
1	A	371	VAL	3.7
1	A	393	ILE	3.7
1	A	394	TYR	3.7
1	A	179	LEU	3.6
1	A	256	LEU	3.6
1	A	322	ASP	3.6
1	A	385	LEU	3.6
1	A	383	GLY	3.6
1	A	616	ILE	3.6
1	A	411	HIS	3.6
1	A	258	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	443	ARG	3.5
1	A	332	GLU	3.5
1	A	470	ILE	3.5
1	A	702	ILE	3.5
1	A	128	ASN	3.5
1	A	303	LYS	3.4
1	A	480	LEU	3.4
1	A	436	GLU	3.4
1	A	329	PRO	3.4
1	A	65	LEU	3.4
1	A	449	GLN	3.4
1	A	384	ARG	3.3
1	A	521	CYS	3.3
1	A	13	GLY	3.3
1	A	24	LEU	3.3
1	A	334	GLU	3.2
1	A	127	GLU	3.2
1	A	230	LEU	3.2
1	A	671	VAL	3.2
1	A	353	PHE	3.2
1	A	425	GLN	3.2
1	A	376	ILE	3.1
1	A	302	ASP	3.1
1	A	490	GLU	3.1
1	A	523	VAL	3.1
1	A	115	ILE	3.1
1	A	474	GLU	3.0
1	A	273	ILE	3.0
1	A	429	THR	3.0
1	A	396	ARG	3.0
1	A	192	ILE	3.0
1	A	497	GLU	2.9
1	A	202	LYS	2.9
1	A	465	ARG	2.9
1	A	488	TYR	2.9
1	A	203	LEU	2.8
1	A	23	ARG	2.8
1	A	595	MET	2.8
1	A	9	GLN	2.8
1	A	356	VAL	2.8
1	A	491	ARG	2.8
1	A	33	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	410	ILE	2.8
1	A	596	THR	2.8
1	A	70	ALA	2.7
1	A	6	ASN	2.7
1	A	224	TYR	2.7
1	A	417	GLY	2.7
1	A	5	ILE	2.6
1	A	378	SER	2.6
1	A	617	VAL	2.6
1	A	196	LEU	2.6
1	A	442	ALA	2.6
1	A	649	GLY	2.6
1	A	699	ILE	2.6
1	A	585	MET	2.6
1	A	423	THR	2.6
1	A	12	GLU	2.5
1	A	418	GLU	2.5
1	A	19	LYS	2.5
1	A	162	ILE	2.5
1	A	76	VAL	2.5
1	A	667	LEU	2.4
1	A	68	ILE	2.4
1	A	175	ILE	2.4
1	A	323	LEU	2.4
1	A	432	ARG	2.4
1	A	648	MET	2.4
1	A	672	TRP	2.4
1	A	191	GLU	2.3
1	A	487	LYS	2.3
1	A	469	THR	2.3
1	A	200	ASN	2.3
1	A	66	PRO	2.3
1	A	119	LEU	2.3
1	A	605	MET	2.3
1	A	207	TYR	2.3
1	A	546	ASN	2.3
1	A	292	LYS	2.3
1	A	673	MET	2.3
1	A	606	ALA	2.3
1	A	448	GLY	2.2
1	A	201	VAL	2.2
1	A	102	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	2.2
1	A	295	PHE	2.2
1	A	351	PRO	2.2
1	A	352	SER	2.2
1	A	359	VAL	2.1
1	A	335	SER	2.1
1	A	392	ASP	2.1
1	A	225	ALA	2.1
1	A	293	ASP	2.1
1	A	174	LYS	2.1
1	A	226	LEU	2.1
1	A	614	PHE	2.0
1	A	615	MET	2.0
1	A	315	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	966	6/6	0.33	0.33	6.04	63,84,90,92	0
4	GOL	A	965	6/6	0.71	0.32	4.35	74,96,108,109	0
4	GOL	A	962	6/6	0.69	0.36	3.00	48,59,66,71	0
4	GOL	A	970	6/6	0.65	0.25	2.25	95,107,113,115	0
4	GOL	A	959	6/6	0.85	0.20	1.33	85,98,102,107	0
4	GOL	A	960	6/6	0.71	0.19	1.06	88,101,102,103	0
2	NI	A	735	1/1	1.00	0.09	-0.68	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SF4	A	733	8/8	0.95	0.07	-1.24	44,47,48,48	0
2	NI	A	734	1/1	0.95	0.04	-1.50	53,53,53,53	0
4	GOL	A	967	6/6	0.81	0.34	-	85,95,101,101	0
4	GOL	A	961	6/6	0.81	0.20	-	94,104,108,113	0
4	GOL	A	968	6/6	0.54	0.41	-	79,83,92,94	0
4	GOL	A	963	6/6	0.52	0.48	-	108,119,123,125	0
4	GOL	A	964	6/6	0.47	0.49	-	90,106,110,114	0
4	GOL	A	969	6/6	0.66	0.43	-	63,70,84,87	0

6.5 Other polymers

There are no such residues in this entry.