Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 02:05 AM EDT

PDB ID	:	1RE5
Title	:	Crystal structure of 3-carboxy-cis,cis-muconate lactonizing enzyme from Pseudomonas putida
Authors	:	Yang, J.; Wang, Y.; Woolridge, E.M.; Petsko, G.A.; Kozarich, J.W.; Ringe, D.
Deposited on	:	2003-11-06
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

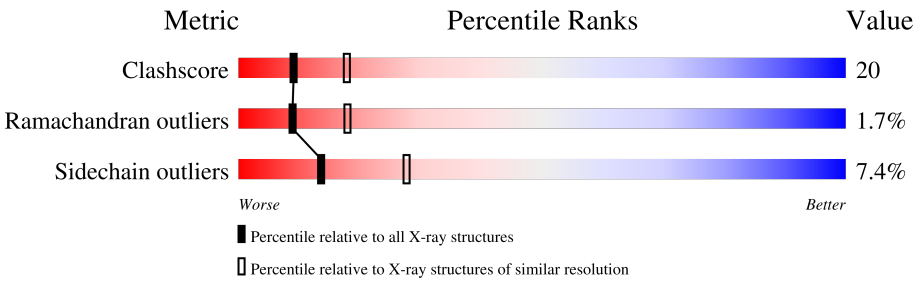
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	450	66% 27% • •
1	B	450	64% 29% • •
1	C	450	66% 27% 5% •
1	D	450	63% 31% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTT	A	802	X	X	X	-
2	DTT	B	801	X	X	X	-
3	CIT	C	800	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13314 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.

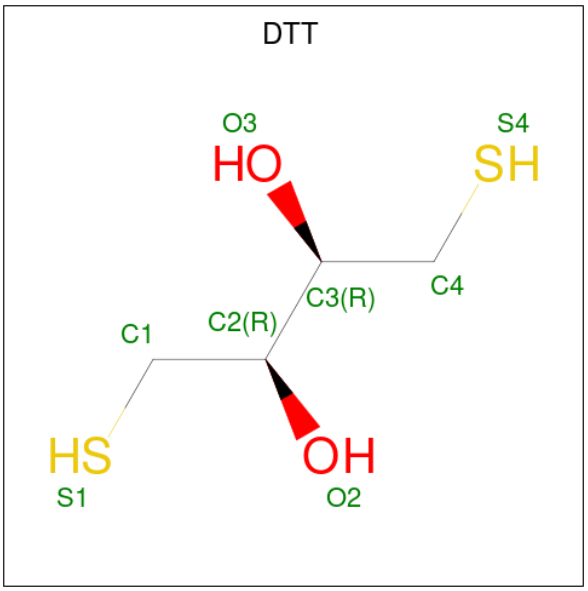
- Molecule 1 is a protein called 3-carboxy-cis,cis-muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3268	2049	595	610	14	0	0	0
1	B	441	3297	2068	601	613	15	0	0	0
1	C	440	3289	2062	600	613	14	0	0	0
1	D	448	3331	2086	608	622	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

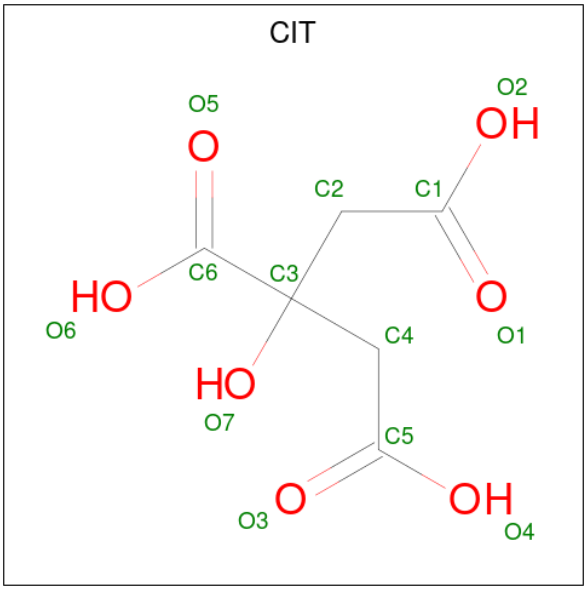
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	THR	VAL	conflict	UNP Q88N37
B	64	THR	VAL	conflict	UNP Q88N37
C	64	THR	VAL	conflict	UNP Q88N37
D	64	THR	VAL	conflict	UNP Q88N37

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	8	4	2	2	0	0
			Total	C	O	S		
2	B	1	8	4	2	2	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	13	6	7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	25	25	25	0	0
			Total	O		
4	B	23	23	23	0	0
			Total	O		
4	C	19	19	19	0	0
			Total	O		
4	D	33	33	33	0	0

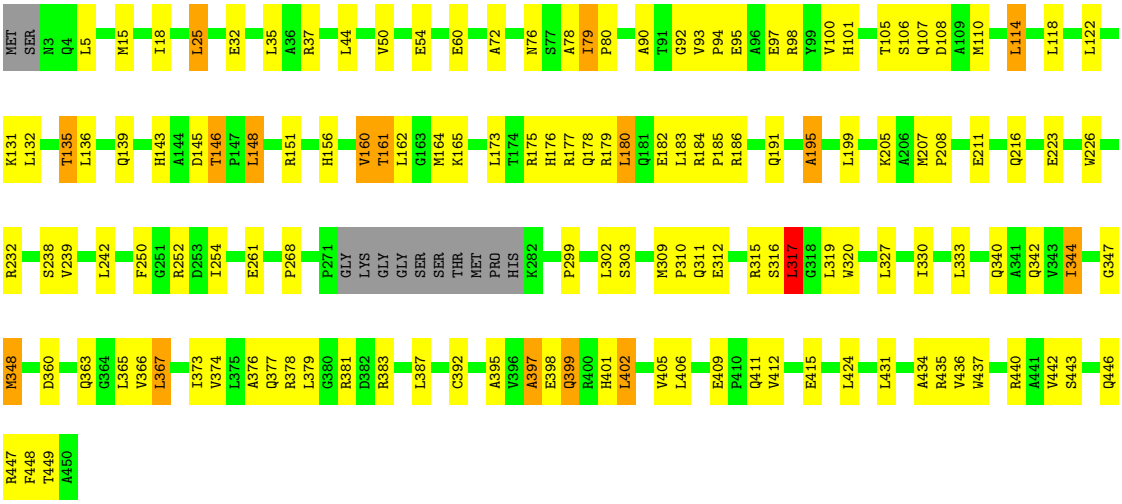
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

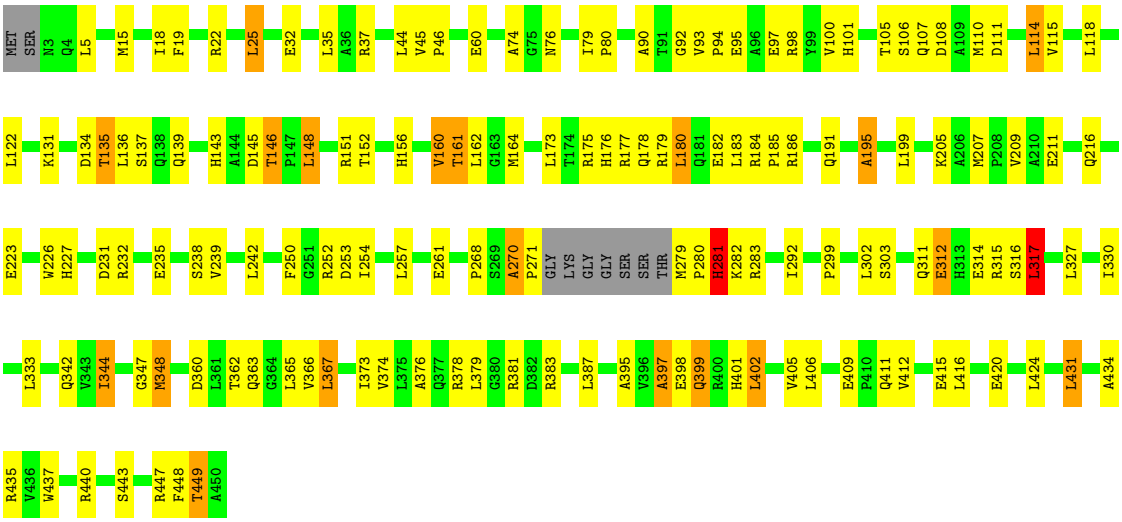
• Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase

Chain A: 66% 27%



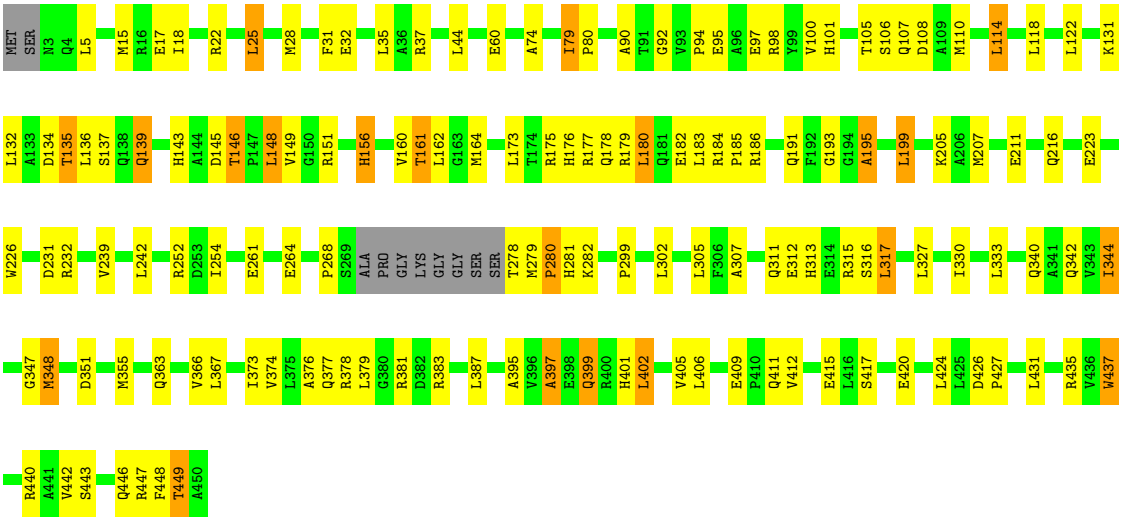
• Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase

Chain B: 64% 29%



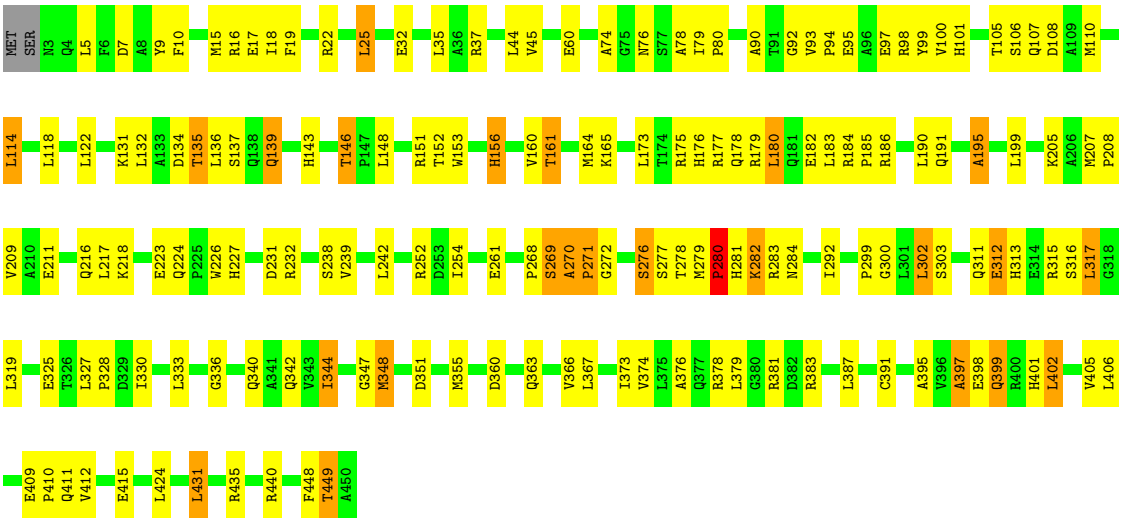
• Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase

Chain C:



• Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	231.52Å 231.52Å 78.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	86.4 (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13314	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, DTT

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	0.37	0/3321	0.62	2/4512 (0.0%)
1	B	0.38	0/3352	0.63	2/4553 (0.0%)
1	C	0.38	0/3343	0.62	1/4541 (0.0%)
1	D	0.39	0/3387	0.62	1/4601 (0.0%)
All	All	0.38	0/13403	0.62	6/18207 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	148	LEU	CA-CB-CG	6.97	131.33	115.30
1	B	148	LEU	CA-CB-CG	6.85	131.06	115.30
1	C	148	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	148	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	317	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	317	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3268	0	3277	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3297	0	3311	150	0
1	C	3289	0	3299	138	0
1	D	3331	0	3335	169	0
2	A	8	0	9	5	0
2	B	8	0	8	5	0
3	C	13	0	5	4	0
4	A	25	0	0	3	0
4	B	23	0	0	4	0
4	C	19	0	0	2	0
4	D	33	0	0	6	0
All	All	13314	0	13244	531	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 20.

All (531) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:MET:HA	1:C:282:LYS:HE3	1.32	1.11
1:B:362:THR:HB	1:D:280:PRO:HG3	1.34	1.10
1:C:161:THR:HG22	1:C:164:MET:HB2	1.40	1.04
1:C:135:THR:HG21	1:C:342:GLN:HE22	1.23	1.01
1:B:107:GLN:HE21	1:B:315:ARG:HH11	1.05	1.00
1:C:107:GLN:HE21	1:C:315:ARG:HH11	1.06	1.00
1:A:107:GLN:HE21	1:A:315:ARG:HH11	1.01	1.00
1:B:107:GLN:HE21	1:B:315:ARG:NH1	1.63	0.97
1:D:135:THR:HG21	1:D:342:GLN:HE22	1.29	0.97
1:C:191:GLN:HE22	1:C:226:TRP:H	1.05	0.96
1:D:191:GLN:HE22	1:D:226:TRP:H	1.08	0.94
1:A:191:GLN:HE22	1:A:226:TRP:H	0.99	0.94
1:B:135:THR:HG21	1:B:342:GLN:HE22	1.28	0.94
1:D:107:GLN:HE21	1:D:315:ARG:HH11	1.15	0.94
1:D:37:ARG:HH11	1:D:216:GLN:NE2	1.67	0.92
1:A:161:THR:HG22	1:A:164:MET:HB2	1.49	0.92
1:C:107:GLN:NE2	1:C:315:ARG:HH11	1.67	0.92
1:B:107:GLN:NE2	1:B:315:ARG:HH11	1.68	0.91
1:A:107:GLN:HE21	1:A:315:ARG:NH1	1.70	0.90
1:A:381:ARG:HH11	1:B:98:ARG:HD2	1.37	0.89
1:A:135:THR:HG21	1:A:342:GLN:HE22	1.35	0.89
1:B:191:GLN:HE22	1:B:226:TRP:H	1.17	0.89
1:A:107:GLN:NE2	1:A:315:ARG:HH11	1.69	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:HG22	1:B:164:MET:HB2	1.54	0.88
1:D:161:THR:HG22	1:D:164:MET:HB2	1.53	0.87
1:A:79:ILE:HG12	1:A:80:PRO:HD3	1.56	0.86
1:C:107:GLN:HE21	1:C:315:ARG:NH1	1.72	0.86
1:C:98:ARG:HD2	1:D:381:ARG:HH11	1.40	0.85
1:D:107:GLN:HE21	1:D:315:ARG:NH1	1.75	0.84
1:D:107:GLN:NE2	1:D:315:ARG:HH11	1.76	0.83
1:C:37:ARG:HH11	1:C:216:GLN:NE2	1.76	0.83
1:A:37:ARG:HH11	1:A:216:GLN:NE2	1.77	0.82
1:B:37:ARG:HH11	1:B:216:GLN:NE2	1.77	0.82
1:C:381:ARG:HH11	1:D:98:ARG:HD2	1.44	0.81
1:C:280:PRO:HG2	1:C:281:HIS:ND1	1.95	0.81
1:B:365:LEU:HB2	1:D:280:PRO:HG2	1.63	0.80
2:A:802:DTT:H3	1:D:299:PRO:HB2	1.63	0.80
1:D:176:HIS:HD2	1:D:179:ARG:HH11	1.31	0.79
1:A:98:ARG:HH11	1:B:381:ARG:HD2	1.46	0.79
1:B:161:THR:CG2	1:B:164:MET:H	1.95	0.79
1:D:79:ILE:HG12	1:D:80:PRO:HD3	1.63	0.79
1:C:37:ARG:HD2	1:C:216:GLN:NE2	1.99	0.78
1:C:106:SER:HB3	1:C:110:MET:HE2	1.66	0.78
1:C:79:ILE:HG12	1:C:80:PRO:HD3	1.66	0.78
1:D:161:THR:CG2	1:D:164:MET:H	1.96	0.78
1:A:381:ARG:HD2	1:B:98:ARG:HH11	1.49	0.77
1:B:365:LEU:CB	1:D:280:PRO:HG2	2.14	0.77
1:A:98:ARG:HD2	1:B:381:ARG:HH11	1.49	0.77
1:A:161:THR:CG2	1:A:164:MET:H	1.98	0.76
1:A:299:PRO:HB2	2:B:801:DTT:H11	1.65	0.76
1:A:381:ARG:NH1	1:B:98:ARG:HD2	2.00	0.76
1:D:281:HIS:O	1:D:283:ARG:N	2.17	0.76
1:C:302:LEU:HD12	1:C:330:ILE:HD13	1.68	0.76
1:C:381:ARG:HD2	1:D:98:ARG:HH11	1.49	0.76
1:B:365:LEU:HB2	1:D:280:PRO:CG	2.16	0.75
1:B:79:ILE:HG12	1:B:80:PRO:HD3	1.68	0.75
1:C:279:MET:CA	1:C:282:LYS:HE3	2.16	0.75
1:B:161:THR:HG22	1:B:164:MET:H	1.52	0.74
1:A:32:GLU:OE1	1:A:101:HIS:HD2	1.69	0.74
1:B:107:GLN:NE2	1:B:315:ARG:NH1	2.30	0.74
1:D:143:HIS:HD2	1:D:146:THR:HG21	1.51	0.74
1:D:143:HIS:CD2	1:D:146:THR:HG21	2.23	0.74
1:B:362:THR:CB	1:D:280:PRO:HG3	2.15	0.74
1:A:44:LEU:HD21	1:A:205:LYS:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HD21	1:B:205:LYS:HG3	1.69	0.73
1:D:37:ARG:HD2	1:D:216:GLN:NE2	2.03	0.73
1:A:107:GLN:NE2	1:A:315:ARG:NH1	2.34	0.73
1:C:98:ARG:HD2	1:D:381:ARG:NH1	2.02	0.73
1:C:15:MET:HE3	1:C:18:ILE:HD12	1.69	0.72
1:B:374:VAL:HG21	1:B:424:LEU:HD21	1.72	0.72
1:A:374:VAL:HG21	1:A:424:LEU:HD21	1.71	0.71
1:C:381:ARG:NH1	1:D:98:ARG:HD2	2.05	0.71
1:B:37:ARG:HD2	1:B:216:GLN:NE2	2.05	0.71
1:D:44:LEU:HD21	1:D:205:LYS:HG3	1.71	0.71
1:C:161:THR:CG2	1:C:164:MET:H	2.02	0.71
1:A:161:THR:HG23	1:A:164:MET:H	1.56	0.70
1:A:381:ARG:HH11	1:B:98:ARG:CD	2.04	0.70
1:D:156:HIS:HD2	4:D:474:HOH:O	1.75	0.70
1:C:311:GLN:HB3	1:C:316:SER:HB3	1.74	0.70
1:D:180:LEU:HD13	1:D:239:VAL:HG11	1.73	0.70
1:B:431:LEU:HD23	1:B:435:ARG:HH12	1.56	0.69
1:D:374:VAL:HG21	1:D:424:LEU:HD21	1.74	0.69
1:A:98:ARG:HD2	1:B:381:ARG:NH1	2.07	0.69
2:B:801:DTT:H3	1:C:299:PRO:HB2	1.74	0.69
1:D:278:THR:C	1:D:280:PRO:HD2	2.12	0.69
1:D:435:ARG:HG3	1:D:435:ARG:HH11	1.58	0.69
1:A:431:LEU:HD23	1:A:435:ARG:HH12	1.55	0.69
1:C:98:ARG:CD	1:D:381:ARG:HH11	2.05	0.69
1:B:15:MET:HE3	1:B:18:ILE:HD12	1.74	0.69
1:A:15:MET:HE3	1:A:18:ILE:HD12	1.74	0.69
1:A:60:GLU:CD	1:A:60:GLU:H	1.96	0.68
1:C:98:ARG:HH11	1:D:381:ARG:HD2	1.57	0.68
1:C:180:LEU:HD13	1:C:239:VAL:HG11	1.75	0.68
1:A:143:HIS:CD2	1:A:146:THR:HG21	2.28	0.68
1:B:114:LEU:HD22	1:B:118:LEU:HG	1.75	0.68
1:C:44:LEU:HD21	1:C:205:LYS:HG3	1.75	0.68
1:D:252:ARG:HD3	4:D:471:HOH:O	1.94	0.68
1:A:98:ARG:CD	1:B:381:ARG:HH11	2.07	0.68
1:A:143:HIS:HD2	1:A:146:THR:HG21	1.59	0.68
1:A:379:LEU:HD21	1:A:415:GLU:HG3	1.76	0.68
1:D:114:LEU:HD22	1:D:118:LEU:HG	1.76	0.68
1:C:176:HIS:HD2	1:C:179:ARG:HH11	1.40	0.67
1:D:15:MET:HE3	1:D:18:ILE:HD12	1.77	0.67
1:C:186:ARG:O	1:C:232:ARG:HD3	1.94	0.67
1:D:105:THR:HG22	1:D:108:ASP:OD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLN:HB3	1:B:316:SER:HB3	1.75	0.67
1:C:92:GLY:O	1:C:94:PRO:HD3	1.96	0.66
1:D:32:GLU:OE1	1:D:101:HIS:HD2	1.77	0.66
1:C:173:LEU:O	1:C:177:ARG:HG3	1.96	0.66
1:C:161:THR:HG23	1:C:164:MET:H	1.59	0.66
1:C:32:GLU:OE1	1:C:101:HIS:HD2	1.79	0.66
1:C:431:LEU:HD23	1:C:435:ARG:HH12	1.60	0.66
1:C:252:ARG:HD3	4:C:818:HOH:O	1.95	0.65
1:C:279:MET:N	1:C:280:PRO:HD3	2.11	0.65
1:A:176:HIS:HD2	1:A:179:ARG:HH11	1.45	0.65
1:C:381:ARG:HH11	1:D:98:ARG:CD	2.07	0.65
1:A:238:SER:HA	1:A:302:LEU:HD21	1.79	0.65
1:A:173:LEU:O	1:A:177:ARG:HG3	1.97	0.65
1:D:161:THR:HG22	1:D:164:MET:H	1.60	0.65
1:B:79:ILE:CG1	1:B:80:PRO:HD3	2.28	0.64
1:A:25:LEU:HD13	1:D:5:LEU:HD11	1.80	0.64
1:C:139:GLN:HA	1:C:139:GLN:HE21	1.62	0.64
1:A:180:LEU:HD13	1:A:239:VAL:HG11	1.80	0.64
1:D:60:GLU:CD	1:D:60:GLU:H	2.02	0.63
1:C:107:GLN:NE2	1:C:315:ARG:NH1	2.39	0.63
1:B:180:LEU:HD13	1:B:239:VAL:HG11	1.81	0.63
1:D:161:THR:HG22	1:D:164:MET:CB	2.29	0.63
1:A:402:LEU:HD22	1:A:406:LEU:HG	1.79	0.63
1:D:37:ARG:HH11	1:D:216:GLN:HE22	1.45	0.63
1:A:143:HIS:HB3	1:A:146:THR:HG23	1.81	0.63
1:D:107:GLN:NE2	1:D:315:ARG:NH1	2.40	0.63
1:B:176:HIS:HD2	1:B:179:ARG:HH11	1.46	0.62
1:A:186:ARG:O	1:A:232:ARG:HD3	1.99	0.62
1:C:105:THR:HG22	1:C:108:ASP:OD2	1.99	0.62
1:D:92:GLY:O	1:D:94:PRO:HD3	1.99	0.62
1:A:145:ASP:HB3	1:A:435:ARG:HH11	1.64	0.62
1:B:37:ARG:HH11	1:B:216:GLN:HE21	1.48	0.61
1:D:79:ILE:CG1	1:D:80:PRO:HD3	2.29	0.61
1:B:92:GLY:O	1:B:94:PRO:HD3	2.01	0.61
1:B:106:SER:HB3	1:B:110:MET:HE2	1.82	0.61
1:B:139:GLN:HE21	1:B:139:GLN:HA	1.65	0.61
1:A:252:ARG:HD3	4:A:825:HOH:O	2.00	0.61
1:A:92:GLY:O	1:A:94:PRO:HD3	1.99	0.61
1:B:281:HIS:O	1:B:283:ARG:N	2.33	0.61
1:C:60:GLU:CD	1:C:60:GLU:H	2.04	0.61
1:A:254:ILE:HG13	1:A:344:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:OE1	1:C:151:ARG:NH1	2.33	0.61
1:B:151:ARG:NH1	1:D:261:GLU:OE1	2.34	0.61
1:A:37:ARG:HD2	1:A:216:GLN:NE2	2.15	0.60
1:D:270:ALA:HB1	1:D:271:PRO:HD2	1.81	0.60
1:D:139:GLN:HA	1:D:139:GLN:HE21	1.65	0.60
1:A:440:ARG:HD3	1:B:223:GLU:O	2.01	0.59
1:C:374:VAL:HG21	1:C:424:LEU:HD21	1.83	0.59
1:D:207:MET:O	1:D:211:GLU:HG3	2.03	0.59
1:A:299:PRO:HB2	2:B:801:DTT:C1	2.32	0.59
1:C:383:ARG:NH2	1:C:411:GLN:HG2	2.17	0.59
1:A:191:GLN:NE2	1:A:226:TRP:H	1.84	0.59
1:B:60:GLU:H	1:B:60:GLU:CD	2.04	0.59
1:C:223:GLU:O	1:D:440:ARG:HD3	2.02	0.59
1:C:252:ARG:CD	4:C:818:HOH:O	2.50	0.59
1:D:252:ARG:CD	4:D:471:HOH:O	2.49	0.59
1:B:186:ARG:O	1:B:232:ARG:HD3	2.03	0.59
1:B:252:ARG:HD3	4:B:815:HOH:O	2.03	0.59
1:D:402:LEU:HD22	1:D:406:LEU:HG	1.85	0.59
1:D:435:ARG:HG3	1:D:435:ARG:NH1	2.18	0.58
1:C:114:LEU:HD22	1:C:118:LEU:HG	1.85	0.58
1:D:161:THR:HG23	1:D:164:MET:H	1.68	0.58
1:B:402:LEU:HD22	1:B:406:LEU:HG	1.85	0.58
1:D:270:ALA:HB1	1:D:271:PRO:CD	2.34	0.58
1:B:145:ASP:HB3	1:B:435:ARG:HH11	1.68	0.58
1:B:302:LEU:HD12	1:B:330:ILE:HD13	1.84	0.58
1:B:397:ALA:C	1:B:399:GLN:H	2.07	0.57
1:A:363:GLN:HB3	1:A:401:HIS:HA	1.86	0.57
1:A:302:LEU:HD12	1:A:330:ILE:HD13	1.86	0.57
1:D:378:ARG:HG2	1:D:378:ARG:HH11	1.68	0.57
1:A:317:LEU:HD22	1:D:292:ILE:HD12	1.85	0.57
1:D:311:GLN:HB3	1:D:316:SER:HB3	1.85	0.57
1:A:79:ILE:CG1	1:A:80:PRO:HD3	2.31	0.57
1:D:254:ILE:HG13	1:D:344:ILE:CD1	2.33	0.57
1:C:254:ILE:HG13	1:C:344:ILE:CD1	2.35	0.57
1:D:176:HIS:CD2	1:D:179:ARG:HH11	2.16	0.57
1:A:254:ILE:HG13	1:A:344:ILE:HD11	1.87	0.57
1:D:173:LEU:O	1:D:177:ARG:HG3	2.05	0.56
1:A:397:ALA:C	1:A:399:GLN:H	2.08	0.56
1:B:131:LYS:HE3	4:B:818:HOH:O	2.04	0.56
1:C:440:ARG:HD3	1:D:223:GLU:O	2.05	0.56
1:B:105:THR:HG22	1:B:108:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ILE:HG13	1:B:344:ILE:CD1	2.34	0.56
1:C:79:ILE:CG1	1:C:80:PRO:HD3	2.34	0.56
1:C:373:ILE:O	1:C:376:ALA:HB3	2.06	0.56
1:A:114:LEU:HD22	1:A:118:LEU:HG	1.87	0.56
1:A:195:ALA:O	1:A:315:ARG:NH2	2.39	0.55
1:B:238:SER:HA	1:B:302:LEU:HD21	1.88	0.55
1:C:254:ILE:HG13	1:C:344:ILE:HD11	1.87	0.55
1:C:387:LEU:HD11	1:C:409:GLU:CD	2.27	0.55
1:C:268:PRO:HG3	1:C:347:GLY:C	2.27	0.55
1:D:45:VAL:HG22	1:D:99:TYR:CD2	2.41	0.55
1:D:383:ARG:NH2	1:D:411:GLN:HG2	2.21	0.55
1:C:145:ASP:HB3	1:C:435:ARG:HH11	1.70	0.55
1:C:363:GLN:HB3	1:C:401:HIS:HA	1.89	0.55
1:D:270:ALA:O	1:D:272:GLY:N	2.40	0.55
1:A:97:GLU:O	1:A:100:VAL:HG12	2.07	0.55
1:B:173:LEU:O	1:B:177:ARG:HG3	2.07	0.55
3:C:800:CIT:C1	3:C:800:CIT:O5	2.55	0.55
1:D:271:PRO:HB2	1:D:276:SER:CB	2.37	0.55
1:C:143:HIS:CD2	1:C:146:THR:HG21	2.42	0.55
1:D:93:VAL:HG13	1:D:95:GLU:OE2	2.07	0.55
1:B:161:THR:HG22	1:B:164:MET:CB	2.33	0.54
1:B:363:GLN:HB3	1:B:401:HIS:HA	1.88	0.54
1:A:207:MET:O	1:A:211:GLU:HG3	2.07	0.54
1:C:135:THR:HG21	1:C:342:GLN:NE2	2.07	0.54
1:C:344:ILE:O	1:C:348:MET:HG3	2.07	0.54
1:A:161:THR:HG22	1:A:164:MET:CB	2.30	0.54
1:B:280:PRO:O	1:B:281:HIS:HB2	2.06	0.54
1:B:311:GLN:HB3	1:B:316:SER:CB	2.37	0.54
1:C:191:GLN:NE2	1:C:226:TRP:H	1.90	0.54
1:B:379:LEU:HD21	1:B:415:GLU:HG3	1.89	0.54
1:A:383:ARG:NH2	1:A:411:GLN:HG2	2.22	0.54
1:B:443:SER:O	1:B:447:ARG:HG2	2.07	0.54
1:D:381:ARG:NH2	4:D:475:HOH:O	2.40	0.54
1:D:397:ALA:C	1:D:399:GLN:H	2.10	0.54
1:C:302:LEU:HD12	1:C:330:ILE:CD1	2.38	0.54
1:D:165:LYS:HE3	4:D:454:HOH:O	2.07	0.54
1:A:76:ASN:HB2	1:A:110:MET:HE1	1.90	0.54
1:D:344:ILE:O	1:D:348:MET:HG3	2.07	0.54
1:A:311:GLN:HB3	1:A:316:SER:HB3	1.90	0.53
1:C:37:ARG:HH11	1:C:216:GLN:HE22	1.55	0.53
1:D:282:LYS:O	1:D:284:ASN:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ALA:C	1:C:399:GLN:H	2.11	0.53
2:A:802:DTT:C1	1:B:299:PRO:HB2	2.38	0.53
1:C:178:GLN:O	1:C:182:GLU:HG3	2.09	0.53
1:D:223:GLU:HG2	1:D:224:GLN:HG2	1.90	0.53
1:D:302:LEU:HD12	1:D:330:ILE:HD13	1.90	0.53
1:A:161:THR:HG22	1:A:164:MET:H	1.74	0.53
1:A:344:ILE:O	1:A:348:MET:HG3	2.09	0.53
1:D:90:ALA:O	1:D:94:PRO:HG3	2.09	0.53
1:D:176:HIS:CD2	1:D:179:ARG:NH1	2.77	0.53
1:D:238:SER:HA	1:D:302:LEU:HD21	1.91	0.52
1:B:362:THR:HG21	1:D:280:PRO:HA	1.91	0.52
1:A:76:ASN:HB2	1:A:110:MET:CE	2.39	0.52
1:D:143:HIS:HB3	1:D:146:THR:HG23	1.91	0.52
1:A:435:ARG:HH11	1:A:435:ARG:HG3	1.74	0.52
1:B:134:ASP:O	1:B:137:SER:HB3	2.10	0.52
1:D:205:LYS:O	1:D:209:VAL:HG23	2.09	0.52
1:D:448:PHE:O	1:D:449:THR:C	2.47	0.52
1:A:90:ALA:O	1:A:94:PRO:HG3	2.10	0.52
1:D:15:MET:HE1	1:D:19:PHE:HE2	1.74	0.52
2:A:802:DTT:H2	1:C:307:ALA:HB2	1.91	0.52
1:B:106:SER:HB3	1:B:110:MET:CE	2.40	0.52
1:B:161:THR:HG22	1:B:164:MET:N	2.24	0.52
1:B:344:ILE:O	1:B:348:MET:HG3	2.09	0.52
1:C:402:LEU:HD22	1:C:406:LEU:HG	1.92	0.52
1:B:261:GLU:OE1	1:D:151:ARG:NH1	2.43	0.51
1:A:5:LEU:HD11	1:D:25:LEU:HD13	1.92	0.51
1:A:261:GLU:HB2	1:C:261:GLU:HB2	1.93	0.51
1:D:395:ALA:HA	1:D:405:VAL:HG21	1.93	0.51
1:D:186:ARG:O	1:D:232:ARG:HD3	2.11	0.51
1:B:395:ALA:HA	1:B:405:VAL:HG21	1.92	0.51
1:B:448:PHE:O	1:B:449:THR:C	2.49	0.51
1:C:90:ALA:O	1:C:94:PRO:HG3	2.10	0.51
3:C:800:CIT:C5	1:D:152:THR:HG21	2.41	0.51
1:D:176:HIS:HD2	1:D:179:ARG:NH1	2.04	0.51
1:D:195:ALA:O	1:D:315:ARG:NH2	2.43	0.51
1:D:363:GLN:HB3	1:D:401:HIS:HA	1.92	0.51
1:C:195:ALA:O	1:C:315:ARG:NH2	2.44	0.51
1:C:311:GLN:HB3	1:C:316:SER:CB	2.39	0.51
1:A:93:VAL:HG13	1:A:95:GLU:OE2	2.10	0.50
1:A:160:VAL:CG1	1:A:161:THR:N	2.74	0.50
1:C:139:GLN:HA	1:C:139:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:HIS:HB3	1:A:146:THR:CG2	2.40	0.50
1:D:254:ILE:HG13	1:D:344:ILE:HD11	1.92	0.50
1:B:90:ALA:O	1:B:94:PRO:HG3	2.12	0.50
1:B:143:HIS:HD2	1:B:146:THR:HG21	1.77	0.50
1:B:205:LYS:O	1:B:209:VAL:HG23	2.12	0.50
1:B:161:THR:HG23	1:B:164:MET:H	1.73	0.50
1:B:381:ARG:HG3	4:B:816:HOH:O	2.11	0.50
1:B:15:MET:HE1	1:B:19:PHE:HE2	1.77	0.49
1:B:253:ASP:O	1:B:257:LEU:HG	2.12	0.49
1:C:148:LEU:CD2	1:C:162:LEU:N	2.75	0.49
1:C:282:LYS:HG3	1:C:282:LYS:O	2.11	0.49
1:D:37:ARG:NH1	1:D:216:GLN:NE2	2.48	0.49
1:A:223:GLU:O	1:B:440:ARG:HD3	2.12	0.49
1:C:435:ARG:HH11	1:C:435:ARG:HG3	1.77	0.49
1:B:15:MET:HE1	1:B:19:PHE:CE2	2.47	0.49
1:D:183:LEU:HD12	1:D:183:LEU:C	2.32	0.49
1:D:184:ARG:N	1:D:185:PRO:HD2	2.27	0.49
1:B:183:LEU:HD12	1:B:183:LEU:C	2.33	0.49
1:B:207:MET:O	1:B:211:GLU:HG3	2.11	0.49
1:B:395:ALA:O	1:B:399:GLN:HA	2.13	0.49
1:A:268:PRO:HG3	1:A:347:GLY:C	2.33	0.49
1:A:303:SER:OG	2:A:802:DTT:H42	2.12	0.49
1:C:268:PRO:HG3	1:C:347:GLY:O	2.12	0.49
1:C:279:MET:HA	1:C:282:LYS:CE	2.23	0.49
1:A:395:ALA:HA	1:A:405:VAL:HG21	1.93	0.49
1:D:268:PRO:HG3	1:D:347:GLY:C	2.33	0.49
1:B:108:ASP:OD1	1:B:227:HIS:HE1	1.96	0.49
1:B:395:ALA:CA	1:B:405:VAL:HG21	2.43	0.49
1:C:160:VAL:CG1	1:C:161:THR:N	2.76	0.49
1:B:254:ILE:HG13	1:B:344:ILE:HD11	1.94	0.49
1:A:402:LEU:CD2	1:A:406:LEU:HG	2.42	0.48
1:A:448:PHE:O	1:A:449:THR:C	2.50	0.48
1:C:132:LEU:O	1:C:136:LEU:HB2	2.13	0.48
1:B:25:LEU:HD13	1:C:5:LEU:HD11	1.95	0.48
1:C:106:SER:HB3	1:C:110:MET:CE	2.38	0.48
1:C:143:HIS:HB3	1:C:146:THR:HG23	1.95	0.48
1:C:143:HIS:HD2	1:C:146:THR:HG21	1.78	0.48
1:A:95:GLU:H	1:A:95:GLU:CD	2.17	0.48
1:A:232:ARG:NH2	4:A:821:HOH:O	2.45	0.48
1:A:131:LYS:O	1:A:135:THR:HG23	2.12	0.48
1:B:139:GLN:HA	1:B:139:GLN:NE2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLN:O	1:B:182:GLU:HG3	2.14	0.48
1:C:379:LEU:HD21	1:C:415:GLU:HG3	1.95	0.48
1:C:395:ALA:HA	1:C:405:VAL:HG21	1.95	0.48
1:A:145:ASP:HB3	1:A:435:ARG:NH1	2.29	0.48
1:B:152:THR:HG22	1:D:281:HIS:HE1	1.79	0.48
1:B:164:MET:HE2	1:B:434:ALA:CB	2.43	0.48
1:D:15:MET:HE1	1:D:19:PHE:CE2	2.49	0.48
1:B:268:PRO:HG3	1:B:347:GLY:C	2.34	0.48
1:C:160:VAL:HA	1:C:164:MET:HE3	1.95	0.48
1:D:379:LEU:HD21	1:D:415:GLU:HG3	1.95	0.48
1:A:78:ALA:HB3	1:A:106:SER:HB3	1.95	0.47
1:A:365:LEU:HB3	1:C:281:HIS:CE1	2.49	0.47
1:B:378:ARG:HG2	1:B:378:ARG:HH11	1.79	0.47
1:B:160:VAL:CG1	1:B:161:THR:N	2.77	0.47
1:B:184:ARG:N	1:B:185:PRO:HD2	2.29	0.47
1:D:317:LEU:H	1:D:317:LEU:CD1	2.26	0.47
1:A:186:ARG:HH21	1:B:178:GLN:HE21	1.63	0.47
1:A:252:ARG:CD	4:A:825:HOH:O	2.59	0.47
1:A:442:VAL:O	1:A:446:GLN:HG3	2.15	0.47
1:B:402:LEU:CD2	1:B:406:LEU:HG	2.44	0.47
1:A:139:GLN:HE21	1:A:139:GLN:HA	1.80	0.47
1:A:395:ALA:O	1:A:399:GLN:HA	2.14	0.47
1:B:143:HIS:HB3	1:B:146:THR:HG23	1.96	0.47
1:B:93:VAL:HG13	1:B:95:GLU:OE2	2.15	0.47
1:A:178:GLN:O	1:A:182:GLU:HG3	2.14	0.47
1:A:317:LEU:CD2	1:D:292:ILE:HD12	2.44	0.47
1:A:395:ALA:CA	1:A:405:VAL:HG21	2.44	0.47
1:C:161:THR:HG22	1:C:164:MET:H	1.78	0.47
1:C:176:HIS:CD2	1:C:179:ARG:HH11	2.28	0.47
1:C:417:SER:OG	1:C:420:GLU:HG3	2.14	0.47
1:C:448:PHE:O	1:C:449:THR:C	2.53	0.47
1:A:381:ARG:HD2	1:B:98:ARG:NH1	2.23	0.47
1:D:311:GLN:HB3	1:D:316:SER:CB	2.45	0.47
1:A:443:SER:O	1:A:447:ARG:HG2	2.15	0.47
1:C:17:GLU:OE2	1:C:22:ARG:NH1	2.48	0.47
1:C:105:THR:OG1	3:C:800:CIT:O5	2.32	0.47
1:D:373:ILE:O	1:D:376:ALA:HB3	2.14	0.47
1:B:143:HIS:CD2	1:B:146:THR:HG21	2.50	0.47
1:B:152:THR:CG2	1:D:281:HIS:CE1	2.98	0.47
1:C:395:ALA:CA	1:C:405:VAL:HG21	2.45	0.47
1:A:436:VAL:O	1:A:440:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:ALA:CA	1:D:405:VAL:HG21	2.45	0.46
1:C:184:ARG:N	1:C:185:PRO:HD2	2.31	0.46
1:C:231:ASP:OD2	1:D:175:ARG:NH1	2.48	0.46
1:C:252:ARG:NH1	1:D:312:GLU:HG3	2.29	0.46
1:D:279:MET:N	1:D:280:PRO:HD2	2.31	0.46
1:B:74:ALA:HB1	1:B:79:ILE:HG12	1.96	0.46
1:D:317:LEU:HD13	1:D:317:LEU:O	2.15	0.46
1:A:373:ILE:O	1:A:376:ALA:HB3	2.15	0.46
1:B:32:GLU:OE1	1:B:101:HIS:HD2	1.98	0.46
1:B:79:ILE:CG1	1:B:80:PRO:CD	2.94	0.46
1:D:37:ARG:HH11	1:D:216:GLN:HE21	1.54	0.46
1:A:435:ARG:HG3	1:A:435:ARG:NH1	2.30	0.46
1:C:97:GLU:O	1:C:100:VAL:HG12	2.14	0.46
1:D:134:ASP:O	1:D:137:SER:HB3	2.15	0.46
1:C:340:GLN:O	1:C:344:ILE:HG23	2.16	0.46
1:C:280:PRO:HG2	1:C:281:HIS:H	1.80	0.46
1:D:402:LEU:CD2	1:D:406:LEU:HG	2.46	0.46
1:B:365:LEU:HB3	1:D:280:PRO:HG2	1.94	0.46
1:C:378:ARG:HG2	1:C:378:ARG:HH11	1.81	0.46
1:D:395:ALA:O	1:D:399:GLN:HA	2.16	0.46
1:B:97:GLU:O	1:B:100:VAL:HG12	2.16	0.46
1:C:134:ASP:O	1:C:137:SER:HB3	2.16	0.46
1:B:435:ARG:HH11	1:B:435:ARG:HG3	1.80	0.46
1:D:387:LEU:HD11	1:D:409:GLU:CD	2.36	0.45
1:B:152:THR:HG22	1:D:281:HIS:CE1	2.51	0.45
1:A:107:GLN:HG3	1:A:320:TRP:CZ2	2.50	0.45
1:D:152:THR:HG23	1:D:153:TRP:HD1	1.81	0.45
1:D:351:ASP:O	1:D:355:MET:HG3	2.17	0.45
1:A:151:ARG:NH1	1:C:261:GLU:OE1	2.49	0.45
1:A:392:CYS:SG	1:C:278:THR:HG21	2.56	0.45
1:C:175:ARG:NH1	1:D:231:ASP:OD2	2.50	0.45
1:D:131:LYS:O	1:D:135:THR:HG23	2.16	0.45
1:B:79:ILE:HG13	1:B:80:PRO:N	2.31	0.45
1:C:207:MET:O	1:C:211:GLU:HG3	2.16	0.45
1:D:106:SER:HB3	1:D:110:MET:HE2	1.99	0.45
1:A:161:THR:CG2	1:A:164:MET:N	2.75	0.45
1:A:175:ARG:NH1	1:B:231:ASP:OD2	2.50	0.45
1:B:161:THR:CG2	1:B:164:MET:N	2.74	0.45
1:D:391:CYS:SG	1:D:406:LEU:HD23	2.57	0.45
1:D:17:GLU:OE2	1:D:22:ARG:NH1	2.50	0.45
1:A:37:ARG:HH11	1:A:216:GLN:HE21	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:THR:CG2	1:D:164:MET:N	2.74	0.45
1:A:105:THR:HG22	1:A:108:ASP:OD2	2.17	0.44
1:C:381:ARG:HD2	1:D:98:ARG:NH1	2.26	0.44
3:C:800:CIT:O3	1:D:152:THR:HG21	2.18	0.44
1:D:37:ARG:HD2	1:D:216:GLN:HE22	1.82	0.44
1:A:92:GLY:C	1:A:94:PRO:HD3	2.38	0.44
1:A:374:VAL:O	1:A:377:GLN:HG2	2.17	0.44
1:B:365:LEU:CB	1:D:280:PRO:CG	2.86	0.44
1:C:302:LEU:CD1	1:C:330:ILE:HD13	2.42	0.44
1:D:178:GLN:O	1:D:182:GLU:HG3	2.17	0.44
1:B:365:LEU:HD12	1:D:280:PRO:HD3	1.99	0.44
1:C:131:LYS:O	1:C:135:THR:HG23	2.18	0.44
1:A:183:LEU:C	1:A:183:LEU:HD12	2.38	0.44
1:C:435:ARG:HG3	1:C:435:ARG:NH1	2.32	0.44
1:D:7:ASP:OD2	1:D:16:ARG:HD2	2.18	0.44
1:C:383:ARG:NH2	1:C:411:GLN:CG	2.81	0.44
1:D:136:LEU:HD12	1:D:136:LEU:HA	1.87	0.44
1:A:50:VAL:O	1:A:54:GLU:HG3	2.17	0.44
1:B:387:LEU:HD11	1:B:409:GLU:CD	2.39	0.44
1:C:395:ALA:O	1:C:399:GLN:HA	2.17	0.44
1:D:279:MET:N	1:D:280:PRO:CD	2.79	0.44
1:B:367:LEU:HD12	1:B:367:LEU:HA	1.74	0.43
1:C:92:GLY:C	1:C:94:PRO:HD3	2.38	0.43
1:C:193:GLY:C	1:C:199:LEU:HD13	2.38	0.43
1:A:98:ARG:NH1	1:B:381:ARG:HD2	2.23	0.43
1:B:107:GLN:HE22	1:B:227:HIS:HB3	1.83	0.43
1:C:161:THR:HG22	1:C:164:MET:CB	2.27	0.43
1:C:351:ASP:O	1:C:355:MET:HG3	2.18	0.43
1:A:176:HIS:CD2	1:A:179:ARG:HH11	2.30	0.43
1:D:76:ASN:HB2	1:D:110:MET:CE	2.49	0.43
1:A:132:LEU:O	1:A:136:LEU:HB2	2.19	0.43
1:B:92:GLY:C	1:B:94:PRO:HD3	2.39	0.43
1:B:270:ALA:HA	1:B:271:PRO:HD3	1.90	0.43
1:A:184:ARG:N	1:A:185:PRO:HD2	2.34	0.43
1:A:387:LEU:HD11	1:A:409:GLU:CD	2.39	0.43
1:A:131:LYS:HE2	1:A:131:LYS:HB3	1.85	0.43
1:A:340:GLN:O	1:A:344:ILE:HG23	2.17	0.43
2:A:802:DTT:S4	1:D:300:GLY:N	2.92	0.43
1:B:5:LEU:HD11	1:C:25:LEU:HD13	2.01	0.43
1:B:409:GLU:HG3	1:B:412:VAL:H	1.83	0.43
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:O	1:D:100:VAL:HG12	2.19	0.43
1:D:410:PRO:HB2	1:D:411:GLN:OE1	2.19	0.43
1:B:186:ARG:NH1	1:B:235:GLU:OE2	2.52	0.42
1:B:435:ARG:HG3	1:B:435:ARG:NH1	2.34	0.42
1:C:176:HIS:HD2	1:C:179:ARG:NH1	2.12	0.42
1:A:378:ARG:HH11	1:A:378:ARG:HG2	1.85	0.42
1:A:395:ALA:HB2	1:A:405:VAL:HG21	2.02	0.42
1:C:74:ALA:HB1	1:C:79:ILE:HG12	1.99	0.42
1:C:151:ARG:NH2	1:C:264:GLU:OE1	2.52	0.42
1:B:95:GLU:CD	1:B:95:GLU:H	2.23	0.42
1:C:443:SER:O	1:C:447:ARG:HG2	2.19	0.42
1:D:281:HIS:CE1	1:D:284:ASN:HD21	2.37	0.42
1:C:149:VAL:HG21	1:C:156:HIS:CD2	2.54	0.42
1:C:183:LEU:C	1:C:183:LEU:HD12	2.40	0.42
1:A:165:LYS:NZ	1:B:314:GLU:OE2	2.51	0.42
1:A:268:PRO:HG3	1:A:347:GLY:O	2.20	0.42
1:D:92:GLY:C	1:D:94:PRO:HD3	2.39	0.42
1:D:409:GLU:HG3	1:D:412:VAL:H	1.84	0.42
1:D:78:ALA:HB3	1:D:106:SER:HB3	2.01	0.42
1:D:139:GLN:HA	1:D:139:GLN:NE2	2.34	0.42
1:A:25:LEU:CD1	1:D:5:LEU:HD11	2.47	0.42
1:B:76:ASN:HB2	1:B:110:MET:HE1	2.02	0.42
1:B:250:PHE:O	1:B:254:ILE:HG12	2.20	0.42
1:B:312:GLU:H	1:B:312:GLU:HG3	1.54	0.42
1:B:416:LEU:HA	1:B:420:GLU:OE1	2.19	0.42
2:B:801:DTT:O2	1:D:303:SER:HB2	2.20	0.42
1:D:95:GLU:CD	1:D:95:GLU:H	2.23	0.42
1:A:379:LEU:HD21	1:A:415:GLU:CG	2.48	0.42
1:B:373:ILE:O	1:B:376:ALA:HB3	2.20	0.42
1:D:10:PHE:O	1:D:336:GLY:HA3	2.20	0.42
1:D:268:PRO:O	1:D:269:SER:CB	2.67	0.42
1:D:325:GLU:C	1:D:328:PRO:HD2	2.40	0.42
1:B:148:LEU:CD2	1:B:162:LEU:N	2.83	0.42
1:B:383:ARG:NH2	1:B:411:GLN:HG2	2.35	0.42
1:D:74:ALA:HB1	1:D:79:ILE:HD11	2.02	0.42
1:D:227:HIS:HD2	4:D:464:HOH:O	2.03	0.42
1:D:431:LEU:HD23	1:D:435:ARG:HH12	1.83	0.42
1:B:111:ASP:HB2	1:B:191:GLN:HG2	2.02	0.41
1:C:95:GLU:H	1:C:95:GLU:CD	2.24	0.41
1:C:37:ARG:HH11	1:C:216:GLN:HE21	1.61	0.41
1:A:79:ILE:CG1	1:A:80:PRO:CD	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:HE2	1:A:434:ALA:CB	2.50	0.41
1:A:250:PHE:O	1:A:254:ILE:HG12	2.20	0.41
1:B:160:VAL:HG13	1:B:161:THR:N	2.34	0.41
1:D:79:ILE:CG1	1:D:80:PRO:CD	2.96	0.41
1:B:176:HIS:CD2	1:B:179:ARG:HH11	2.33	0.41
1:B:292:ILE:HD12	1:C:317:LEU:HD22	2.03	0.41
1:B:437:TRP:HE3	1:B:437:TRP:HA	1.85	0.41
1:D:160:VAL:CG1	1:D:161:THR:N	2.83	0.41
1:A:148:LEU:CD2	1:A:162:LEU:N	2.83	0.41
1:B:111:ASP:O	1:B:115:VAL:HG23	2.19	0.41
1:B:131:LYS:O	1:B:135:THR:HG23	2.20	0.41
1:B:437:TRP:HA	1:B:437:TRP:CE3	2.56	0.41
1:A:309:MET:N	1:A:310:PRO:HD2	2.35	0.41
1:A:373:ILE:HG13	1:A:374:VAL:N	2.36	0.41
1:B:303:SER:OG	2:B:801:DTT:H42	2.21	0.41
1:B:395:ALA:HB2	1:B:405:VAL:HG21	2.03	0.41
1:C:252:ARG:HH22	1:D:319:LEU:HD11	1.85	0.41
1:A:348:MET:HG3	1:A:348:MET:H	1.69	0.41
1:A:367:LEU:HD12	1:A:367:LEU:HA	1.85	0.41
1:C:437:TRP:HA	1:C:437:TRP:CE3	2.55	0.41
1:B:195:ALA:O	1:B:315:ARG:NH2	2.53	0.41
1:C:409:GLU:HG3	1:C:412:VAL:H	1.86	0.41
1:A:72:ALA:HA	1:D:9:TYR:CD1	2.56	0.41
1:A:139:GLN:HA	1:A:139:GLN:NE2	2.35	0.41
1:C:161:THR:CG2	1:C:164:MET:N	2.77	0.41
1:C:313:HIS:CD2	1:D:151:ARG:HD2	2.56	0.41
1:C:373:ILE:HG13	1:C:374:VAL:N	2.35	0.41
1:D:17:GLU:HG3	1:D:22:ARG:HH12	1.86	0.41
1:D:132:LEU:O	1:D:136:LEU:HB2	2.21	0.41
1:D:205:LYS:C	1:D:208:PRO:HD2	2.41	0.41
1:B:45:VAL:HG13	1:B:46:PRO:HD2	2.02	0.41
1:B:180:LEU:HD12	1:B:180:LEU:HA	1.91	0.41
1:B:379:LEU:HD21	1:B:415:GLU:CG	2.50	0.41
1:D:325:GLU:OE1	1:D:325:GLU:HA	2.21	0.41
1:D:340:GLN:O	1:D:344:ILE:HG23	2.21	0.41
1:A:319:LEU:HD11	1:B:252:ARG:HH22	1.85	0.40
1:B:139:GLN:HE21	1:B:139:GLN:CA	2.28	0.40
1:C:151:ARG:HD2	1:D:313:HIS:CD2	2.56	0.40
1:C:374:VAL:O	1:C:377:GLN:HG2	2.21	0.40
1:A:90:ALA:HB2	1:A:97:GLU:OE1	2.21	0.40
1:B:175:ARG:NH2	4:B:813:HOH:O	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ASP:HA	1:C:427:PRO:HD3	1.93	0.40
1:C:437:TRP:HA	1:C:437:TRP:HE3	1.85	0.40
1:D:190:LEU:HG	1:D:191:GLN:N	2.36	0.40
1:D:217:LEU:O	1:D:218:LYS:HB2	2.21	0.40
1:A:207:MET:HB2	1:A:208:PRO:HD3	2.03	0.40
1:B:136:LEU:HD12	1:B:136:LEU:HA	1.95	0.40
1:D:378:ARG:HG2	1:D:378:ARG:NH1	2.34	0.40
1:A:106:SER:HB3	1:A:110:MET:HE2	2.03	0.40
1:C:28:MET:O	1:C:31:PHE:HB3	2.21	0.40
1:C:442:VAL:O	1:C:446:GLN:HG3	2.22	0.40
1:D:74:ALA:CB	1:D:79:ILE:HD11	2.51	0.40
1:D:105:THR:HB	1:D:195:ALA:N	2.37	0.40
1:D:199:LEU:HD12	1:D:199:LEU:HA	1.97	0.40
1:A:409:GLU:HG3	1:A:412:VAL:H	1.86	0.40
1:B:74:ALA:HB1	1:B:79:ILE:CD1	2.51	0.40
1:B:317:LEU:CD1	1:B:317:LEU:H	2.34	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	434/450 (96%)	411 (95%)	19 (4%)	4 (1%)	17 35
1	B	437/450 (97%)	408 (93%)	21 (5%)	8 (2%)	8 16
1	C	436/450 (97%)	412 (94%)	19 (4%)	5 (1%)	14 30
1	D	446/450 (99%)	411 (92%)	23 (5%)	12 (3%)	5 8
All	All	1753/1800 (97%)	1642 (94%)	82 (5%)	29 (2%)	9 18

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	GLN
1	B	281	HIS
1	B	282	LYS
1	B	399	GLN
1	C	280	PRO
1	C	399	GLN
1	D	269	SER
1	D	277	SER
1	D	282	LYS
1	D	399	GLN
1	B	195	ALA
1	D	195	ALA
1	D	271	PRO
1	A	397	ALA
1	B	397	ALA
1	C	397	ALA
1	C	449	THR
1	D	397	ALA
1	A	195	ALA
1	B	398	GLU
1	B	449	THR
1	C	195	ALA
1	D	276	SER
1	D	398	GLU
1	D	449	THR
1	A	398	GLU
1	B	270	ALA
1	D	270	ALA
1	D	280	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	326/343 (95%)	302 (93%)	24 (7%)	13 28
1	B	330/343 (96%)	304 (92%)	26 (8%)	12 24
1	C	329/343 (96%)	306 (93%)	23 (7%)	15 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	332/343 (97%)	308 (93%)	24 (7%)	14	29
All	All	1317/1372 (96%)	1220 (93%)	97 (7%)	13	28

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	35	LEU
1	A	79	ILE
1	A	114	LEU
1	A	122	LEU
1	A	135	THR
1	A	146	THR
1	A	156	HIS
1	A	160	VAL
1	A	161	THR
1	A	180	LEU
1	A	199	LEU
1	A	242	LEU
1	A	312	GLU
1	A	317	LEU
1	A	327	LEU
1	A	333	LEU
1	A	344	ILE
1	A	348	MET
1	A	360	ASP
1	A	366	VAL
1	A	367	LEU
1	A	402	LEU
1	A	437	TRP
1	B	22	ARG
1	B	25	LEU
1	B	35	LEU
1	B	114	LEU
1	B	122	LEU
1	B	135	THR
1	B	146	THR
1	B	156	HIS
1	B	160	VAL
1	B	161	THR
1	B	180	LEU
1	B	199	LEU

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Mol	Chain	Res	Type
1	B	242	LEU
1	B	279	MET
1	B	281	HIS
1	B	312	GLU
1	B	317	LEU
1	B	327	LEU
1	B	333	LEU
1	B	344	ILE
1	B	348	MET
1	B	360	ASP
1	B	366	VAL
1	B	367	LEU
1	B	402	LEU
1	B	431	LEU
1	C	25	LEU
1	C	35	LEU
1	C	79	ILE
1	C	114	LEU
1	C	122	LEU
1	C	135	THR
1	C	139	GLN
1	C	146	THR
1	C	156	HIS
1	C	161	THR
1	C	180	LEU
1	C	199	LEU
1	C	242	LEU
1	C	312	GLU
1	C	317	LEU
1	C	327	LEU
1	C	333	LEU
1	C	344	ILE
1	C	348	MET
1	C	366	VAL
1	C	367	LEU
1	C	402	LEU
1	C	437	TRP
1	D	25	LEU
1	D	35	LEU
1	D	114	LEU
1	D	122	LEU
1	D	135	THR

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Mol	Chain	Res	Type
1	D	139	GLN
1	D	146	THR
1	D	156	HIS
1	D	161	THR
1	D	180	LEU
1	D	242	LEU
1	D	280	PRO
1	D	302	LEU
1	D	312	GLU
1	D	317	LEU
1	D	327	LEU
1	D	333	LEU
1	D	344	ILE
1	D	348	MET
1	D	360	ASP
1	D	366	VAL
1	D	367	LEU
1	D	402	LEU
1	D	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	GLN
1	A	101	HIS
1	A	107	GLN
1	A	117	GLN
1	A	138	GLN
1	A	139	GLN
1	A	143	HIS
1	A	176	HIS
1	A	191	GLN
1	A	216	GLN
1	A	224	GLN
1	A	227	HIS
1	A	284	ASN
1	A	342	GLN
1	A	399	GLN
1	A	429	HIS
1	B	4	GLN
1	B	101	HIS

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Mol	Chain	Res	Type
1	B	107	GLN
1	B	117	GLN
1	B	138	GLN
1	B	139	GLN
1	B	143	HIS
1	B	156	HIS
1	B	176	HIS
1	B	178	GLN
1	B	191	GLN
1	B	216	GLN
1	B	227	HIS
1	B	284	ASN
1	B	342	GLN
1	B	399	GLN
1	B	429	HIS
1	C	4	GLN
1	C	101	HIS
1	C	107	GLN
1	C	117	GLN
1	C	138	GLN
1	C	139	GLN
1	C	143	HIS
1	C	176	HIS
1	C	178	GLN
1	C	191	GLN
1	C	216	GLN
1	C	227	HIS
1	C	284	ASN
1	C	342	GLN
1	C	399	GLN
1	D	3	ASN
1	D	4	GLN
1	D	101	HIS
1	D	107	GLN
1	D	117	GLN
1	D	138	GLN
1	D	139	GLN
1	D	143	HIS
1	D	156	HIS
1	D	176	HIS
1	D	178	GLN
1	D	191	GLN

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Mol	Chain	Res	Type
1	D	216	GLN
1	D	227	HIS
1	D	284	ASN
1	D	342	GLN
1	D	399	GLN
1	D	429	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DTT	B	801	-	7,7,7	6.40	4 (57%)	4,8,8	5.30	4 (100%)
2	DTT	A	802	-	7,7,7	6.37	4 (57%)	4,8,8	5.61	4 (100%)
3	CIT	C	800	-	12,12,12	4.68	4 (33%)	17,17,17	8.04	9 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	B	801	-	2/2/2/2	6/8/8/8	-
2	DTT	A	802	-	2/2/2/2	5/8/8/8	-
3	CIT	C	800	-	-	11/16/16/16	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	DTT	O2-C2	-16.01	1.09	1.43
2	A	802	DTT	O2-C2	-15.72	1.10	1.43
3	C	800	CIT	C3-C6	14.91	1.68	1.53
2	A	802	DTT	C4-S4	-4.04	1.73	1.81
3	C	800	CIT	O7-C3	3.58	1.50	1.43
3	C	800	CIT	C2-C3	3.41	1.58	1.53
2	B	801	DTT	C4-S4	-3.23	1.74	1.81
2	B	801	DTT	O3-C3	-3.17	1.36	1.43
2	A	802	DTT	O3-C3	-2.86	1.37	1.43
2	A	802	DTT	C3-C2	-2.61	1.46	1.52
2	B	801	DTT	C3-C2	-2.58	1.46	1.52
3	C	800	CIT	O5-C6	2.30	1.29	1.22

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	800	CIT	O7-C3-C6	-27.31	70.53	108.86
3	C	800	CIT	C4-C3-C6	-12.38	83.51	110.11
3	C	800	CIT	O7-C3-C4	8.84	130.08	109.40
2	A	802	DTT	C3-C4-S4	-7.96	91.33	114.47
2	B	801	DTT	C3-C4-S4	-7.51	92.62	114.47
2	A	802	DTT	C2-C1-S1	-6.36	95.98	114.47
2	B	801	DTT	C2-C1-S1	-5.95	97.17	114.47
3	C	800	CIT	C3-C2-C1	5.87	128.01	113.81
3	C	800	CIT	O5-C6-C3	-4.85	115.39	122.25
3	C	800	CIT	O7-C3-C2	4.67	120.33	109.40
2	A	802	DTT	O2-C2-C3	3.90	117.74	109.72
3	C	800	CIT	C3-C4-C5	3.87	123.19	113.81
2	B	801	DTT	O2-C2-C3	3.42	116.75	109.72
2	B	801	DTT	O3-C3-C2	-2.97	103.62	109.72
3	C	800	CIT	O2-C1-C2	2.78	123.27	114.35
2	A	802	DTT	O3-C3-C2	-2.65	104.27	109.72
3	C	800	CIT	O4-C5-O3	-2.57	116.90	123.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	802	DTT	C2
2	A	802	DTT	C3
2	B	801	DTT	C2
2	B	801	DTT	C3

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	DTT	S1-C1-C2-O2
2	A	802	DTT	S1-C1-C2-C3
2	A	802	DTT	C1-C2-C3-C4
2	B	801	DTT	S1-C1-C2-C3
2	B	801	DTT	C1-C2-C3-C4
2	B	801	DTT	O2-C2-C3-O3
2	B	801	DTT	C2-C3-C4-S4
2	B	801	DTT	O3-C3-C4-S4
3	C	800	CIT	C1-C2-C3-C6
3	C	800	CIT	O7-C3-C4-C5
3	C	800	CIT	C2-C3-C6-O5
3	C	800	CIT	C2-C3-C6-O6
3	C	800	CIT	O7-C3-C6-O5
3	C	800	CIT	O7-C3-C6-O6
3	C	800	CIT	C1-C2-C3-C4
2	A	802	DTT	O2-C2-C3-O3
2	A	802	DTT	O3-C3-C4-S4
2	B	801	DTT	S1-C1-C2-O2
3	C	800	CIT	C4-C3-C6-O6
3	C	800	CIT	C4-C3-C6-O5
3	C	800	CIT	C3-C4-C5-O4
3	C	800	CIT	C3-C4-C5-O3

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	DTT	5	0
2	A	802	DTT	5	0
3	C	800	CIT	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.