WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 10:54 AM EDT

PDB ID	:	3C8D
Title	:	Crystal structure of the enterobactin esterase FES from Shigella flexneri in the presence of 2,3-Di-hydroxy-N-benzoyl-glycine
Authors	:	Kim, Y.; Maltseva, N.; Abergel, R.; Holzle, D.; Raymond, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-02-11
Resolution	:	1.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	Percentile Ranks	Value
Rfree		0.184
Clashscore		17
Ramachandran outliers		0.2%
Sidechain outliers		5.8%
RSRZ outliers		2.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
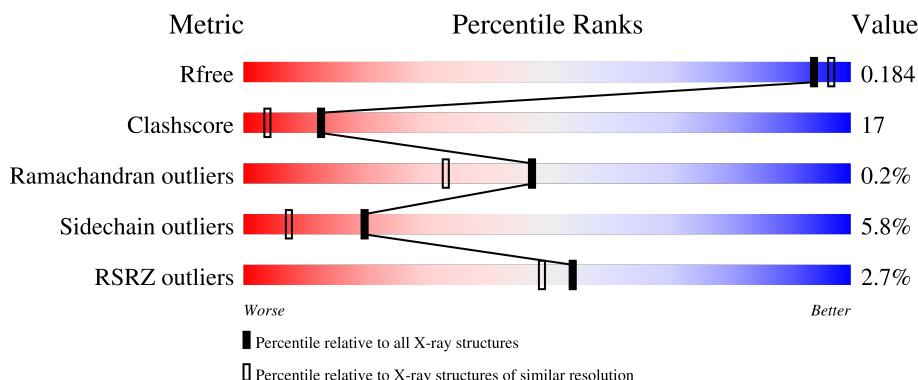
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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% 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	403	3% / 65% / 27% / • / 6%
1	B	403	3% / 67% / 24% / • / 6%
1	C	403	2% / 64% / 28% / • / 6%
1	D	403	2% / 66% / 27% / • / 6%
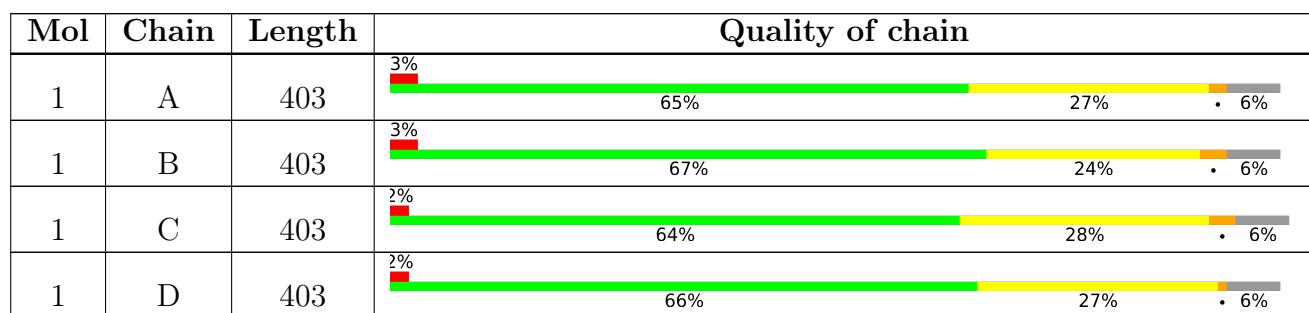
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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	CIT	C	501	-	X	-	-
2	CIT	C	502	-	X	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13727 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 Enterochelin esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total 3146	C 2019	N 553	O 562	S 12	0	11	0
1	B	379	Total 3134	C 2013	N 548	O 561	S 12	0	9	0
1	C	379	Total 3118	C 2003	N 544	O 559	S 12	0	8	0
1	D	378	Total 3157	C 2029	N 552	O 564	S 12	0	11	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q83SB9
A	-1	ASN	-	expression tag	UNP Q83SB9
A	0	ALA	-	expression tag	UNP Q83SB9
B	-2	SER	-	expression tag	UNP Q83SB9
B	-1	ASN	-	expression tag	UNP Q83SB9
B	0	ALA	-	expression tag	UNP Q83SB9
C	-2	SER	-	expression tag	UNP Q83SB9
C	-1	ASN	-	expression tag	UNP Q83SB9
C	0	ALA	-	expression tag	UNP Q83SB9
D	-2	SER	-	expression tag	UNP Q83SB9
D	-1	ASN	-	expression tag	UNP Q83SB9
D	0	ALA	-	expression tag	UNP Q83SB9

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
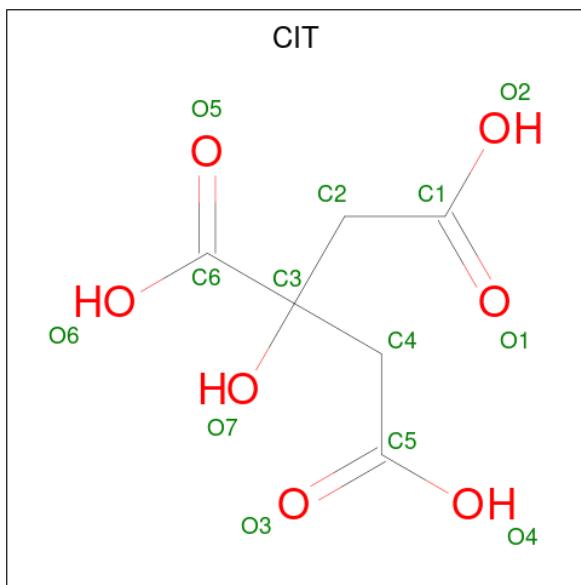
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 6	O 7	0	0
2	B	1	Total 13	C 6	O 7	0	0
2	C	1	Total 13	C 6	O 7	0	0
2	C	1	Total 13	C 6	O 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total 247	O 247	0	0
3	B	314	Total 314	O 314	0	0
3	C	270	Total 270	O 270	0	0
3	D	289	Total 289	O 289	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Enterochelin esterase
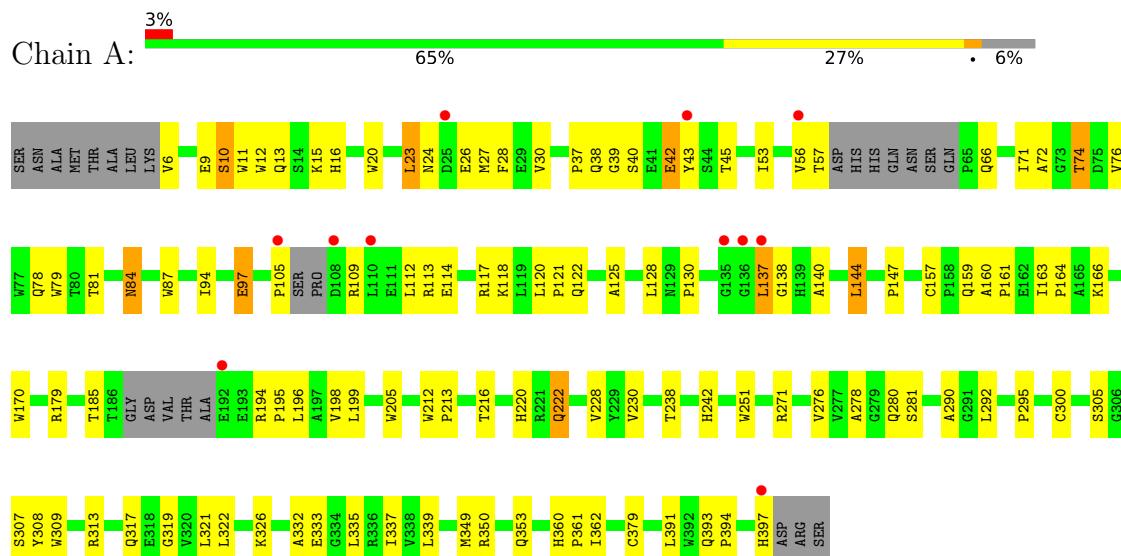
Chain A:

- Molecule 1: Enterochelin esterase

Chain B:

- Molecule 1: Enterochelin esterase

Chain C:

• Molecule 1: Enterochelin esterase

Chain D:
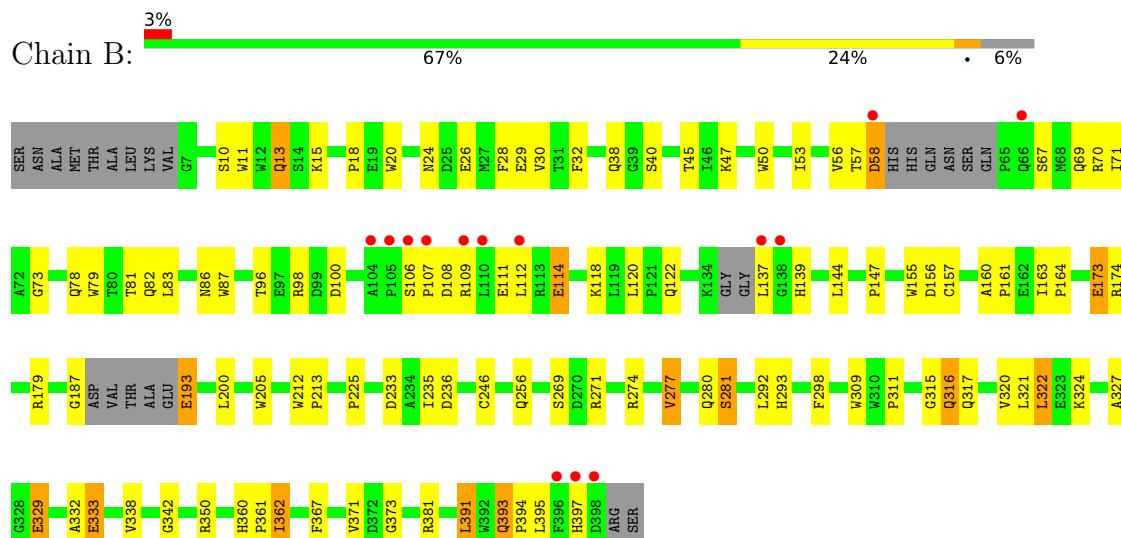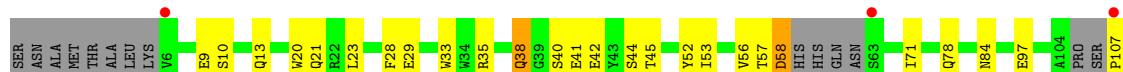
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.30Å 155.97Å 48.48Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	48.48 – 1.80 48.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.48-1.80) 98.0 (48.48-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.79Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.150 , 0.194 0.153 , 0.184	Depositor DCC
R_{free} test set	14892 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.3	EDS
L-test for twinning[2]	$< |L| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.368 for -h,-k,l	Xtriage
Reported twinning fraction	0.354 for h,-k,-l	Depositor
Outliers	0 of 149411 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13727	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2427e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CIT

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	0.34	0/3244	0.51	0/4425
1	B	0.35	0/3233	0.55	2/4409 (0.0%)
1	C	0.33	0/3217	0.53	1/4390 (0.0%)
1	D	0.34	0/3255	0.53	1/4438 (0.0%)
All	All	0.34	0/12949	0.53	4/17662 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	193	GLU	N-CA-C	-7.79	89.97	111.00
1	D	193	GLU	N-CA-C	-5.94	94.96	111.00
1	B	187	GLY	N-CA-C	5.82	127.64	113.10
1	C	193	GLU	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3146	0	3040	110	1
1	B	3134	0	3027	103	1
1	C	3118	0	3011	116	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3157	0	3045	98	1
2	A	13	0	5	2	0
2	B	13	0	5	1	0
2	C	26	0	10	9	0
3	A	247	0	0	23	0
3	B	314	0	0	15	0
3	C	270	0	0	15	0
3	D	289	0	0	24	0
All	All	13727	0	12143	411	2

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 17.

All (411) 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:A:137:LEU:HB3	1:B:317:GLN:CD	1.75	1.07
1:C:194:ARG:HG3	1:C:194:ARG:HH21	1.15	1.07
1:C:74[A]:THR:HG23	1:C:76:VAL:H	1.24	1.02
1:D:175:LEU:HB3	3:D:837:HOH:O	1.62	0.98
2:A:501:CIT:H42	3:B:587:HOH:O	1.66	0.95
1:D:38:GLN:HE21	1:D:45:THR:H	1.15	0.94
1:C:297:ARG:HB3	3:C:915:HOH:O	1.68	0.94
1:C:71:ILE:O	1:C:74[A]:THR:HG22	1.65	0.93
1:C:350:ARG:HD3	1:C:353:GLN:HE21	1.33	0.93
1:C:337[A]:ILE:HD11	1:C:339:LEU:HG	1.54	0.89
1:A:109:ARG:HH12	1:A:113:ARG:HH11	1.12	0.89
1:D:174:ARG:HG2	3:D:844:HOH:O	1.74	0.86
1:A:23:LEU:HD11	1:A:27:MET:HB3	1.57	0.86
1:A:137:LEU:HD22	3:B:749:HOH:O	1.76	0.86
1:C:350:ARG:HH11	1:C:353:GLN:NE2	1.73	0.85
1:C:170:TRP:HE1	1:C:257[B]:GLU:HG2	1.41	0.84
1:A:137:LEU:HB3	1:B:317:GLN:OE1	1.77	0.84
1:D:185:THR:HG21	1:D:194:ARG:NH2	1.92	0.84
1:A:394:PRO:O	1:A:397:HIS:ND1	2.11	0.83
1:B:174:ARG:HH11	1:B:256:GLN:HE22	1.22	0.83
1:A:24:ASN:HB3	1:A:26:GLU:H	1.44	0.82
1:C:193:GLU:HG3	1:C:193:GLU:O	1.78	0.81
1:D:175:LEU:HD23	3:D:844:HOH:O	1.80	0.81
1:B:69:GLN:HG3	3:B:704:HOH:O	1.81	0.81
1:C:65:PRO:HG2	1:C:102:PHE:CD2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PRO:HA	3:A:653:HOH:O	1.81	0.80
1:A:121:PRO:HB2	3:A:608:HOH:O	1.80	0.80
1:B:24:ASN:HD22	1:B:26[A]:GLU:H	1.27	0.80
1:D:174:ARG:HH21	1:D:256:GLN:HE22	1.30	0.79
1:D:169:ILE:HD11	1:D:178:SER:HB3	1.65	0.79
1:B:24:ASN:HD22	1:B:26[B]:GLU:H	1.28	0.78
1:D:38:GLN:NE2	1:D:45:THR:H	1.81	0.78
1:D:148:GLN:HG3	3:D:879:HOH:O	1.83	0.77
1:D:320[A]:VAL:HG12	1:D:324:LYS:HE2	1.65	0.77
1:D:9:GLU:O	1:D:13:GLN:HG2	1.83	0.77
1:A:397:HIS:O	1:A:397:HIS:CD2	2.38	0.76
1:A:179:ARG:HD2	3:A:506:HOH:O	1.84	0.75
1:C:170:TRP:NE1	1:C:257[B]:GLU:HG2	2.01	0.75
1:D:179:ARG:HB2	1:D:233:ASP:HB3	1.69	0.75
1:C:109:ARG:HH11	1:C:113:ARG:HH11	1.34	0.75
1:C:106:SER:HB2	3:C:948:HOH:O	1.87	0.74
1:C:312:HIS:HA	2:C:501:CIT:O2	1.89	0.73
1:C:194:ARG:HB3	1:C:227:ALA:HA	1.70	0.73
1:A:30:VAL:HG13	3:A:694:HOH:O	1.89	0.72
1:A:170:TRP:CE3	1:A:179:ARG:HD3	2.25	0.72
1:C:194:ARG:HG3	1:C:194:ARG:NH2	1.93	0.72
1:A:212:TRP:HB2	1:A:213:PRO:HD3	1.71	0.72
1:C:336:ARG:HH11	1:C:367:PHE:HZ	1.37	0.71
1:C:20:TRP:HB3	1:C:30:VAL:HG22	1.72	0.71
1:A:45:THR:HG22	1:A:97:GLU:HB3	1.73	0.70
1:A:238[B]:THR:HG23	1:B:320[B]:VAL:HG11	1.73	0.69
1:C:49:VAL:HB	1:C:68:MET:HB2	1.75	0.68
1:A:276:VAL:HG22	1:A:300:CYS:HB2	1.75	0.68
1:D:270:ASP:HA	1:D:297:ARG:HH22	1.58	0.68
1:A:137:LEU:HD13	1:B:317:GLN:HB2	1.76	0.68
1:C:393:GLN:HB3	1:C:394:PRO:HD3	1.76	0.68
1:C:9:GLU:O	1:C:13:GLN:HG3	1.94	0.68
1:D:137:LEU:HD13	3:D:887:HOH:O	1.94	0.67
1:A:72:ALA:HB3	3:A:655:HOH:O	1.95	0.66
1:B:57:THR:OG1	3:B:557:HOH:O	2.12	0.66
1:C:292:LEU:O	3:C:967:HOH:O	2.12	0.66
1:D:111:GLU:HA	1:D:114[A]:GLU:HG2	1.77	0.66
1:C:22:ARG:HG2	1:C:28:PHE:CZ	2.30	0.66
1:A:350:ARG:CZ	1:B:114:GLU:HG3	2.26	0.66
1:B:205:TRP:HE1	1:B:280:GLN:HE22	1.43	0.65
1:C:350:ARG:HH11	1:C:353:GLN:HE22	1.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:GLN:HA	3:D:851:HOH:O	1.96	0.65
1:B:292:LEU:HD12	1:B:321[A]:LEU:HD11	1.79	0.65
1:A:53:ILE:HB	1:A:57:THR:H	1.62	0.65
1:B:78:GLN:HG3	3:B:798:HOH:O	1.97	0.65
1:D:131:GLN:OE1	3:D:909:HOH:O	2.13	0.64
1:B:371:VAL:HG12	1:B:373:GLY:H	1.61	0.64
1:B:393:GLN:N	1:B:394:PRO:HD2	2.13	0.64
1:A:23:LEU:HD12	1:A:24:ASN:HB2	1.78	0.64
1:C:349:MET:O	1:C:353:GLN:HG2	1.98	0.64
1:D:44:SER:O	3:D:739:HOH:O	2.15	0.64
1:B:11:TRP:CH2	1:B:15:LYS:HE3	2.32	0.64
1:B:137:LEU:N	1:B:139:HIS:CD2	2.66	0.64
1:C:369:ARG:HH22	1:C:386:GLN:HG3	1.62	0.63
1:A:84:ASN:HD22	1:A:84:ASN:N	1.97	0.63
1:A:335:LEU:HD23	1:A:337:ILE:HD11	1.80	0.63
1:C:371:VAL:HG12	1:C:373:GLY:H	1.64	0.63
1:B:107:PRO:HB2	1:B:112:LEU:HD22	1.81	0.63
1:C:271:ARG:HB3	1:C:273:ASP:OD1	1.99	0.63
1:A:23:LEU:CD1	1:A:27:MET:HB3	2.29	0.62
1:A:87:TRP:HZ3	1:A:144:LEU:HB3	1.65	0.62
1:C:350:ARG:HD3	1:C:353:GLN:NE2	2.11	0.62
1:D:35:ARG:HD3	3:D:722:HOH:O	2.00	0.62
1:C:261:LEU:HD12	3:C:841:HOH:O	1.99	0.61
1:D:349:MET:CG	3:D:779:HOH:O	2.47	0.61
1:C:106:SER:N	1:C:107:PRO:CD	2.62	0.61
1:C:318:GLU:HB2	3:C:830:HOH:O	2.00	0.61
1:A:125:ALA:HB2	1:A:140:ALA:HB1	1.83	0.61
1:C:74[B]:THR:HG22	1:C:76:VAL:HG23	1.81	0.61
1:B:293:HIS:HE1	1:B:324[A]:LYS:NZ	1.98	0.61
1:D:107:PRO:HD2	1:D:108:ASP:N	2.16	0.61
1:A:16:HIS:HB3	3:A:683:HOH:O	2.00	0.60
1:A:205:TRP:HE1	1:A:280:GLN:HE22	1.47	0.60
1:A:313:ARG:HD2	1:B:309:TRP:CE2	2.36	0.60
1:D:131:GLN:CD	3:D:909:HOH:O	2.38	0.60
1:D:177:ASN:ND2	3:D:837:HOH:O	2.33	0.60
1:D:205:TRP:HE1	1:D:280:GLN:HE22	1.49	0.60
1:C:113:ARG:HH21	1:D:316:GLN:HG3	1.66	0.60
1:D:71:ILE:HG22	3:D:890:HOH:O	2.02	0.60
1:B:338:VAL:HG23	1:B:391:LEU:HD13	1.84	0.60
1:C:6:VAL:HA	1:C:11:TRP:CD1	2.36	0.60
1:D:155:TRP:CZ2	1:D:381:ARG:HB2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLN:HB2	3:A:626:HOH:O	2.00	0.60
1:A:6:VAL:HA	1:A:11:TRP:CG	2.36	0.60
1:A:222:GLN:N	1:A:222:GLN:HE21	1.99	0.60
1:D:180:ARG:O	1:D:233:ASP:HB2	2.02	0.60
1:C:368:TRP:HZ2	1:C:370:GLN:HE21	1.49	0.60
1:C:106:SER:N	1:C:107:PRO:HD3	2.17	0.60
1:C:24:ASN:OD1	1:C:27:MET:CB	2.50	0.59
1:A:137:LEU:O	1:B:317:GLN:NE2	2.35	0.59
1:B:50:TRP:CZ3	1:B:67:SER:HB2	2.37	0.59
1:B:367:PHE:CE1	3:B:760:HOH:O	2.52	0.59
2:C:502:CIT:H21	2:C:502:CIT:O4	2.01	0.59
1:D:323:GLU:O	1:D:326:LYS:HD3	2.03	0.59
1:A:137:LEU:CB	1:B:317:GLN:CD	2.63	0.59
1:C:155:TRP:CZ2	1:C:381:ARG:HB2	2.38	0.58
1:B:205:TRP:HE1	1:B:280:GLN:NE2	2.02	0.58
1:D:349:MET:HG3	3:D:779:HOH:O	2.03	0.58
1:A:114:GLU:HG3	1:B:350:ARG:HD3	1.85	0.58
1:C:20:TRP:O	1:C:21:GLN:HG3	2.04	0.58
1:A:9:GLU:O	1:A:13:GLN:HG3	2.03	0.57
1:A:130:PRO:HD3	3:A:683:HOH:O	2.04	0.57
1:B:293:HIS:CE1	1:B:324[A]:LYS:NZ	2.73	0.57
1:A:122:GLN:HG3	3:A:608:HOH:O	2.02	0.57
1:A:394:PRO:O	1:A:397:HIS:CE1	2.57	0.57
1:A:109:ARG:HH12	1:A:113:ARG:NH1	1.94	0.56
1:B:155:TRP:CZ2	1:B:381:ARG:HB2	2.40	0.56
1:C:74[B]:THR:CG2	1:C:76:VAL:HG23	2.34	0.56
1:C:137:LEU:HB3	1:C:139:HIS:CD2	2.40	0.56
1:B:322:LEU:HD12	3:B:676:HOH:O	2.05	0.56
1:C:84:ASN:C	1:C:86:ASN:H	2.09	0.56
1:D:58:ASP:HB2	3:D:757:HOH:O	2.04	0.56
1:B:53:ILE:HB	1:B:56:VAL:HB	1.86	0.56
1:D:338:VAL:HA	1:D:367:PHE:HB2	1.87	0.56
1:D:347:MET:HB2	3:D:878:HOH:O	2.04	0.56
1:B:395:LEU:HD13	3:B:589:HOH:O	2.06	0.56
1:C:78:GLN:HG3	3:C:791:HOH:O	2.06	0.56
1:B:293:HIS:HE1	1:B:324[A]:LYS:HZ1	1.52	0.56
2:C:502:CIT:H21	3:D:645:HOH:O	2.05	0.56
1:D:41:GLU:CD	1:D:41:GLU:H	2.09	0.55
1:A:78:GLN:HG2	1:A:79:TRP:N	2.19	0.55
1:C:137:LEU:HD23	1:C:137:LEU:O	2.06	0.55
1:B:87:TRP:HZ3	1:B:144:LEU:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ARG:HB2	1:D:313:ARG:HH21	1.72	0.55
1:A:117:ARG:HA	1:B:316:GLN:O	2.07	0.55
1:A:397:HIS:O	1:A:397:HIS:CG	2.59	0.55
1:C:369:ARG:NH2	1:C:390:ASP:OD1	2.40	0.55
1:A:66:GLN:HA	3:A:731:HOH:O	2.06	0.55
1:D:125:ALA:HB2	1:D:140:ALA:CB	2.37	0.55
1:B:53:ILE:HG21	1:B:56:VAL:HG21	1.88	0.55
1:A:198:VAL:HA	1:A:230[B]:VAL:HG23	1.88	0.55
1:A:292:LEU:CD2	1:A:332:ALA:HB2	2.36	0.55
1:D:125:ALA:HB2	1:D:140:ALA:HB1	1.88	0.55
1:D:311:PRO:HD3	1:D:320[A]:VAL:HG23	1.89	0.55
1:A:159:GLN:O	1:A:213:PRO:HA	2.07	0.54
1:A:10:SER:HA	1:A:13:GLN:HE21	1.72	0.54
1:A:12:TRP:CZ2	1:A:76:VAL:HG22	2.42	0.54
1:A:23:LEU:HD12	1:A:23:LEU:C	2.28	0.54
1:A:84:ASN:HD22	1:A:84:ASN:H	1.56	0.54
1:A:360:HIS:HB3	1:A:361:PRO:HD3	1.90	0.54
1:C:120:LEU:HD13	1:C:137:LEU:HD13	1.89	0.54
1:C:134:LYS:HG3	1:C:134:LYS:O	2.09	0.53
1:C:179:ARG:HD3	1:C:233[B]:ASP:O	2.08	0.53
1:A:251:TRP:CE2	1:A:290:ALA:HB2	2.43	0.53
1:C:114:GLU:OE2	1:C:114:GLU:HA	2.08	0.53
1:C:186:THR:O	1:C:187:GLY:C	2.47	0.53
1:D:259:LEU:HB2	1:D:260:PRO:HD3	1.89	0.53
1:C:336:ARG:NH1	1:C:367:PHE:HZ	2.05	0.53
1:D:369:ARG:NH2	1:D:390:ASP:OD1	2.39	0.53
1:A:42:GLU:HG3	1:A:43:TYR:CD2	2.44	0.52
2:C:501:CIT:O1	1:D:309:TRP:CZ2	2.62	0.52
1:C:107:PRO:HB2	1:C:112:LEU:HD21	1.92	0.52
1:C:318:GLU:HG3	1:C:322:LEU:HD23	1.92	0.52
1:A:281:SER:HB2	2:A:501:CIT:O6	2.09	0.52
1:A:37:PRO:HA	3:A:707:HOH:O	2.10	0.52
1:C:179:ARG:HD3	1:C:233[A]:ASP:O	2.09	0.52
1:C:244:LEU:O	1:C:286:SER:HB2	2.09	0.52
1:B:225:PRO:HG3	1:B:395:LEU:HD12	1.92	0.52
2:C:502:CIT:O4	2:C:502:CIT:C2	2.58	0.51
1:D:349:MET:HG2	3:D:779:HOH:O	2.07	0.51
1:D:120:LEU:N	1:D:121:PRO:HD2	2.26	0.51
1:D:162:GLU:HB2	3:D:896:HOH:O	2.09	0.51
1:C:109:ARG:NH1	1:C:113:ARG:HH11	2.06	0.51
1:D:53:ILE:HB	1:D:56:VAL:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ILE:HD13	1:B:362:ILE:N	2.26	0.51
1:D:23:LEU:HD21	1:D:29:GLU:HB2	1.91	0.51
1:A:212:TRP:CB	1:A:213:PRO:HD3	2.40	0.51
1:C:24:ASN:OD1	1:C:27:MET:HB2	2.11	0.51
1:B:32:PHE:O	1:B:78:GLN:HA	2.11	0.51
1:B:70:ARG:HG2	1:B:71:ILE:N	2.25	0.51
1:B:315:GLY:HA2	3:B:543:HOH:O	2.10	0.51
1:B:293:HIS:CE1	1:B:324[A]:LYS:HZ2	2.29	0.51
1:D:323:GLU:HA	1:D:326:LYS:HD2	1.93	0.51
1:A:20:TRP:HE3	3:A:694:HOH:O	1.93	0.50
1:A:94:ILE:HD11	1:A:120:LEU:HD23	1.94	0.50
1:C:170:TRP:HE1	1:C:257[B]:GLU:CG	2.17	0.50
1:B:30:VAL:HG21	1:B:83:LEU:HD12	1.93	0.50
1:D:71:ILE:HA	3:D:865:HOH:O	2.12	0.50
1:B:114:GLU:HA	1:B:114:GLU:OE1	2.11	0.50
1:C:344:ARG:NH1	1:C:373:GLY:HA2	2.27	0.50
1:A:11:TRP:CZ2	1:A:15:LYS:HE2	2.47	0.50
1:B:107:PRO:HB2	1:B:112:LEU:CD2	2.41	0.50
2:C:501:CIT:O1	1:D:309:TRP:HZ2	1.94	0.49
1:A:332:ALA:O	1:A:362:ILE:HD13	2.11	0.49
1:B:120:LEU:HD13	1:B:137:LEU:HD22	1.94	0.49
1:B:24:ASN:ND2	1:B:26[A]:GLU:H	2.03	0.49
1:B:107:PRO:HB3	1:B:111:GLU:HB2	1.95	0.49
1:A:199:LEU:HD22	1:A:278:ALA:HB3	1.94	0.49
1:D:270:ASP:OD2	1:D:270:ASP:C	2.51	0.49
1:A:40:SER:OG	1:A:42:GLU:HB3	2.13	0.49
1:A:53:ILE:CG2	1:A:56:VAL:HB	2.43	0.49
2:C:502:CIT:O4	2:C:502:CIT:O1	2.31	0.49
1:B:271:ARG:HD2	3:B:556:HOH:O	2.13	0.49
1:D:107:PRO:HD2	1:D:108:ASP:H	1.76	0.49
1:B:13:GLN:HE21	1:B:13:GLN:HA	1.78	0.48
1:D:311:PRO:CD	1:D:320[A]:VAL:HG23	2.43	0.48
1:D:343:ILE:HA	1:D:349:MET:CE	2.43	0.48
1:B:24:ASN:ND2	1:B:26[B]:GLU:H	2.04	0.48
1:C:334:GLY:O	1:C:335:LEU:HD23	2.12	0.48
1:A:238[B]:THR:HG21	3:A:638:HOH:O	2.12	0.48
1:C:109:ARG:NH2	1:D:109:ARG:HD3	2.28	0.48
1:D:393:GLN:HB3	1:D:394:PRO:HD3	1.95	0.48
1:C:205:TRP:HE1	1:C:280:GLN:HE22	1.60	0.48
1:C:337[A]:ILE:HD12	1:C:338:VAL:C	2.35	0.48
1:A:379:CYS:HB3	3:A:697:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:TRP:CB	3:C:915:HOH:O	2.62	0.47
1:C:135:GLY:HA2	3:C:906:HOH:O	2.13	0.47
1:A:56:VAL:O	1:A:57:THR:HB	2.15	0.47
1:A:166:LYS:HE3	3:A:565:HOH:O	2.13	0.47
1:D:155:TRP:CE2	1:D:381:ARG:HB2	2.50	0.47
1:C:313:ARG:O	1:D:313:ARG:NH2	2.47	0.47
1:C:98:ARG:HE	1:C:100:ASP:CG	2.18	0.47
1:B:53:ILE:HG22	1:B:56:VAL:CG2	2.45	0.47
1:B:53:ILE:CG2	1:B:56:VAL:CG2	2.92	0.47
1:C:350:ARG:NH1	1:C:353:GLN:HE22	2.09	0.47
1:A:238[B]:THR:CG2	1:B:320[B]:VAL:HG11	2.43	0.47
1:B:236:ASP:HB2	3:B:632:HOH:O	2.15	0.47
1:D:137:LEU:O	1:D:137:LEU:HD23	2.15	0.47
1:D:360:HIS:N	1:D:361:PRO:HD2	2.29	0.47
1:C:109:ARG:O	1:C:113:ARG:HG2	2.15	0.46
1:C:168:ILE:HG22	3:C:935:HOH:O	2.15	0.46
1:B:20:TRP:HA	1:B:29:GLU:O	2.16	0.46
1:B:96:THR:HA	1:B:122:GLN:HE22	1.80	0.46
1:C:98:ARG:HG3	1:C:100:ASP:OD2	2.14	0.46
1:C:240:ARG:HH12	2:C:502:CIT:H41	1.80	0.46
1:A:307:SER:HB3	1:A:309:TRP:NE1	2.29	0.46
1:B:212:TRP:HB2	1:B:213:PRO:HD3	1.97	0.46
1:B:174:ARG:HH11	1:B:256:GLN:NE2	2.02	0.46
1:A:79:TRP:CH2	1:A:81:THR:HB	2.51	0.46
1:A:185[B]:THR:HG23	3:A:675:HOH:O	2.15	0.46
1:B:50:TRP:CE3	1:B:67:SER:HB2	2.51	0.46
1:D:336:ARG:NH2	1:D:391:LEU:O	2.46	0.46
1:A:10:SER:HA	1:A:13:GLN:HG3	1.97	0.46
1:C:84:ASN:OD1	1:C:86:ASN:HB2	2.16	0.46
1:C:125:ALA:HB2	1:C:140:ALA:HB1	1.98	0.46
1:C:294:TRP:HB3	3:C:915:HOH:O	2.15	0.46
1:B:107:PRO:CB	1:B:111:GLU:HB2	2.45	0.46
1:C:276:VAL:HG22	1:C:300:CYS:HB2	1.98	0.46
1:C:316:GLN:OE1	1:D:58:ASP:OD2	2.34	0.46
1:A:308:TYR:O	1:A:319:GLY:HA3	2.16	0.46
1:D:129:ASN:HA	1:D:130:PRO:HD2	1.86	0.46
1:C:195:PRO:HG2	1:C:227:ALA:HB2	1.98	0.45
1:C:251:TRP:O	1:C:255:GLN:HG3	2.16	0.45
1:C:240:ARG:NH1	2:C:502:CIT:H41	2.32	0.45
1:A:23:LEU:HD12	1:A:24:ASN:CB	2.44	0.45
1:B:342:GLY:HA2	1:B:371:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99[A]:ASP:OD1	1:C:99[A]:ASP:O	2.34	0.45
1:C:71:ILE:HB	1:C:74[A]:THR:CG2	2.46	0.45
1:A:28:PHE:CZ	1:A:147:PRO:HG2	2.52	0.45
1:A:74:THR:CG2	1:A:76:VAL:HG23	2.47	0.45
1:B:316:GLN:H	1:B:316:GLN:HG3	1.51	0.45
1:C:137:LEU:HG	1:D:317:GLN:HB2	1.98	0.45
1:C:205:TRP:O	1:C:210:PRO:HA	2.17	0.45
1:C:280:GLN:HA	1:C:304:GLN:O	2.16	0.45
1:C:317:GLN:OE1	1:D:137:LEU:HA	2.17	0.45
1:B:292:LEU:CD1	1:B:321[A]:LEU:HD11	2.47	0.45
1:D:107:PRO:CD	1:D:108:ASP:N	2.79	0.45
1:A:205:TRP:HE1	1:A:280:GLN:NE2	2.13	0.45
1:B:137:LEU:HD13	1:B:139:HIS:NE2	2.32	0.45
1:D:194:ARG:HB3	1:D:227:ALA:HA	1.99	0.45
1:A:74:THR:HG22	1:A:76:VAL:HG23	1.99	0.45
1:C:74[A]:THR:HG23	1:C:76:VAL:N	2.08	0.45
1:D:324:LYS:HB3	1:D:330:VAL:HG22	1.98	0.45
1:B:40[B]:SER:OG	1:B:73:GLY:HA2	2.17	0.44
1:B:277[B]:VAL:CG2	1:B:298:PHE:CD2	3.00	0.44
1:B:281:SER:HB2	2:B:501:CIT:O6	2.16	0.44
1:C:6:VAL:HA	1:C:11:TRP:CG	2.52	0.44
1:D:225:PRO:HG3	1:D:395:LEU:HD22	1.99	0.44
1:A:117:ARG:HH22	1:A:118:LYS:HG3	1.82	0.44
1:C:155:TRP:CE2	1:C:381:ARG:HB2	2.52	0.44
1:D:120:LEU:N	1:D:121:PRO:CD	2.80	0.44
1:D:205:TRP:HE1	1:D:280:GLN:NE2	2.14	0.44
1:B:57:THR:O	1:B:58:ASP:C	2.55	0.44
1:C:74[B]:THR:HG23	3:C:735:HOH:O	2.18	0.44
1:D:9:GLU:OE2	1:D:13:GLN:NE2	2.51	0.44
1:D:38:GLN:H	1:D:38:GLN:HG2	1.52	0.44
1:C:22:ARG:HG2	1:C:28:PHE:CE2	2.52	0.44
1:D:28:PHE:CZ	1:D:147:PRO:HG2	2.53	0.44
1:A:38:GLN:HE22	1:A:45:THR:HB	1.82	0.44
1:B:174:ARG:NH1	1:B:256:GLN:HE22	2.02	0.44
1:A:39:GLY:HA2	3:A:611:HOH:O	2.18	0.44
1:D:296:GLU:HA	3:D:833:HOH:O	2.17	0.44
1:B:18:PRO:HG2	1:B:144:LEU:HD13	1.99	0.44
1:B:360:HIS:HB3	1:B:361:PRO:HD3	1.99	0.44
1:C:146:MET:HA	1:C:146:MET:CE	2.48	0.43
1:C:110:LEU:HD21	3:D:878:HOH:O	2.18	0.43
1:C:212:TRP:HB2	1:C:213:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLN:NE2	1:B:45:THR:H	2.17	0.43
1:C:292:LEU:HD13	1:C:330:VAL:HG11	2.00	0.43
1:D:57:THR:O	1:D:58:ASP:OD1	2.36	0.43
1:B:28:PHE:CZ	1:B:147:PRO:HG2	2.54	0.43
1:D:33[A]:TRP:HZ3	1:D:78:GLN:OE1	2.01	0.43
1:A:281:SER:HA	1:A:305:SER:O	2.19	0.43
1:A:349:MET:O	1:A:353:GLN:HG3	2.19	0.43
1:C:84:ASN:C	1:C:86:ASN:N	2.71	0.43
1:A:212:TRP:HB2	1:A:213:PRO:CD	2.43	0.43
1:A:216:THR:HG23	1:A:220:HIS:CE1	2.54	0.43
1:A:317:GLN:HB2	1:B:137:LEU:HD23	2.00	0.43
1:B:11:TRP:CZ2	1:B:15:LYS:HE3	2.53	0.43
1:C:150:PRO:HG3	3:C:820:HOH:O	2.18	0.43
1:B:79:TRP:CH2	1:B:81:THR:HB	2.54	0.43
1:C:316:GLN:NE2	1:D:52:TYR:OH	2.52	0.43
1:C:337[A]:ILE:HG13	1:C:366:ILE:HG23	2.00	0.43
1:D:20:TRP:HA	1:D:29:GLU:O	2.19	0.43
1:A:300:CYS:HB3	1:A:391:LEU:HD13	2.01	0.43
1:A:397:HIS:CD2	1:A:397:HIS:C	2.92	0.43
1:D:119:LEU:C	1:D:121:PRO:HD2	2.38	0.43
1:D:185:THR:HG21	1:D:194:ARG:HH21	1.74	0.43
1:D:268:PHE:HD2	1:D:269:SER:O	2.02	0.43
1:A:6:VAL:HA	1:A:11:TRP:CD1	2.54	0.42
1:C:155:TRP:CE3	1:C:214:VAL:HG21	2.53	0.42
1:D:270:ASP:HA	1:D:297:ARG:NH2	2.31	0.42
1:C:261:LEU:HD21	3:C:953:HOH:O	2.20	0.42
1:D:170:TRP:CE3	1:D:179:ARG:HD2	2.54	0.42
1:D:221[B]:ARG:O	1:D:222:GLN:HB2	2.19	0.42
1:D:251:TRP:O	1:D:255:GLN:HG3	2.18	0.42
1:B:58:ASP:OD2	1:B:58:ASP:N	2.52	0.42
1:B:82:GLN:HG3	3:B:628:HOH:O	2.18	0.42
1:D:392:TRP:O	1:D:395:LEU:HB2	2.19	0.42
1:D:111:GLU:HA	1:D:114[A]:GLU:CG	2.46	0.42
1:A:196:LEU:HD11	1:A:230[B]:VAL:CG2	2.50	0.42
1:D:302:LEU:HD13	1:D:338:VAL:HB	2.01	0.42
1:A:295:PRO:HG3	3:A:531:HOH:O	2.19	0.42
1:A:393[B]:GLN:N	1:A:394:PRO:CD	2.82	0.42
1:B:98:ARG:HB3	1:B:100:ASP:OD1	2.19	0.42
1:C:26:GLU:O	1:C:26:GLU:HG3	2.18	0.42
1:C:41:GLU:HB3	1:C:70:ARG:CD	2.49	0.42
1:D:224[B]:LEU:HD13	1:D:389:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:HA	1:A:161:PRO:HD3	1.90	0.42
1:C:134:LYS:HG2	3:C:958:HOH:O	2.20	0.42
1:A:97:GLU:HG2	3:A:624:HOH:O	2.18	0.42
1:A:163:ILE:HA	1:A:164:PRO:HD3	1.74	0.42
1:B:179:ARG:HB2	1:B:233:ASP:HB3	2.01	0.42
1:C:108:ASP:O	1:C:112:LEU:HD23	2.20	0.42
1:C:195:PRO:HB3	1:C:274:ARG:HG3	2.01	0.42
1:C:23:LEU:HD22	1:C:29:GLU:HB3	2.02	0.41
1:D:139:HIS:HE1	3:D:743:HOH:O	2.02	0.41
1:D:169:ILE:C	1:D:169:ILE:HD13	2.40	0.41
1:D:273:ASP:HB2	3:D:774:HOH:O	2.20	0.41
1:B:53:ILE:CG2	1:B:56:VAL:HG21	2.50	0.41
1:B:107:PRO:HB3	1:B:111:GLU:CB	2.50	0.41
1:B:155:TRP:CE2	1:B:381:ARG:HB2	2.55	0.41
1:B:163:ILE:HA	1:B:164:PRO:HD2	1.81	0.41
1:A:222:GLN:HA	3:A:734:HOH:O	2.20	0.41
1:B:173:GLU:H	1:B:173:GLU:HG2	1.52	0.41
1:C:185:THR:HG22	1:C:228:VAL:HG22	2.02	0.41
1:A:185[A]:THR:HG22	1:A:228:VAL:HG22	2.02	0.41
1:A:360:HIS:N	1:A:361:PRO:CD	2.83	0.41
1:B:107:PRO:HG2	1:B:112:LEU:HD11	2.02	0.41
1:C:244:LEU:N	1:C:245:PRO:CD	2.84	0.41
1:A:194:ARG:HA	1:A:195:PRO:HD2	1.92	0.41
1:B:58:ASP:HB3	3:B:739:HOH:O	2.20	0.41
1:C:22:ARG:HG3	3:C:825:HOH:O	2.20	0.41
1:A:125:ALA:HB2	1:A:140:ALA:CB	2.49	0.41
1:B:327:ALA:HB3	1:B:329:GLU:HG2	2.03	0.41
1:D:293:HIS:CE1	1:D:330:VAL:HG11	2.56	0.41
1:A:71:ILE:HD11	3:A:626:HOH:O	2.21	0.41
1:A:128:LEU:HD12	3:A:642:HOH:O	2.20	0.41
1:A:393[B]:GLN:HB3	1:A:394:PRO:HD3	2.02	0.41
1:B:333:GLU:HG2	3:B:642:HOH:O	2.20	0.41
1:C:35:ARG:O	1:C:37:PRO:HD3	2.20	0.41
1:A:242:HIS:HE1	1:B:246:CYS:O	2.03	0.41
1:B:160:ALA:HA	1:B:161:PRO:HD3	1.90	0.41
1:B:311:PRO:HD3	1:B:320[B]:VAL:HG23	2.03	0.41
1:B:321[B]:LEU:HB3	3:B:676:HOH:O	2.20	0.41
1:B:393:GLN:N	1:B:394:PRO:CD	2.83	0.41
1:A:393[A]:GLN:N	1:A:394:PRO:CD	2.83	0.40
1:B:332:ALA:HB3	1:B:362:ILE:CD1	2.51	0.40
1:C:98:ARG:NE	1:C:100:ASP:OD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337[A]:ILE:HD11	1:C:339:LEU:CG	2.38	0.40
1:D:316:GLN:HE21	1:D:316:GLN:HB3	1.74	0.40
1:A:117:ARG:HH21	1:A:117:ARG:HB3	1.85	0.40
1:B:269:SER:CB	1:B:274:ARG:HD2	2.52	0.40
1:B:277[A]:VAL:HG13	1:B:298:PHE:CD2	2.56	0.40
1:D:84:ASN:O	1:D:146:MET:HG3	2.21	0.40
1:B:20:TRP:HB3	1:B:30:VAL:HG22	2.02	0.40
1:C:316:GLN:HE21	1:C:316:GLN:HB3	1.71	0.40
1:B:156:ASP:OD2	1:B:156:ASP:N	2.44	0.40
1:C:23:LEU:HD12	1:C:23:LEU:HA	1.78	0.40
1:D:111:GLU:CA	1:D:114[A]:GLU:HG2	2.46	0.40
1:A:114:GLU:HG3	1:B:350:ARG:CD	2.51	0.40
1:A:321:LEU:HB3	3:A:526:HOH:O	2.22	0.40
1:D:97:GLU:CD	1:D:97:GLU:H	2.24	0.40
1:D:311:PRO:HD3	1:D:320[B]:VAL:HG13	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:CYS:SG	1:D:157:CYS:SG[2_646]	1.87	0.33
1:A:157:CYS:SG	1:B:157:CYS:SG[2_545]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/403 (94%)	367 (96%)	13 (3%)	1 (0%)	41	27
1	B	380/403 (94%)	368 (97%)	11 (3%)	1 (0%)	41	27
1	C	381/403 (94%)	362 (95%)	19 (5%)	0	100	100
1	D	379/403 (94%)	369 (97%)	9 (2%)	1 (0%)	41	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1521/1612 (94%)	1466 (96%)	52 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLY
1	D	235	ILE
1	B	235	ILE

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	331/341 (97%)	316 (96%)	15 (4%)	27	13
1	B	331/341 (97%)	307 (93%)	24 (7%)	14	4
1	C	328/341 (96%)	308 (94%)	20 (6%)	18	7
1	D	332/341 (97%)	315 (95%)	17 (5%)	24	10
All	All	1322/1364 (97%)	1246 (94%)	76 (6%)	20	8

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	23	LEU
1	A	42	GLU
1	A	74	THR
1	A	84	ASN
1	A	97	GLU
1	A	112	LEU
1	A	137	LEU
1	A	144	LEU
1	A	222	GLN
1	A	271	ARG
1	A	322	LEU

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Mol	Chain	Res	Type
1	A	326	LYS
1	A	333	GLU
1	A	339	LEU
1	B	10	SER
1	B	13	GLN
1	B	47	LYS
1	B	58	ASP
1	B	86	ASN
1	B	106	SER
1	B	108	ASP
1	B	109	ARG
1	B	114	GLU
1	B	118	LYS
1	B	173	GLU
1	B	193	GLU
1	B	200	LEU
1	B	277[A]	VAL
1	B	277[B]	VAL
1	B	281	SER
1	B	316	GLN
1	B	322	LEU
1	B	329	GLU
1	B	333	GLU
1	B	362	ILE
1	B	391	LEU
1	B	393	GLN
1	B	397	HIS
1	C	23	LEU
1	C	24	ASN
1	C	48	ARG
1	C	57	THR
1	C	109	ARG
1	C	111	GLU
1	C	156	ASP
1	C	157	CYS
1	C	194	ARG
1	C	200	LEU
1	C	264	VAL
1	C	274	ARG
1	C	302	LEU
1	C	318	GLU
1	C	326	LYS

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Mol	Chain	Res	Type
1	C	330	VAL
1	C	337[A]	ILE
1	C	337[B]	ILE
1	C	347	MET
1	C	369	ARG
1	D	10	SER
1	D	21	GLN
1	D	38	GLN
1	D	40	SER
1	D	42	GLU
1	D	58	ASP
1	D	113	ARG
1	D	134	LYS
1	D	156	ASP
1	D	169	ILE
1	D	261	LEU
1	D	313	ARG
1	D	322	LEU
1	D	326	LYS
1	D	330	VAL
1	D	350	ARG
1	D	396	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	24	ASN
1	A	84	ASN
1	A	222	GLN
1	A	255	GLN
1	A	280	GLN
1	A	304	GLN
1	A	317	GLN
1	B	13	GLN
1	B	24	ASN
1	B	38	GLN
1	B	84	ASN
1	B	86	ASN
1	B	122	GLN
1	B	131	GLN
1	B	139	HIS

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Mol	Chain	Res	Type
1	B	255	GLN
1	B	256	GLN
1	B	280	GLN
1	B	293	HIS
1	B	304	GLN
1	B	386	GLN
1	C	69	GLN
1	C	78	GLN
1	C	86	ASN
1	C	159	GLN
1	C	280	GLN
1	C	304	GLN
1	C	316	GLN
1	C	353	GLN
1	C	370	GLN
1	D	38	GLN
1	D	69	GLN
1	D	207	GLN
1	D	256	GLN
1	D	280	GLN
1	D	293	HIS
1	D	316	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	CIT	B	501	-	12,12,12	2.14	6 (50%)	17,17,17	1.87	7 (41%)
2	CIT	A	501	-	12,12,12	1.15	0	17,17,17	1.88	5 (29%)
2	CIT	C	501	-	12,12,12	1.86	5 (41%)	17,17,17	2.76	7 (41%)
2	CIT	C	502	-	12,12,12	1.89	5 (41%)	17,17,17	2.53	8 (47%)

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	CIT	B	501	-	-	2/16/16/16	-
2	CIT	A	501	-	-	8/16/16/16	-
2	CIT	C	501	-	-	7/16/16/16	-
2	CIT	C	502	-	-	11/16/16/16	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	CIT	C3-C6	-4.91	1.48	1.53
2	C	501	CIT	O2-C1	-3.60	1.18	1.30
2	C	502	CIT	O7-C3	3.38	1.49	1.43
2	B	501	CIT	C2-C3	-3.19	1.49	1.53
2	C	501	CIT	C3-C6	-2.96	1.50	1.53
2	C	502	CIT	C3-C6	-2.77	1.50	1.53
2	C	501	CIT	O4-C5	-2.66	1.21	1.30
2	C	502	CIT	O4-C5	-2.38	1.22	1.30
2	B	501	CIT	O2-C1	-2.37	1.22	1.30
2	B	501	CIT	C4-C3	-2.26	1.51	1.53
2	C	501	CIT	O6-C6	-2.20	1.22	1.30
2	C	502	CIT	C2-C3	-2.14	1.51	1.53
2	B	501	CIT	O4-C5	-2.11	1.23	1.30
2	C	501	CIT	C2-C1	2.09	1.57	1.50
2	C	502	CIT	O6-C6	-2.07	1.22	1.30
2	B	501	CIT	O6-C6	-2.06	1.22	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	CIT	O2-C1-O1	-7.66	104.20	123.30
2	C	502	CIT	C2-C3-C6	-5.20	98.93	110.11
2	C	502	CIT	O6-C6-C3	4.69	121.20	113.05
2	C	501	CIT	O2-C1-C2	4.16	127.70	114.35
2	A	501	CIT	C2-C3-C6	-3.86	101.82	110.11
2	C	501	CIT	O6-C6-C3	3.75	119.56	113.05
2	C	502	CIT	O5-C6-C3	-3.63	117.11	122.25
2	A	501	CIT	O6-C6-C3	3.45	119.03	113.05
2	C	502	CIT	O4-C5-O3	-3.40	114.82	123.30
2	B	501	CIT	C3-C2-C1	-3.09	106.34	113.81
2	B	501	CIT	C2-C3-C6	-2.96	103.75	110.11
2	A	501	CIT	O7-C3-C6	2.91	112.95	108.86
2	C	502	CIT	C3-C2-C1	-2.82	106.97	113.81
2	B	501	CIT	O7-C3-C2	2.72	115.77	109.40
2	C	501	CIT	O4-C5-C4	2.69	123.00	114.35
2	B	501	CIT	C3-C4-C5	-2.51	107.73	113.81
2	C	502	CIT	O4-C5-C4	2.51	122.41	114.35
2	A	501	CIT	O4-C5-C4	2.39	122.02	114.35
2	B	501	CIT	O5-C6-C3	-2.38	118.88	122.25
2	C	502	CIT	C4-C3-C6	2.36	115.18	110.11
2	C	502	CIT	O7-C3-C2	2.29	114.77	109.40
2	C	501	CIT	O7-C3-C2	2.29	114.77	109.40
2	B	501	CIT	O6-C6-C3	2.25	116.95	113.05
2	A	501	CIT	O4-C5-O3	-2.20	117.81	123.30
2	B	501	CIT	O4-C5-C4	2.20	121.42	114.35
2	C	501	CIT	O4-C5-O3	-2.18	117.87	123.30
2	C	501	CIT	O7-C3-C4	-2.09	104.52	109.40

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C1-C2-C3-C4
2	A	501	CIT	O7-C3-C6-O5
2	A	501	CIT	O7-C3-C6-O6
2	A	501	CIT	C4-C3-C6-O5
2	A	501	CIT	C4-C3-C6-O6
2	C	501	CIT	C1-C2-C3-O7
2	C	501	CIT	C1-C2-C3-C4
2	C	501	CIT	C2-C3-C6-O5
2	C	501	CIT	C2-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	501	CIT	O7-C3-C6-O5
2	C	501	CIT	O7-C3-C6-O6
2	C	502	CIT	C2-C3-C4-C5
2	C	502	CIT	O7-C3-C4-C5
2	C	502	CIT	C2-C3-C6-O5
2	C	502	CIT	C2-C3-C6-O6
2	C	502	CIT	O7-C3-C6-O5
2	C	502	CIT	O7-C3-C6-O6
2	A	501	CIT	C1-C2-C3-C6
2	C	501	CIT	C1-C2-C3-C6
2	C	502	CIT	C6-C3-C4-C5
2	A	501	CIT	C1-C2-C3-O7
2	C	502	CIT	C1-C2-C3-C6
2	C	502	CIT	C1-C2-C3-C4
2	B	501	CIT	O1-C1-C2-C3
2	C	502	CIT	C3-C4-C5-O3
2	B	501	CIT	O2-C1-C2-C3
2	C	502	CIT	C3-C4-C5-O4
2	A	501	CIT	C6-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	CIT	1	0
2	A	501	CIT	2	0
2	C	501	CIT	3	0
2	C	502	CIT	6	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(Å²)	Q<0.9
1	A	378/403 (93%)	-0.02	11 (2%)	51	46	18, 35, 73, 167	0
1	B	379/403 (94%)	-0.06	14 (3%)	41	36	15, 30, 72, 114	0
1	C	379/403 (94%)	-0.09	7 (1%)	68	64	18, 34, 71, 102	0
1	D	378/403 (93%)	-0.04	9 (2%)	59	54	18, 36, 71, 98	0
All	All	1514/1612 (93%)	-0.05	41 (2%)	54	49	15, 34, 71, 167	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	LEU	16.8
1	B	105	PRO	6.6
1	B	398	ASP	6.5
1	D	137	LEU	5.6
1	C	137	LEU	5.1
1	B	137	LEU	5.0
1	A	136	GLY	4.9
1	B	397	HIS	4.8
1	D	396	PHE	4.5
1	C	110	LEU	4.5
1	A	397	HIS	4.4
1	B	110	LEU	4.1
1	A	110	LEU	3.4
1	B	138	GLY	3.4
1	D	135	GLY	3.4
1	B	106	SER	3.3
1	B	109	ARG	3.2
1	A	192	GLU	3.1
1	C	112	LEU	3.1
1	D	270	ASP	3.0
1	C	134	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	135	GLY	2.8
1	D	107	PRO	2.7
1	D	6	VAL	2.6
1	B	104	ALA	2.6
1	C	136	GLY	2.6
1	B	396	PHE	2.6
1	A	25	ASP	2.6
1	B	112	LEU	2.5
1	A	108	ASP	2.4
1	A	105	PRO	2.3
1	D	193	GLU	2.3
1	C	372	ASP	2.3
1	C	117	ARG	2.2
1	A	56	VAL	2.2
1	D	63	SER	2.1
1	B	58	ASP	2.1
1	A	43	TYR	2.0
1	D	360	HIS	2.0
1	B	107	PRO	2.0
1	B	66	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	C	502	13/13	0.64	0.21	83,88,93,94	0
2	CIT	B	501	13/13	0.68	0.15	87,92,94,96	0
2	CIT	C	501	13/13	0.70	0.22	64,68,71,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	A	501	13/13	0.84	0.15	38,54,72,76	0

6.5　Other polymers ⓘ

There are no such residues in this entry.