Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:52 PM GMT

PDB ID : 1HOP
Title : STRUCTURE OF GUANINE NUCLEOTIDE (GPPCP) COMPLEX OF ADENYLOSUCCINATE SYNTHETASE FROM ESCHERICHIA COLI AT PH 6.5 AND 25 DEGREES CELSIUS
Authors : Poland, B.W.; Hou, Z.; Bruns, C.; Fromm, H.J.; Honzatko, R.B.
Deposited on : 1996-04-26
Resolution : 2.30 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

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

The reported resolution of this entry is 2.30 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		0.207
Clashscore		27
Ramachandran outliers		4.1%
Sidechain outliers		9.2%
RSRZ outliers		6.0%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
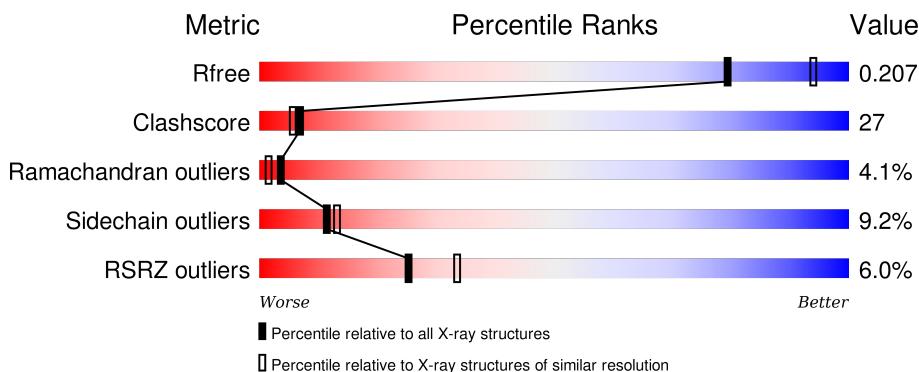
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	431	8% / 50% / 43% / 7%
1	B	431	4% / 53% / 41% / 5% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9261 atoms, of which 2210 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 ADENYLOSUCCINATE SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total 4069	C 2092	H 748	N 576	O 640	S 13	0	0	0
1	B	431	Total 4069	C 2092	H 748	N 576	O 640	S 13	0	0	0

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).
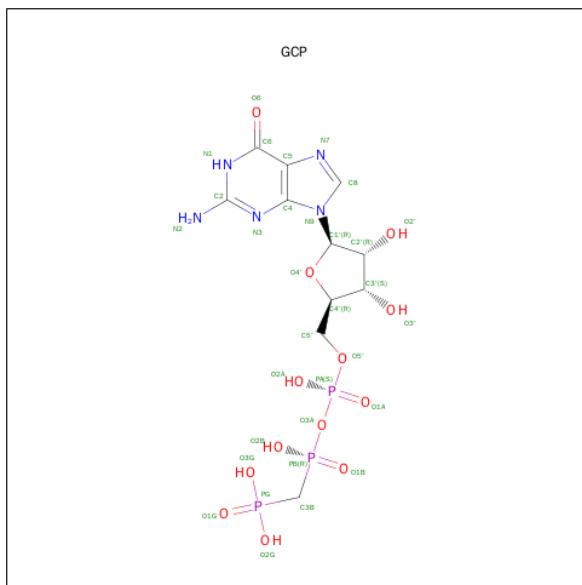
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 44	C 11	H 12	N 5	O 13	P 3	0	0
2	B	1	Total 44	C 11	H 12	N 5	O 13	P 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	162	Total 486	H 324	O 162	0	0
3	B	183	Total 549	H 366	O 183	0	0

3 Residue-property plots ⓘ

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: ADENYLOSUCCINATE SYNTHETASE
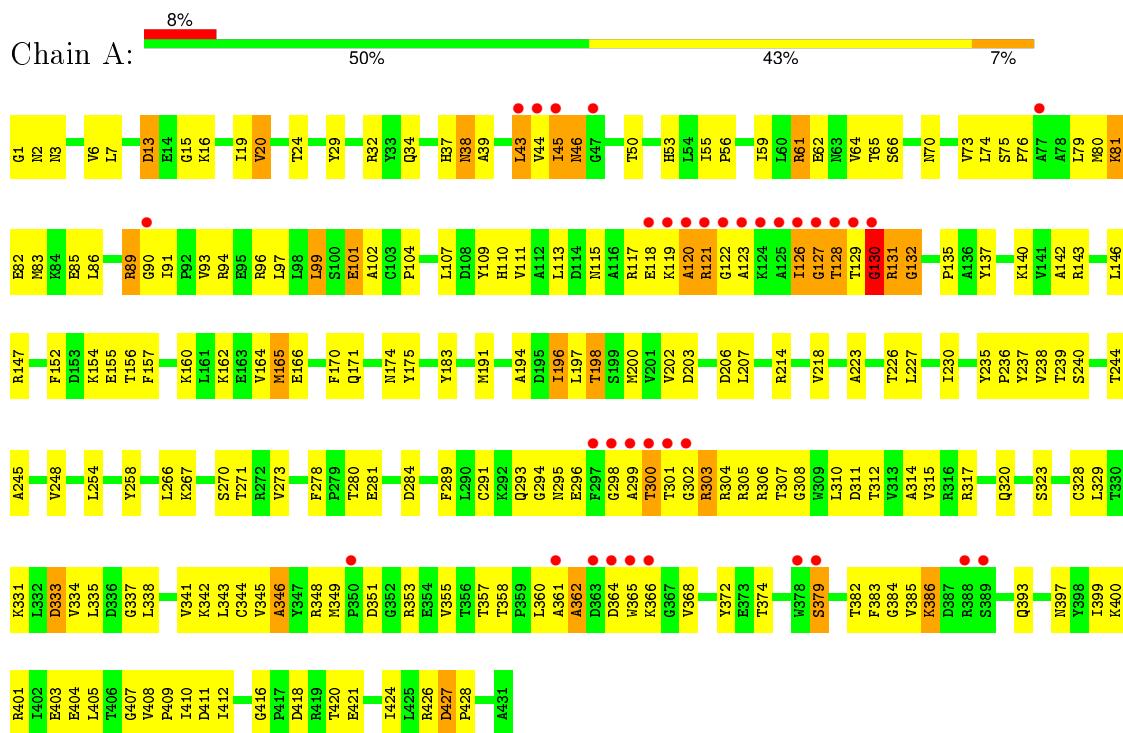
- Molecule 1: ADENYLOSUCCINATE SYNTHETASE
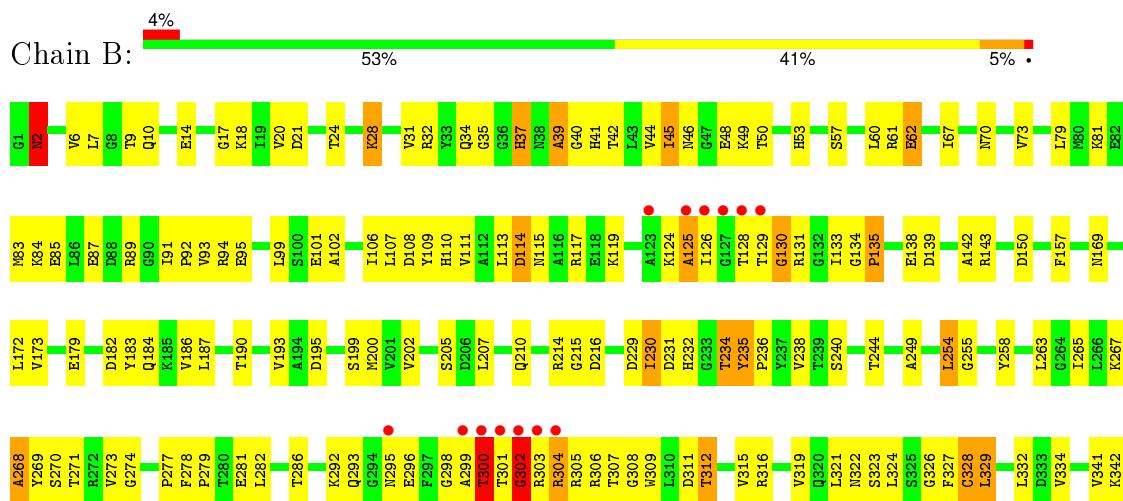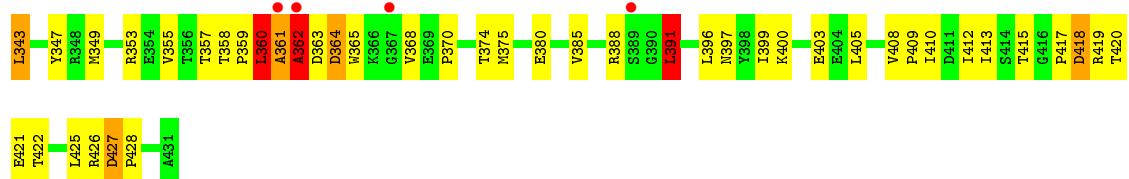
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.85Å 94.06Å 119.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 5.05 – 2.32	Depositor EDS
% Data completeness (in resolution range)	70.0 (15.00-2.30) 71.3 (5.05-2.32)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.32Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , 0.227 0.192 , 0.207	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.14 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.29$	Xtriage
Outliers	0 of 23665 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9261	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 27.40 % 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 2.2155e-03.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.83	2/3379 (0.1%)	0.95	2/4577 (0.0%)
1	B	0.83	2/3379 (0.1%)	0.98	6/4577 (0.1%)
All	All	0.83	4/6758 (0.1%)	0.96	8/9154 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ILE	C-N	20.97	1.70	1.33
1	B	300	THR	C-N	14.74	1.68	1.34
1	A	130	GLY	C-N	12.37	1.62	1.34
1	B	328	CYS	CB-SG	7.63	1.95	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	GLY	O-C-N	-12.22	103.14	122.70
1	B	302	GLY	CA-C-N	-8.34	98.84	117.20
1	A	126	ILE	O-C-N	-8.14	109.36	123.20
1	B	302	GLY	C-N-CA	-7.23	103.63	121.70
1	B	343	LEU	CA-CB-CG	6.67	130.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	364	ASP	N-CA-C	6.19	127.72	111.00
1	B	150	ASP	CB-CG-OD2	5.72	123.44	118.30
1	B	391	LEU	CA-CB-CG	5.55	128.08	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	GLY	Mainchain,Peptide
1	A	237	TYR	Sidechain
1	B	302	GLY	Mainchain
1	B	362	ALA	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3321	748	3325	182	0
1	B	3321	748	3326	180	0
2	A	32	12	14	1	0
2	B	32	12	14	3	0
3	A	162	324	0	13	0
3	B	183	366	0	18	0
All	All	7051	2210	6679	357	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 27.

All (357) 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:B:300:THR:C	1:B:301:THR:N	1.68	1.45
1:A:126:ILE:C	1:A:127:GLY:N	1.70	1.43
1:A:129:THR:HG22	1:A:129:THR:O	1.64	0.94
1:A:16:LYS:HD2	3:A:543:HOH:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:O	1:A:128:THR:CG2	2.20	0.90
1:A:226:THR:HG23	1:A:244:THR:HG22	1.58	0.86
1:A:81:LYS:HA	1:A:81:LYS:HE2	1.61	0.82
1:A:101:GLU:HG3	1:A:102:ALA:N	1.95	0.82
3:A:479:HOH:O	1:B:235:TYR:HE2	1.65	0.79
1:A:46:ASN:HB3	1:A:89:ARG:HG3	1.65	0.79
1:A:128:THR:O	1:A:128:THR:HG22	1.82	0.78
1:A:384:GLY:HA2	1:A:421:GLU:HG3	1.63	0.78
1:B:311:ASP:O	1:B:315:VAL:HG23	1.83	0.78
1:A:271:THR:HG22	1:A:307:THR:HG22	1.67	0.77
1:A:349:MET:SD	1:A:368:VAL:HG12	2.25	0.76
1:B:31:VAL:HG22	1:B:67:ILE:HD12	1.66	0.75
1:A:131:ARG:HH11	1:A:131:ARG:HB3	1.50	0.75
1:B:32:ARG:HH11	1:B:32:ARG:HG3	1.51	0.75
1:A:399:ILE:HG23	1:A:410:ILE:HD12	1.68	0.75
1:A:109:TYR:O	1:A:113:LEU:HD23	1.87	0.74
3:A:524:HOH:O	1:B:143:ARG:HD3	1.87	0.73
1:B:235:TYR:O	1:B:238:VAL:HG22	1.87	0.73
1:B:61:ARG:HD2	3:B:593:HOH:O	1.89	0.73
1:B:244:THR:HB	1:B:322:ASN:OD1	1.89	0.72
1:A:56:PRO:HB2	1:A:66:SER:HB3	1.70	0.72
1:A:426:ARG:O	1:A:427:ASP:HB3	1.89	0.72
1:B:282:LEU:HG	1:B:308:GLY:HA2	1.71	0.71
1:A:128:THR:O	1:A:129:THR:HB	1.89	0.71
1:A:46:ASN:CB	1:A:89:ARG:HG3	2.19	0.71
1:A:89:ARG:N	1:A:89:ARG:HD3	2.05	0.71
1:B:334:VAL:HA	3:B:439:HOH:O	1.91	0.71
1:B:312:THR:HG21	1:B:405:LEU:HB3	1.73	0.71
1:B:360:LEU:HD23	1:B:360:LEU:H	1.54	0.70
1:B:319:VAL:HA	1:B:324:LEU:HD12	1.73	0.70
1:A:115:ASN:OD1	1:A:130:GLY:HA2	1.91	0.70
1:B:328:CYS:SG	1:B:412:ILE:HG22	2.31	0.69
1:A:162:LYS:O	1:A:166:GLU:HG3	1.92	0.69
1:A:117:ARG:HH12	1:A:135:PRO:HG3	1.57	0.69
1:A:39:ALA:HA	1:A:223:ALA:HB1	1.73	0.69
1:A:129:THR:CG2	1:A:129:THR:O	2.37	0.69
1:B:9:THR:HG21	1:B:327:PHE:HE1	1.57	0.69
1:A:305:ARG:HD3	3:A:471:HOH:O	1.92	0.68
1:A:335:LEU:HD13	1:A:341:VAL:HG11	1.76	0.67
1:A:310:LEU:HD23	1:A:343:LEU:CD2	2.24	0.67
1:A:203:ASP:OD2	1:A:206:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:NH1	1:A:131:ARG:HB3	2.09	0.67
1:B:129:THR:HA	1:B:131:ARG:NH1	2.09	0.67
1:B:397:ASN:HA	1:B:400:LYS:NZ	2.09	0.67
1:B:20:VAL:O	1:B:24:THR:HG23	1.95	0.66
1:A:19:ILE:HD12	1:A:19:ILE:H	1.60	0.66
1:A:254:LEU:HD12	3:A:472:HOH:O	1.94	0.66
1:B:85:GLU:O	1:B:89:ARG:HG2	1.96	0.66
1:B:32:ARG:HG3	1:B:32:ARG:NH1	2.11	0.65
1:B:281:GLU:HA	1:B:307:THR:O	1.97	0.65
1:A:345:VAL:HG12	1:A:405:LEU:HD13	1.78	0.65
1:A:245:ALA:O	1:A:248:VAL:HG23	1.97	0.64
1:A:117:ARG:NH1	1:A:135:PRO:HG3	2.12	0.64
1:A:152:PHE:CZ	1:A:198:THR:HG22	2.32	0.64
1:B:41:HIS:CE1	1:B:57:SER:HB3	2.33	0.64
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.62	0.63
1:A:62:GLU:HA	1:A:96:ARG:NH1	2.13	0.63
1:A:55:ILE:HG12	1:A:82:GLU:OE1	1.97	0.63
1:B:18:LYS:HE3	1:B:419:ARG:HA	1.81	0.63
1:B:300:THR:C	1:B:301:THR:CA	2.64	0.63
1:A:97:LEU:HD23	1:A:200:MET:CE	2.28	0.62
1:B:234:THR:HG21	1:B:277:PRO:HD2	1.80	0.62
1:A:293:GLN:HB3	1:A:334:VAL:HG13	1.82	0.62
1:B:388:ARG:HH11	1:B:425:LEU:HD22	1.66	0.61
1:A:19:ILE:HD12	1:A:19:ILE:N	2.15	0.61
1:A:19:ILE:HG12	1:A:328:CYS:SG	2.41	0.60
1:A:43:LEU:HD12	1:A:50:THR:O	2.01	0.60
1:B:249:ALA:HA	1:B:254:LEU:O	2.00	0.60
1:B:286:THR:HG21	1:B:309:TRP:CH2	2.36	0.60
1:A:73:VAL:HG12	1:A:104:PRO:HB2	1.83	0.60
1:B:302:GLY:O	1:B:303:ARG:C	2.40	0.60
1:A:345:VAL:O	1:A:346:ALA:HB2	2.01	0.60
1:A:258:TYR:CE2	1:B:323:SER:HB3	2.37	0.60
1:B:299:ALA:O	1:B:300:THR:HB	2.00	0.60
1:B:349:MET:HG3	1:B:353:ARG:NH2	2.16	0.60
1:B:142:ALA:O	1:B:143:ARG:C	2.40	0.59
1:B:397:ASN:CG	1:B:400:LYS:HZ1	2.04	0.59
1:A:128:THR:O	1:A:128:THR:HG23	1.99	0.59
1:B:328:CYS:SG	1:B:412:ILE:CG2	2.91	0.59
1:A:118:GLU:O	1:A:119:LYS:C	2.40	0.59
1:B:128:THR:HG23	1:B:128:THR:O	2.03	0.59
1:A:128:THR:HG21	3:A:438:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:PRO:HB3	1:B:365:TRP:HB3	1.84	0.59
1:B:45:ILE:HD13	1:B:60:LEU:HD11	1.85	0.58
1:A:160:LYS:O	1:A:164:VAL:HG23	2.03	0.58
1:A:97:LEU:HD23	1:A:200:MET:HE1	1.83	0.58
1:B:184:GLN:HE22	1:B:187:LEU:HD23	1.69	0.58
1:B:42:THR:HG23	3:B:539:HOH:O	2.04	0.58
1:B:186:VAL:HG13	3:B:477:HOH:O	2.04	0.58
1:B:399:ILE:O	1:B:403:GLU:HG3	2.04	0.58
1:B:83:MET:O	1:B:87:GLU:HG3	2.02	0.58
1:A:365:TRP:O	1:A:368:VAL:HG22	2.03	0.58
1:A:79:LEU:CD1	1:A:83:MET:SD	2.92	0.58
1:A:301:THR:HB	1:A:303:ARG:NH2	2.19	0.57
1:A:74:LEU:CD2	1:A:99:LEU:HD22	2.34	0.57
1:B:360:LEU:H	1:B:360:LEU:CD2	2.17	0.57
1:B:397:ASN:O	1:B:400:LYS:HG3	2.05	0.57
1:B:129:THR:HA	1:B:131:ARG:CZ	2.35	0.56
1:A:101:GLU:CD	1:A:147:ARG:HH21	2.08	0.56
1:B:282:LEU:HD11	1:B:309:TRP:NE1	2.20	0.56
1:B:107:LEU:H	1:B:110:HIS:HD2	1.53	0.56
1:A:382:THR:O	1:A:385:VAL:HG23	2.05	0.56
1:A:416:GLY:HA3	1:A:421:GLU:HG2	1.88	0.55
1:A:118:GLU:HG2	1:A:123:ALA:HA	1.88	0.55
1:A:62:GLU:HG3	1:A:96:ARG:HH12	1.70	0.55
1:B:426:ARG:O	1:B:427:ASP:HB3	2.07	0.55
1:A:311:ASP:HA	1:A:344:CYS:HB3	1.89	0.55
1:B:182:ASP:HA	3:B:511:HOH:O	2.07	0.55
1:A:364:ASP:OD1	1:A:366:LYS:HB3	2.06	0.55
1:A:152:PHE:CE1	1:A:198:THR:HG22	2.42	0.55
1:A:1:GLY:HA2	3:A:461:HOH:O	2.06	0.54
1:B:131:ARG:HD2	1:B:133:ILE:HD12	1.90	0.54
1:A:90:GLY:C	1:A:91:ILE:HD12	2.27	0.54
1:B:37:HIS:CD2	1:B:37:HIS:H	2.25	0.54
1:A:146:LEU:HD22	1:A:157:PHE:CE1	2.43	0.54
1:B:169:ASN:O	1:B:173:VAL:HG22	2.08	0.54
1:B:9:THR:HG21	1:B:327:PHE:CE1	2.42	0.53
1:B:114:ASP:HB3	1:B:130:GLY:HA2	1.89	0.53
1:A:418:ASP:HB3	1:A:421:GLU:OE1	2.08	0.53
1:A:312:THR:HG21	1:A:405:LEU:HB3	1.89	0.53
1:A:15:GLY:HA2	2:A:432:GCP:C5'	2.39	0.53
1:A:351:ASP:OD1	1:A:353:ARG:HG2	2.09	0.53
1:B:312:THR:HG21	1:B:405:LEU:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TYR:O	1:B:236:PRO:C	2.46	0.53
1:A:384:GLY:HA2	1:A:421:GLU:CG	2.35	0.53
1:B:282:LEU:HD11	1:B:309:TRP:CE2	2.44	0.53
1:B:235:TYR:HB3	1:B:236:PRO:HD3	1.90	0.52
1:A:357:THR:HG22	3:B:607:HOH:O	2.09	0.52
1:B:418:ASP:HB3	1:B:421:GLU:OE1	2.09	0.52
1:B:92:PRO:HB2	1:B:95:GLU:HG2	1.91	0.52
1:A:91:ILE:HD12	1:A:91:ILE:N	2.25	0.52
1:B:117:ARG:NH1	1:B:135:PRO:HG3	2.25	0.52
1:B:157:PHE:CZ	1:B:190:THR:HG21	2.44	0.52
1:A:74:LEU:HD21	1:A:99:LEU:HD22	1.91	0.52
1:B:129:THR:O	1:B:131:ARG:HG2	2.10	0.52
1:A:196:ILE:HG22	1:A:197:LEU:N	2.23	0.52
1:A:59:ILE:HG21	1:A:86:LEU:HD13	1.92	0.52
1:B:45:ILE:HD12	1:B:60:LEU:HD21	1.92	0.52
2:B:433:GCP:H5'1	3:B:480:HOH:O	2.09	0.52
1:B:41:HIS:CE1	1:B:57:SER:CB	2.93	0.51
1:B:374:THR:HG21	3:B:491:HOH:O	2.10	0.51
1:B:359:PRO:HG2	1:B:365:TRP:CD1	2.45	0.51
1:B:273:VAL:HG22	1:B:305:ARG:HG2	1.93	0.51
1:A:3:ASN:ND2	1:A:258:TYR:O	2.44	0.51
1:B:70:ASN:HB2	1:B:102:ALA:HB3	1.92	0.51
1:A:333:ASP:CB	1:A:383:PHE:HD1	2.24	0.51
1:A:130:GLY:O	1:A:131:ARG:C	2.49	0.51
1:B:21:ASP:HB3	1:B:419:ARG:HH22	1.76	0.51
1:B:355:VAL:HG22	1:B:357:THR:H	1.75	0.51
1:A:29:TYR:HB2	1:A:218:VAL:HG22	1.93	0.51
1:B:286:THR:HG21	1:B:309:TRP:CZ2	2.45	0.51
1:B:184:GLN:NE2	1:B:187:LEU:HD23	2.25	0.51
1:B:300:THR:O	1:B:300:THR:HG23	2.09	0.51
1:B:44:VAL:HA	1:B:49:LYS:HA	1.91	0.51
1:B:214:ARG:NH1	1:B:216:ASP:OD2	2.44	0.51
1:B:111:VAL:HG22	1:B:131:ARG:O	2.11	0.51
1:A:120:ALA:O	1:A:122:GLY:N	2.44	0.51
1:B:417:PRO:HG3	2:B:433:GCP:C4	2.41	0.50
1:B:61:ARG:HD3	3:B:546:HOH:O	2.10	0.50
1:B:292:LYS:HE3	1:B:293:GLN:OE1	2.11	0.50
1:B:35:GLY:O	1:B:73:VAL:HG22	2.12	0.50
1:A:236:PRO:O	1:B:143:ARG:NH1	2.45	0.50
1:A:271:THR:CG2	1:A:307:THR:HG22	2.40	0.50
1:A:97:LEU:O	1:A:200:MET:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:OE1	1:A:306:ARG:HD2	2.12	0.50
1:A:323:SER:HB3	1:B:258:TYR:CE2	2.47	0.49
1:A:411:ASP:HB3	1:A:426:ARG:HB3	1.93	0.49
1:A:317:ARG:O	1:A:320:GLN:HG2	2.13	0.49
1:B:358:THR:HB	1:B:365:TRP:CZ2	2.47	0.49
1:B:44:VAL:O	1:B:46:ASN:N	2.45	0.49
1:B:274:GLY:O	1:B:306:ARG:NH2	2.45	0.49
1:A:301:THR:HB	1:A:303:ARG:HH22	1.76	0.49
1:B:360:LEU:HD23	1:B:360:LEU:N	2.24	0.49
1:B:6:VAL:HG22	1:B:263:LEU:HD23	1.94	0.49
1:B:329:LEU:HD21	1:B:332:LEU:HB2	1.95	0.49
1:B:399:ILE:HG23	1:B:410:ILE:HD12	1.95	0.49
1:A:304:ARG:HG3	1:A:304:ARG:NH1	2.27	0.49
1:A:64:VAL:HG12	1:A:65:THR:N	2.27	0.49
1:A:266:LEU:O	1:A:329:LEU:HA	2.13	0.49
1:A:46:ASN:ND2	3:A:541:HOH:O	2.46	0.49
1:A:238:VAL:HG23	1:B:143:ARG:HD2	1.95	0.49
1:A:56:PRO:CB	1:A:66:SER:HB3	2.42	0.49
1:A:113:LEU:O	1:A:117:ARG:HD2	2.13	0.48
1:A:13:ASP:OD2	1:A:305:ARG:CZ	2.61	0.48
1:B:83:MET:HE1	1:B:94:ARG:HD2	1.95	0.48
1:A:393:GLN:O	1:A:397:ASN:ND2	2.46	0.48
1:A:310:LEU:HD23	1:A:343:LEU:HD21	1.95	0.48
1:A:196:ILE:HG22	1:A:197:LEU:HD23	1.94	0.48
1:B:62:GLU:H	1:B:62:GLU:HG3	1.42	0.48
1:A:97:LEU:HB3	1:A:200:MET:CE	2.43	0.48
1:B:409:PRO:HG3	1:B:426:ARG:HH12	1.78	0.48
1:A:291:CYS:SG	1:A:296:GLU:HB2	2.53	0.48
1:B:10:GLN:HG2	3:B:522:HOH:O	2.13	0.48
1:A:75:SER:O	1:A:76:PRO:C	2.50	0.48
1:A:111:VAL:HG22	1:A:131:ARG:HA	1.95	0.48
1:B:328:CYS:HA	1:B:412:ILE:O	2.14	0.48
1:B:234:THR:HG21	1:B:277:PRO:CD	2.44	0.48
1:B:115:ASN:O	1:B:119:LYS:HG3	2.13	0.48
1:B:268:ALA:HB2	1:B:332:LEU:HA	1.95	0.47
1:A:170:PHE:O	1:A:174:ASN:HB2	2.14	0.47
1:A:358:THR:HG23	1:A:365:TRP:CZ2	2.49	0.47
1:B:263:LEU:HD11	1:B:328:CYS:HB2	1.96	0.47
1:A:70:ASN:OD1	1:B:232:HIS:HE1	1.98	0.47
1:A:24:THR:HG22	1:A:24:THR:O	2.15	0.47
1:A:412:ILE:HG12	1:A:424:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LEU:O	1:B:362:ALA:N	2.48	0.47
1:A:302:GLY:O	1:A:303:ARG:C	2.53	0.47
1:A:280:THR:HG22	1:A:372:TYR:CZ	2.49	0.47
1:B:363:ASP:HB2	3:B:516:HOH:O	2.14	0.47
1:A:64:VAL:CG1	1:A:65:THR:N	2.78	0.47
1:B:172:LEU:HB3	1:B:179:GLU:O	2.15	0.47
1:B:279:PRO:O	1:B:370:PRO:HG3	2.16	0.46
1:A:79:LEU:HD12	1:A:80:MET:CE	2.46	0.46
1:A:79:LEU:HD12	1:A:80:MET:HE2	1.96	0.46
1:B:14:GLU:HB3	1:B:265:ILE:HG22	1.97	0.46
1:A:348:ARG:NH1	1:A:348:ARG:HG2	2.30	0.46
1:A:46:ASN:HB2	1:A:89:ARG:HG3	1.97	0.46
1:A:171:GLN:O	1:A:175:TYR:HB3	2.15	0.46
1:B:210:GLN:O	1:B:214:ARG:HB2	2.16	0.46
1:A:349:MET:SD	1:A:368:VAL:CG1	2.99	0.46
1:A:197:LEU:O	1:A:198:THR:C	2.52	0.46
1:A:299:ALA:O	1:A:300:THR:HB	2.16	0.46
1:A:61:ARG:HD2	1:A:61:ARG:N	2.29	0.46
1:A:360:LEU:O	1:A:362:ALA:N	2.43	0.46
1:B:273:VAL:CG2	1:B:305:ARG:HG2	2.45	0.46
1:B:396:LEU:O	1:B:400:LYS:HG2	2.16	0.45
1:B:388:ARG:HD3	1:B:425:LEU:HD21	1.98	0.45
1:B:326:GLY:HA2	1:B:408:VAL:CG1	2.46	0.45
1:B:271:THR:HG21	1:B:296:GLU:HG3	1.98	0.45
1:A:294:GLY:O	1:A:295:ASN:HB3	2.16	0.45
1:B:418:ASP:OD2	1:B:421:GLU:HG3	2.16	0.45
1:B:388:ARG:HD3	1:B:425:LEU:CD2	2.46	0.45
1:A:165:MET:SD	1:A:183:TYR:HA	2.57	0.45
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.82	0.45
1:B:81:LYS:HB3	1:B:81:LYS:HE2	1.89	0.45
1:B:380:GLU:H	1:B:380:GLU:CD	2.20	0.45
1:B:300:THR:O	1:B:301:THR:C	2.54	0.45
1:B:315:VAL:O	1:B:319:VAL:HG23	2.16	0.45
1:B:300:THR:CA	1:B:301:THR:N	2.73	0.45
1:A:266:LEU:O	1:A:329:LEU:HD12	2.16	0.45
1:B:267:LYS:O	1:B:269:TYR:N	2.50	0.45
1:A:280:THR:O	1:A:308:GLY:HA3	2.16	0.45
1:A:280:THR:HG22	1:A:372:TYR:OH	2.16	0.45
1:A:400:LYS:O	1:A:404:GLU:HG3	2.17	0.45
1:B:45:ILE:N	1:B:48:GLU:O	2.51	0.44
1:B:300:THR:CG2	1:B:300:THR:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TYR:C	1:B:235:TYR:CD1	2.86	0.44
1:A:79:LEU:HD13	1:A:79:LEU:O	2.16	0.44
1:B:329:LEU:HD21	1:B:332:LEU:HD13	1.98	0.44
1:B:39:ALA:HB3	1:B:53:HIS:HA	1.99	0.44
1:A:101:GLU:HG2	3:A:439:HOH:O	2.17	0.44
1:A:19:ILE:H	1:A:19:ILE:CD1	2.28	0.44
1:B:418:ASP:CG	1:B:419:ARG:N	2.71	0.44
1:B:267:LYS:C	1:B:269:TYR:N	2.69	0.44
1:B:214:ARG:HD2	1:B:214:ARG:HH11	1.65	0.44
1:A:314:ALA:O	1:A:317:ARG:HB3	2.17	0.44
1:A:53:HIS:N	1:A:82:GLU:OE2	2.48	0.44
1:A:384:GLY:CA	1:A:421:GLU:HG3	2.40	0.44
1:B:265:ILE:HG13	1:B:328:CYS:HB3	1.99	0.44
1:A:424:ILE:N	3:A:534:HOH:O	2.50	0.44
1:A:107:LEU:H	1:A:110:HIS:HD2	1.65	0.44
1:A:426:ARG:O	1:A:427:ASP:CB	2.57	0.43
1:B:28:LYS:NZ	1:B:28:LYS:O	2.43	0.43
1:B:99:LEU:HD11	1:B:200:MET:HE3	2.00	0.43
1:A:66:SER:O	1:A:97:LEU:HD12	2.18	0.43
1:B:18:LYS:NZ	1:B:418:ASP:O	2.51	0.43
1:B:109:TYR:O	1:B:113:LEU:HG	2.18	0.43
1:B:282:LEU:HD21	1:B:309:TRP:CD1	2.53	0.43
1:B:385:VAL:HG11	1:B:391:LEU:HD13	2.01	0.43
1:A:154:LYS:HG2	1:A:191:MET:CE	2.48	0.43
1:B:397:ASN:CG	1:B:400:LYS:NZ	2.70	0.43
1:B:214:ARG:NH2	3:B:573:HOH:O	2.51	0.43
1:A:386:LYS:HD3	1:A:420:THR:O	2.18	0.43
1:A:345:VAL:O	1:A:346:ALA:CB	2.66	0.43
1:B:302:GLY:O	1:B:304:ARG:N	2.51	0.43
1:B:79:LEU:O	1:B:83:MET:HG3	2.18	0.43
1:A:16:LYS:O	1:A:20:VAL:HG23	2.18	0.43
1:B:195:ASP:O	1:B:199:SER:HB3	2.19	0.43
1:B:397:ASN:HA	1:B:400:LYS:HZ2	1.83	0.43
1:B:183:TYR:HB2	3:B:454:HOH:O	2.19	0.43
1:A:337:GLY:H	1:A:379:SER:HA	1.84	0.43
1:A:113:LEU:HD11	1:A:171:GLN:OE1	2.19	0.43
1:A:83:MET:HG2	1:A:93:VAL:HG11	2.01	0.43
1:B:342:LYS:HG2	1:B:374:THR:OG1	2.19	0.43
1:B:70:ASN:CB	1:B:102:ALA:HB3	2.48	0.43
1:B:129:THR:HA	1:B:131:ARG:NH2	2.34	0.42
1:A:311:ASP:O	1:A:315:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLY:N	2:B:433:GCP:O1A	2.51	0.42
1:A:291:CYS:SG	1:A:304:ARG:NH1	2.78	0.42
1:B:6:VAL:HG13	1:B:265:ILE:HD11	2.00	0.42
1:B:349:MET:HG3	1:B:353:ARG:CZ	2.49	0.42
1:A:107:LEU:O	1:A:110:HIS:HB2	2.19	0.42
1:A:6:VAL:O	1:A:7:LEU:HB3	2.18	0.42
1:B:6:VAL:HG13	1:B:265:ILE:CD1	2.48	0.42
1:A:86:LEU:HB3	1:A:91:ILE:HB	2.00	0.42
1:B:129:THR:HA	1:B:131:ARG:HH12	1.78	0.42
1:A:312:THR:HB	1:A:344:CYS:O	2.20	0.42
1:A:333:ASP:HB2	1:A:383:PHE:HD1	1.84	0.42
1:A:120:ALA:O	1:A:121:ARG:C	2.57	0.42
1:A:94:ARG:HD3	3:A:549:HOH:O	2.19	0.42
1:B:229:ASP:O	1:B:230:ILE:C	2.57	0.42
1:B:110:HIS:HE1	1:B:139:ASP:OD2	2.02	0.42
1:A:79:LEU:HD11	1:A:83:MET:SD	2.59	0.42
1:A:335:LEU:O	1:A:338:LEU:HB2	2.19	0.42
1:A:345:VAL:HG12	1:A:405:LEU:CD1	2.48	0.42
1:B:427:ASP:HA	1:B:428:PRO:HD3	1.77	0.42
1:B:229:ASP:O	1:B:231:ASP:N	2.53	0.42
1:B:360:LEU:O	1:B:361:ALA:C	2.57	0.42
1:B:304:ARG:NE	3:B:518:HOH:O	2.51	0.42
1:B:298:GLY:HA3	3:B:566:HOH:O	2.20	0.42
1:B:303:ARG:O	1:B:304:ARG:C	2.59	0.42
1:A:298:GLY:O	1:A:299:ALA:HB3	2.20	0.42
1:B:91:ILE:O	1:B:93:VAL:N	2.52	0.42
1:B:303:ARG:HD3	1:B:303:ARG:HH11	1.68	0.41
1:B:347:TYR:HB3	1:B:368:VAL:HG13	2.02	0.41
1:B:73:VAL:O	1:B:73:VAL:HG23	2.20	0.41
1:A:299:ALA:O	1:A:300:THR:CB	2.68	0.41
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.81	0.41
1:A:203:ASP:HB3	3:A:441:HOH:O	2.19	0.41
1:A:311:ASP:C	1:A:311:ASP:OD1	2.57	0.41
1:B:388:ARG:NH1	1:B:425:LEU:HD22	2.31	0.41
1:A:170:PHE:HA	3:A:527:HOH:O	2.19	0.41
1:B:232:HIS:HB2	1:B:321:LEU:HD11	2.02	0.41
1:B:316:ARG:HE	1:B:316:ARG:HB2	1.60	0.41
1:A:142:ALA:O	1:A:143:ARG:HB2	2.18	0.41
1:B:134:GLY:O	1:B:138:GLU:HG3	2.20	0.41
1:A:267:LYS:HD2	1:A:331:LYS:HD2	2.01	0.41
1:A:59:ILE:HG21	1:A:86:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:HIS:HA	1:B:53:HIS:O	2.20	0.41
1:A:132:GLY:C	1:A:135:PRO:HD2	2.40	0.41
1:B:73:VAL:HB	1:B:106:ILE:HD11	2.02	0.41
1:B:300:THR:C	1:B:301:THR:C	2.78	0.41
1:B:304:ARG:CZ	3:B:518:HOH:O	2.68	0.41
1:B:277:PRO:HA	3:B:455:HOH:O	2.20	0.41
1:A:335:LEU:HD13	1:A:341:VAL:CG1	2.48	0.41
1:A:289:PHE:CE1	1:A:338:LEU:HD21	2.55	0.41
1:A:361:ALA:N	1:B:101:GLU:OE2	2.53	0.41
1:A:170:PHE:C	1:A:170:PHE:CD1	2.94	0.41
1:A:94:ARG:HH11	1:A:94:ARG:HD2	1.71	0.41
1:A:235:TYR:CG	1:A:236:PRO:HA	2.55	0.41
1:A:427:ASP:HA	1:A:428:PRO:HD3	1.88	0.41
1:B:2:ASN:ND2	1:B:215:GLY:O	2.53	0.41
1:A:342:LYS:HE2	1:A:374:THR:OG1	2.21	0.41
1:A:214:ARG:HH11	1:A:214:ARG:HD2	1.66	0.41
1:B:124:LYS:O	1:B:125:ALA:HB2	2.21	0.41
1:B:361:ALA:HB2	3:B:533:HOH:O	2.21	0.40
1:B:347:TYR:HB3	1:B:349:MET:CE	2.51	0.40
1:B:268:ALA:CB	1:B:332:LEU:HA	2.51	0.40
1:A:32:ARG:NH1	1:A:39:ALA:HB2	2.36	0.40
1:B:131:ARG:HG3	1:B:133:ILE:H	1.86	0.40
1:A:137:TYR:O	1:A:140:LYS:HB3	2.21	0.40
1:A:403:GLU:HG2	1:A:409:PRO:HA	2.02	0.40
1:A:407:GLY:O	1:A:408:VAL:HG23	2.22	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	429/431 (100%)	372 (87%)	41 (10%)	16 (4%)	4	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	429/431 (100%)	366 (85%)	44 (10%)	19 (4%)	3	1
All	All	858/862 (100%)	738 (86%)	85 (10%)	35 (4%)	3	1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	THR
1	B	39	ALA
1	B	45	ILE
1	B	125	ALA
1	B	235	TYR
1	B	300	THR
1	B	361	ALA
1	B	364	ASP
1	A	120	ALA
1	A	121	ARG
1	A	230	ILE
1	B	2	ASN
1	B	108	ASP
1	B	130	GLY
1	B	362	ALA
1	A	38	ASN
1	A	128	THR
1	A	303	ARG
1	A	346	ALA
1	B	40	GLY
1	B	268	ALA
1	B	304	ARG
1	A	127	GLY
1	A	194	ALA
1	A	362	ALA
1	A	427	ASP
1	A	46	ASN
1	B	126	ILE
1	B	255	GLY
1	B	360	LEU
1	B	230	ILE
1	B	427	ASP
1	A	20	VAL
1	A	45	ILE
1	A	132	GLY

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	353/353 (100%)	320 (91%)	33 (9%)	11	13
1	B	353/353 (100%)	321 (91%)	32 (9%)	12	13
All	All	706/706 (100%)	641 (91%)	65 (9%)	11	13

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	13	ASP
1	A	34	GLN
1	A	37	HIS
1	A	38	ASN
1	A	43	LEU
1	A	44	VAL
1	A	45	ILE
1	A	61	ARG
1	A	81	LYS
1	A	85	GLU
1	A	89	ARG
1	A	99	LEU
1	A	101	GLU
1	A	131	ARG
1	A	155	GLU
1	A	156	THR
1	A	165	MET
1	A	196	ILE
1	A	198	THR
1	A	202	VAL
1	A	207	LEU
1	A	239	THR
1	A	240	SER
1	A	270	SER
1	A	273	VAL
1	A	278	PHE

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Mol	Chain	Res	Type
1	A	284	ASP
1	A	333	ASP
1	A	355	VAL
1	A	379	SER
1	A	386	LYS
1	A	401	ARG
1	B	2	ASN
1	B	7	LEU
1	B	28	LYS
1	B	34	GLN
1	B	37	HIS
1	B	50	THR
1	B	62	GLU
1	B	84	LYS
1	B	114	ASP
1	B	135	PRO
1	B	193	VAL
1	B	202	VAL
1	B	205	SER
1	B	207	LEU
1	B	234	THR
1	B	240	SER
1	B	254	LEU
1	B	270	SER
1	B	278	PHE
1	B	295	ASN
1	B	312	THR
1	B	329	LEU
1	B	341	VAL
1	B	343	LEU
1	B	360	LEU
1	B	375	MET
1	B	391	LEU
1	B	413	ILE
1	B	415	THR
1	B	418	ASP
1	B	420	THR
1	B	422	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	393	GLN
1	B	2	ASN
1	B	37	HIS
1	B	41	HIS
1	B	110	HIS
1	B	171	GLN
1	B	232	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 ⓘ

2 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	GCP	A	432	-	26,34,34	1.89	6 (23%)	32,54,54	1.91	7 (21%)
2	GCP	B	433	-	26,34,34	1.68	6 (23%)	32,54,54	2.96	12 (37%)

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	GCP	A	432	-	-	0/15/38/38	0/3/3/3
2	GCP	B	433	-	-	0/15/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	433	GCP	PB-O2B	-3.71	1.47	1.56
2	A	432	GCP	PB-O2B	-3.59	1.47	1.56
2	B	433	GCP	PG-O2G	-2.50	1.48	1.54
2	B	433	GCP	PG-O3G	-2.33	1.49	1.54
2	A	432	GCP	PG-O3G	-2.10	1.49	1.54
2	B	433	GCP	C4-N3	2.25	1.39	1.35
2	A	432	GCP	C6-N1	2.47	1.40	1.36
2	B	433	GCP	C2-N3	2.66	1.36	1.33
2	A	432	GCP	C2'-C3'	3.30	1.62	1.53
2	B	433	GCP	PB-O3A	3.88	1.62	1.58
2	A	432	GCP	PB-O3A	4.03	1.63	1.58
2	A	432	GCP	O4'-C1'	4.63	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	432	GCP	O1G-PG-C3B	-4.29	101.36	111.13
2	B	433	GCP	O4'-C1'-N9	-3.83	100.09	108.10
2	B	433	GCP	O2'-C2'-C3'	-3.57	100.20	111.83
2	B	433	GCP	O5'-PA-O1A	-2.71	99.10	109.62
2	A	432	GCP	O3G-PG-C3B	-2.42	100.52	106.40
2	B	433	GCP	O3G-PG-C3B	-2.18	101.12	106.40
2	A	432	GCP	O2'-C2'-C3'	2.02	118.41	111.83
2	B	433	GCP	C4-C5-N7	2.25	111.55	109.48
2	B	433	GCP	O3G-PG-O2G	2.32	114.92	108.13
2	B	433	GCP	O3'-C3'-C2'	2.35	119.48	111.83
2	A	432	GCP	O2G-PG-C3B	2.43	112.30	106.40
2	A	432	GCP	N1-C2-N3	2.54	125.19	121.79
2	B	433	GCP	O2B-PB-O1B	2.54	118.11	110.12
2	A	432	GCP	C4-C5-N7	2.77	112.02	109.48
2	B	433	GCP	C1'-N9-C4	2.84	131.22	126.94
2	B	433	GCP	O3A-PA-O5'	4.97	116.13	102.94
2	A	432	GCP	C6-N1-C2	5.60	123.36	120.20
2	B	433	GCP	C2'-C1'-N9	6.38	124.05	114.29
2	B	433	GCP	C6-N1-C2	11.06	126.44	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	GCP	1	0
2	B	433	GCP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	431/431 (100%)	0.34	35 (8%)	15	21	10, 29, 58, 80	0
1	B	431/431 (100%)	-0.01	17 (3%)	43	52	8, 24, 47, 69	0
All	All	862/862 (100%)	0.17	52 (6%)	25	33	8, 26, 55, 80	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	ALA	9.1
1	A	129	THR	8.4
1	A	127	GLY	7.2
1	A	128	THR	6.2
1	B	300	THR	5.7
1	A	120	ALA	5.5
1	B	303	ARG	5.3
1	A	123	ALA	4.7
1	A	121	ARG	4.5
1	B	126	ILE	4.5
1	A	299	ALA	4.1
1	A	122	GLY	3.9
1	A	298	GLY	3.8
1	A	300	THR	3.7
1	A	125	ALA	3.7
1	B	123	ALA	3.5
1	A	124	LYS	3.5
1	A	389	SER	3.4
1	B	295	ASN	3.3
1	B	127	GLY	3.3
1	A	301	THR	3.3
1	B	128	THR	3.3
1	B	301	THR	3.2
1	A	297	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	118	GLU	3.1
1	A	126	ILE	3.0
1	A	361	ALA	3.0
1	B	367	GLY	2.9
1	B	361	ALA	2.7
1	A	379	SER	2.6
1	B	304	ARG	2.4
1	A	77	ALA	2.4
1	A	119	LYS	2.4
1	A	130	GLY	2.3
1	B	299	ALA	2.3
1	A	44	VAL	2.3
1	A	47	GLY	2.3
1	A	365	TRP	2.3
1	A	302	GLY	2.2
1	B	129	THR	2.2
1	A	45	ILE	2.2
1	B	362	ALA	2.2
1	A	378	TRP	2.2
1	A	364	ASP	2.1
1	A	388	ARG	2.1
1	B	389	SER	2.1
1	A	90	GLY	2.1
1	B	302	GLY	2.1
1	A	363	ASP	2.0
1	A	43	LEU	2.0
1	A	350	PRO	2.0
1	A	366	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, 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	LLDF	B-factors($Å^2$)	Q<0.9
2	GCP	B	433	32/32	0.88	0.21	1.10	0,53,58,59	0
2	GCP	A	432	32/32	0.91	0.17	0.05	0,42,53,54	0

6.5 Other polymers (i)

There are no such residues in this entry.