



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:20 AM UTC

PDB ID : 3OQN / pdb_00003oqn
Title : Structure of ccpa-hpr-ser46-p-gntr-down cre
Authors : Schumacher, M.A.; Sprehe, M.; Bartholomae, M.; Hillen, W.; Brennan, R.G.
Deposited on : 2010-09-03
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

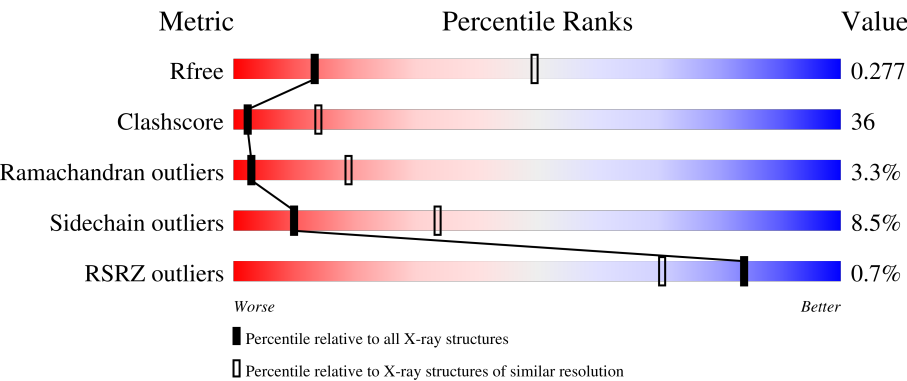
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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.



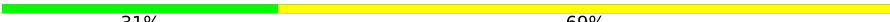
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	339	% 40% 51% 6% .
1	C	339	% 41% 50% 7% .
2	D	87	36% 54% 10%
2	S	87	% 26% 64% 8% .
3	E	16	44% 50% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	16	 31% 69%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7082 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 Catabolite control protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2579	1627	438	502	12			
1	C	332	Total	C	N	O	S	0	0	0
			2579	1627	438	502	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP P25144
A	336	HIS	-	expression tag	UNP P25144
A	337	HIS	-	expression tag	UNP P25144
A	338	HIS	-	expression tag	UNP P25144
A	339	HIS	-	expression tag	UNP P25144
A	340	HIS	-	expression tag	UNP P25144
C	335	HIS	-	expression tag	UNP P25144
C	336	HIS	-	expression tag	UNP P25144
C	337	HIS	-	expression tag	UNP P25144
C	338	HIS	-	expression tag	UNP P25144
C	339	HIS	-	expression tag	UNP P25144
C	340	HIS	-	expression tag	UNP P25144

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	S	87	Total	C	N	O	P	S	0	0	0
			637	389	106	138	1	3			
2	D	87	Total	C	N	O	P	S	0	0	0
			637	389	106	138	1	3			

- Molecule 3 is a DNA chain called 5'-D(*TP*TP*GP*AP*AP*AP*GP*CP*GP*GP*TP*A P*CP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	16	Total	C	N	O	P	0	0	0
			327	157	62	93	15			

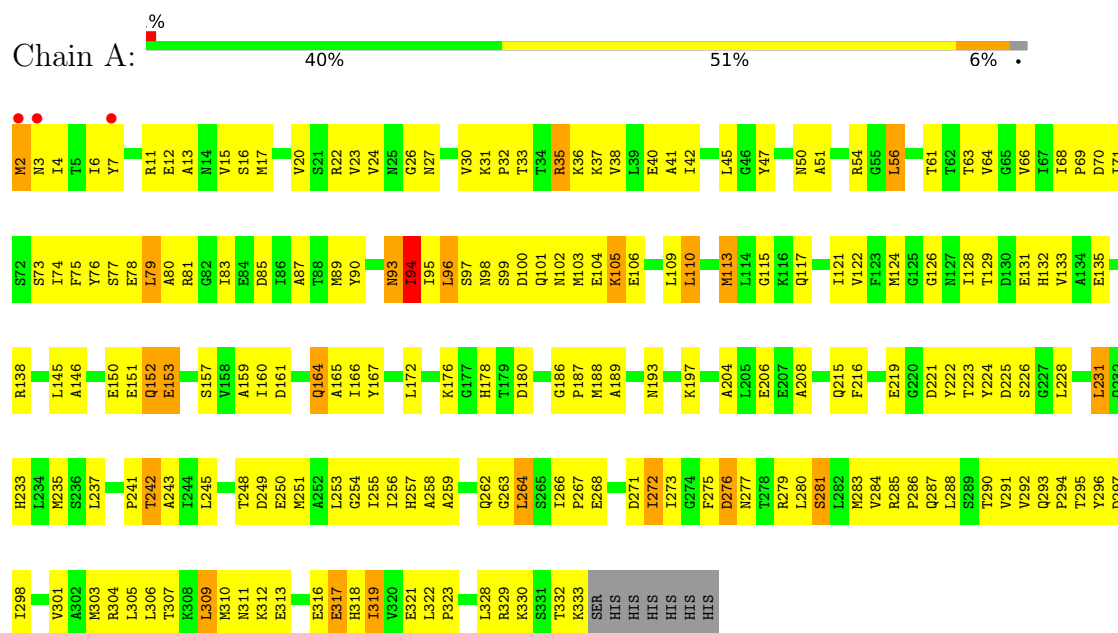
- Molecule 4 is a DNA chain called 5'-D(*AP*TP*GP*GP*TP*AP*CP*CP*GP*CP*TP*TP*TP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	16	Total	C	N	O	P	0	0	0
			323	156	57	95	15			

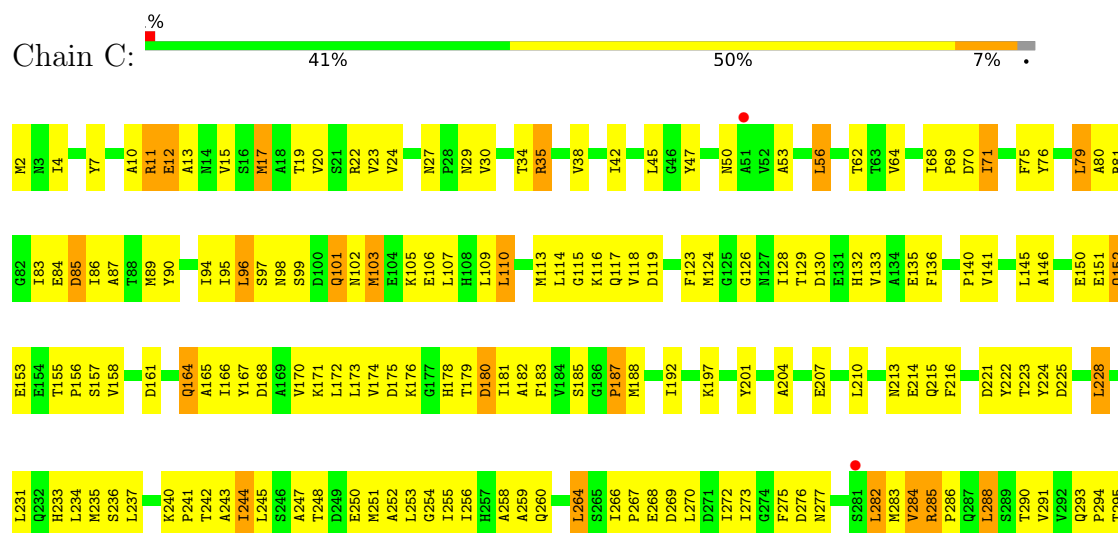
3 Residue-property plots [i](#)

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

• Molecule 1: Catabolite control protein A

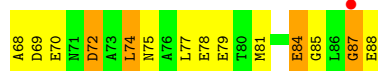
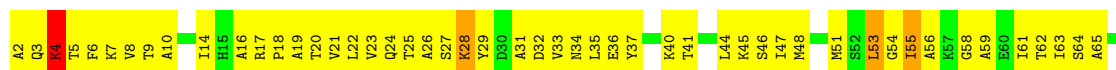


• Molecule 1: Catabolite control protein A





• Molecule 2: Phosphocarrier protein HPr



• Molecule 2: Phosphocarrier protein HPr



• Molecule 3: 5'-D(*TP*TP*GP*AP*AP*AP*GP*CP*GP*GP*TP*AP*CP*CP*AP*T)-3'



• Molecule 4: 5'-D(*AP*TP*GP*GP*TP*AP*CP*CP*GP*CP*TP*TP*TP*CP*AP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.93Å 103.51Å 175.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.70 – 3.30 87.70 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (87.70-3.30) 95.4 (87.70-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.279 0.222 , 0.277	Depositor DCC
R_{free} test set	1374 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7082	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.56	0/2619	0.98	4/3549 (0.1%)
1	C	0.54	0/2619	0.98	7/3549 (0.2%)
2	D	0.47	0/630	0.80	0/846
2	S	0.45	0/630	0.87	1/846 (0.1%)
3	E	0.34	0/367	0.76	0/565
4	B	0.40	0/361	0.86	0/555
All	All	0.52	0/7226	0.94	12/9910 (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
3	E	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	LYS	CA-C-N	6.62	126.64	119.89
1	C	240	LYS	C-N-CA	6.62	126.64	119.89
1	A	94	ILE	N-CA-C	6.05	117.30	108.53
1	C	128	ILE	CB-CA-C	-5.80	105.65	111.80
2	S	87	GLY	N-CA-C	5.52	118.47	112.29
1	C	103	MET	N-CA-C	5.47	116.93	111.07
1	C	85	ASP	N-CA-C	5.41	118.10	111.82
1	A	208	ALA	N-CA-C	-5.39	106.37	113.17
1	C	288	LEU	N-CA-C	5.39	118.05	109.96
1	C	130	ASP	N-CA-C	-5.39	105.57	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ILE	N-CA-C	5.28	115.89	108.17
1	A	121	ILE	N-CA-C	5.22	116.17	108.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	707	DC	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2579	0	2622	203	0
1	C	2579	0	2622	174	0
2	D	637	0	631	61	0
2	S	637	0	631	52	0
3	E	327	0	182	14	0
4	B	323	0	183	15	0
All	All	7082	0	6871	496	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (496) 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:56:LEU:HD22	4:B:707:DC:H1'	1.35	1.02
1:C:23:VAL:HG21	1:C:38:VAL:HG11	1.42	1.01
1:A:23:VAL:HG21	1:A:38:VAL:HG11	1.45	0.97
2:S:22:LEU:HG	2:S:44:LEU:HD21	1.46	0.95
1:A:69:PRO:HB3	1:A:101:GLN:HE21	1.32	0.95
1:C:87:ALA:HB2	1:C:303:MET:HE3	1.48	0.95
1:C:156:PRO:HB3	1:C:318:HIS:HB3	1.47	0.94
2:D:9:THR:HG22	2:D:87:GLY:N	1.83	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:HD22	1:A:105:LYS:HB2	1.29	0.93
1:C:182:ALA:HB3	1:C:244:ILE:HG22	1.50	0.93
1:A:71:ILE:H	1:A:98:ASN:ND2	1.67	0.92
1:A:56:LEU:HD12	1:C:56:LEU:HD12	1.52	0.89
1:A:109:LEU:O	1:A:113:MET:HG3	1.72	0.88
1:A:160:ILE:HD13	1:A:293:GLN:HG3	1.54	0.88
1:A:64:VAL:HG21	1:A:303:MET:HE1	1.57	0.86
1:A:306:LEU:HG	1:A:310:MET:HE2	1.58	0.84
1:A:71:ILE:H	1:A:98:ASN:HD21	1.22	0.83
1:A:83:ILE:HD13	1:A:122:VAL:HG11	1.59	0.83
1:A:294:PRO:HB2	1:A:297:ASP:HB2	1.60	0.82
1:A:277:ASN:HD22	1:A:292:VAL:HG13	1.46	0.81
1:A:228:LEU:HD23	1:A:258:ALA:HB2	1.63	0.81
1:C:228:LEU:HD12	1:C:254:GLY:O	1.81	0.80
1:C:71:ILE:H	1:C:98:ASN:ND2	1.80	0.80
1:A:225:ASP:HA	1:A:228:LEU:HD12	1.65	0.79
2:S:2:ALA:HB1	2:S:74:LEU:HD22	1.64	0.79
2:S:75:ASN:O	2:S:79:GLU:HG3	1.83	0.78
1:A:187:PRO:HD2	1:A:222:TYR:CE2	2.18	0.77
2:S:9:THR:HG23	2:S:87:GLY:HA2	1.65	0.77
4:B:714:DA:C8	4:B:714:DA:H5'	2.20	0.77
1:C:68:ILE:HD11	1:C:76:TYR:HB3	1.64	0.77
2:S:17:ARG:HB2	2:S:18:PRO:HD3	1.66	0.76
1:A:31:LYS:HE3	1:A:33:THR:HB	1.66	0.75
1:A:251:MET:O	1:A:255:ILE:HG12	1.85	0.75
2:D:9:THR:HG22	2:D:87:GLY:H	1.51	0.75
2:S:33:VAL:HG11	2:S:77:LEU:HD11	1.69	0.75
1:C:152:GLN:CD	1:C:152:GLN:H	1.93	0.74
1:C:253:LEU:HD12	1:C:288:LEU:HD22	1.69	0.74
1:C:101:GLN:HE21	1:C:101:GLN:HA	1.53	0.73
2:D:22:LEU:HD22	2:D:81:MET:HE3	1.70	0.73
1:A:63:THR:HG22	1:A:93:ASN:HB2	1.71	0.73
1:A:287:GLN:HB2	1:A:329:ARG:HB3	1.70	0.73
1:A:87:ALA:HB2	1:A:303:MET:HE3	1.71	0.73
1:C:124:MET:HG2	1:C:146:ALA:HB3	1.69	0.72
1:C:13:ALA:O	1:C:15:VAL:HG13	1.89	0.72
1:A:73:SER:HB3	1:A:76:TYR:HB2	1.72	0.71
1:A:277:ASN:H	1:A:290:THR:HG21	1.54	0.71
1:C:64:VAL:HG21	1:C:303:MET:HE1	1.71	0.71
1:C:223:THR:HG22	1:C:225:ASP:H	1.56	0.71
1:A:301:VAL:HG13	2:S:48:MET:HG2	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:CG	2:S:51:MET:HE2	2.16	0.71
1:A:150:GLU:HG2	1:A:152:GLN:HG2	1.73	0.71
2:S:17:ARG:H	2:S:17:ARG:HD2	1.55	0.71
1:A:69:PRO:CB	1:A:101:GLN:HE21	2.03	0.70
1:C:56:LEU:HD22	3:E:707:DC:H1'	1.73	0.70
3:E:708:DG:H1'	3:E:709:DG:H5''	1.72	0.70
4:B:714:DA:H5'	4:B:714:DA:H8	1.55	0.70
2:S:8:VAL:HG23	2:S:58:GLY:H	1.57	0.70
1:A:275:PHE:O	1:A:276:ASP:HB2	1.91	0.69
1:C:7:TYR:HE1	1:C:17:MET:SD	2.14	0.69
1:C:294:PRO:HB2	1:C:297:ASP:HB2	1.75	0.69
1:C:237:LEU:HD12	1:C:237:LEU:H	1.56	0.69
1:A:329:ARG:C	1:A:330:LYS:HE2	2.17	0.69
1:C:178:HIS:CE1	1:C:243:ALA:HB2	2.28	0.69
4:B:700:DA:H2''	4:B:701:DT:O5'	1.92	0.68
1:A:12:GLU:HG3	1:A:45:LEU:HD11	1.76	0.68
1:A:180:ASP:HB3	1:A:216:PHE:HE1	1.56	0.68
1:A:70:ASP:HA	1:A:98:ASN:HD22	1.58	0.67
2:D:81:MET:HE2	2:D:81:MET:HA	1.75	0.67
1:A:172:LEU:C	1:A:172:LEU:HD23	2.19	0.67
1:C:101:GLN:HE22	1:C:126:GLY:N	1.92	0.67
2:D:8:VAL:HG23	2:D:58:GLY:N	2.09	0.67
2:D:42:VAL:HG11	2:D:53:LEU:HD11	1.76	0.67
1:A:94:ILE:C	1:A:95:ILE:HD12	2.19	0.67
1:C:89:MET:HG3	2:D:24:GLN:HE21	1.59	0.67
1:A:20:VAL:O	1:A:24:VAL:HG23	1.95	0.67
1:A:41:ALA:O	1:A:45:LEU:HD13	1.95	0.67
2:S:6:PHE:HZ	2:S:78:GLU:HG2	1.58	0.66
1:C:87:ALA:HB2	1:C:303:MET:CE	2.25	0.66
1:C:244:ILE:HG13	1:C:272:ILE:HG13	1.76	0.66
1:C:75:PHE:HE2	1:C:295:THR:HG1	1.42	0.66
1:C:150:GLU:HG2	1:C:152:GLN:HG2	1.78	0.66
2:D:22:LEU:HG	2:D:44:LEU:HD11	1.78	0.66
2:S:8:VAL:HG23	2:S:58:GLY:N	2.11	0.65
1:A:26:GLY:HA2	1:A:35:ARG:HH22	1.62	0.65
1:C:207:GLU:O	1:C:207:GLU:HG3	1.97	0.65
1:C:309:LEU:HD13	1:C:309:LEU:H	1.61	0.65
1:A:224:TYR:HB2	1:C:283:MET:HE3	1.79	0.65
1:A:61:THR:O	1:A:63:THR:HG23	1.97	0.65
2:D:9:THR:H	2:D:87:GLY:HA2	1.62	0.65
1:A:7:TYR:HE1	1:A:11:ARG:CZ	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:HG23	1:C:210:LEU:HD22	1.79	0.64
2:D:47:ILE:HG23	2:D:51:MET:HE3	1.79	0.64
1:A:22:ARG:HB3	1:A:27:ASN:HB3	1.78	0.64
2:D:9:THR:HG22	2:D:87:GLY:CA	2.28	0.64
1:A:102:ASN:ND2	1:A:105:LYS:H	1.96	0.64
2:S:37:TYR:HE2	2:S:59:ALA:HB1	1.63	0.64
2:S:44:LEU:HD23	2:S:44:LEU:O	1.98	0.64
1:A:63:THR:CG2	1:C:116:LYS:HE3	2.27	0.63
1:C:275:PHE:HA	1:C:290:THR:HG23	1.79	0.63
2:D:20:THR:O	2:D:24:GLN:HG3	1.98	0.63
2:D:22:LEU:HD22	2:D:81:MET:CE	2.29	0.63
3:E:709:DG:H8	3:E:709:DG:H5'	1.64	0.63
1:A:253:LEU:HD11	1:A:284:VAL:HG21	1.79	0.63
1:A:128:ILE:N	1:A:128:ILE:HD12	2.13	0.63
1:C:30:VAL:HB	1:C:35:ARG:NH2	2.13	0.63
1:A:102:ASN:ND2	1:A:105:LYS:HB2	2.09	0.62
1:A:290:THR:CG2	1:A:291:VAL:N	2.63	0.62
1:C:71:ILE:H	1:C:98:ASN:HD21	1.46	0.62
1:A:221:ASP:O	1:A:222:TYR:HB2	1.99	0.62
1:C:69:PRO:HD3	1:C:124:MET:O	1.99	0.62
1:A:129:THR:O	1:A:133:VAL:HG23	1.99	0.62
2:S:21:VAL:HG21	2:S:84:GLU:OE2	1.99	0.62
1:A:96:LEU:HD13	1:A:97:SER:N	2.15	0.61
2:D:9:THR:H	2:D:87:GLY:H	1.48	0.61
1:A:81:ARG:HG3	1:A:296:TYR:HE1	1.65	0.61
1:C:86:ILE:HG22	1:C:303:MET:HG3	1.82	0.61
1:C:157:SER:H	1:C:319:ILE:HD13	1.66	0.61
1:A:284:VAL:HG12	1:A:285:ARG:H	1.65	0.61
3:E:705:DA:H2''	3:E:706:DG:O5'	2.01	0.61
1:A:69:PRO:HB3	1:A:101:GLN:NE2	2.09	0.61
1:A:56:LEU:CD2	4:B:707:DC:H1'	2.21	0.61
1:C:245:LEU:HD12	1:C:273:ILE:O	2.01	0.60
1:A:286:PRO:HB2	1:A:330:LYS:HB2	1.83	0.60
1:A:96:LEU:HD13	1:A:97:SER:H	1.66	0.60
1:A:178:HIS:ND1	1:A:242:THR:HB	2.16	0.60
1:C:42:ILE:HG23	1:C:47:TYR:HB3	1.83	0.60
1:A:223:THR:HG22	1:A:225:ASP:H	1.67	0.60
1:A:319:ILE:N	1:A:319:ILE:HD12	2.17	0.60
2:S:37:TYR:HB2	2:S:61:ILE:HG22	1.81	0.60
2:S:2:ALA:HB1	2:S:74:LEU:HD13	1.83	0.60
1:A:63:THR:HG22	1:A:93:ASN:CB	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:HD13	1:C:97:SER:N	2.17	0.59
1:C:309:LEU:N	1:C:309:LEU:CD1	2.64	0.59
1:A:30:VAL:HG21	1:A:35:ARG:NH1	2.17	0.59
1:C:53:ALA:HB3	4:B:709:DC:H5'	1.83	0.59
1:C:182:ALA:HA	1:C:216:PHE:HB3	1.85	0.59
2:D:8:VAL:HG23	2:D:58:GLY:H	1.67	0.59
1:C:167:TYR:CD1	1:C:204:ALA:HB2	2.37	0.59
1:A:95:ILE:HD12	1:A:95:ILE:N	2.17	0.59
1:A:128:ILE:HD12	1:A:128:ILE:H	1.67	0.59
1:A:231:LEU:HD11	1:A:259:ALA:HB2	1.85	0.58
1:A:281:SER:HB3	1:A:329:ARG:HH12	1.68	0.58
2:D:8:VAL:HG22	2:D:58:GLY:O	2.03	0.58
1:C:256:ILE:O	1:C:260:GLN:HG3	2.03	0.58
2:D:9:THR:H	2:D:87:GLY:CA	2.16	0.58
2:D:9:THR:H	2:D:87:GLY:N	2.01	0.58
1:C:311:ASN:C	1:C:313:GLU:H	2.10	0.58
2:D:42:VAL:HG11	2:D:53:LEU:CD1	2.33	0.58
1:C:187:PRO:HD3	1:C:221:ASP:HA	1.85	0.58
2:D:22:LEU:HD13	2:D:81:MET:HE3	1.84	0.58
1:A:221:ASP:OD1	1:A:223:THR:OG1	2.18	0.58
1:A:26:GLY:HA2	1:A:35:ARG:NH2	2.19	0.58
1:A:63:THR:HG22	1:C:116:LYS:HE3	1.85	0.58
1:C:107:LEU:HD22	1:C:135:GLU:HG3	1.86	0.57
1:C:223:THR:HG22	1:C:224:TYR:N	2.18	0.57
1:A:275:PHE:O	1:A:276:ASP:CB	2.52	0.57
1:A:133:VAL:HG21	1:A:152:GLN:HG3	1.87	0.57
1:A:243:ALA:HB2	1:A:271:ASP:HB2	1.85	0.57
2:S:35:LEU:HD21	2:S:55:ILE:HD11	1.87	0.57
1:A:166:ILE:CG1	1:A:197:LYS:HG2	2.34	0.57
3:E:713:DC:H2''	3:E:714:DA:H5''	1.86	0.57
1:A:216:PHE:CZ	1:A:241:PRO:HG3	2.40	0.57
1:A:23:VAL:HG11	1:A:38:VAL:HG13	1.87	0.56
1:A:316:GLU:HG3	1:A:317:GLU:HG2	1.87	0.56
1:C:174:VAL:C	1:C:176:LYS:H	2.13	0.56
1:A:187:PRO:CD	1:A:222:TYR:CE2	2.89	0.56
1:A:6:ILE:HB	3:E:709:DG:OP2	2.04	0.56
1:A:180:ASP:HB3	1:A:216:PHE:CE1	2.39	0.56
1:C:103:MET:HE1	1:C:129:THR:HG21	1.87	0.56
1:C:71:ILE:HD13	1:C:71:ILE:O	2.05	0.56
1:C:235:MET:HE1	1:C:241:PRO:HD2	1.88	0.56
1:A:167:TYR:CE1	1:A:204:ALA:HA	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:VAL:HG21	1:C:201:TYR:HA	1.87	0.56
2:D:35:LEU:HB2	2:D:44:LEU:HD23	1.88	0.56
1:A:38:VAL:O	1:A:42:ILE:HG13	2.05	0.56
2:D:58:GLY:O	2:D:59:ALA:C	2.49	0.56
1:A:228:LEU:HD23	1:A:258:ALA:CB	2.35	0.55
1:C:269:ASP:C	1:C:270:LEU:HD12	2.32	0.55
1:A:186:GLY:H	1:A:193:ASN:ND2	2.05	0.55
1:C:22:ARG:HB3	1:C:27:ASN:HB3	1.88	0.55
1:C:180:ASP:HB2	1:C:242:THR:HG23	1.86	0.55
2:S:33:VAL:HG11	2:S:77:LEU:CD1	2.34	0.55
1:A:51:ALA:HB3	1:C:116:LYS:HA	1.89	0.55
1:C:68:ILE:O	1:C:98:ASN:HA	2.06	0.55
1:C:152:GLN:H	1:C:152:GLN:NE2	2.05	0.55
1:C:290:THR:CG2	1:C:291:VAL:N	2.70	0.55
1:A:290:THR:HG22	1:A:291:VAL:O	2.06	0.55
2:S:53:LEU:HD23	2:S:55:ILE:HD11	1.88	0.54
1:C:103:MET:HE2	1:C:132:HIS:HE1	1.72	0.54
1:C:192:ILE:HG12	1:C:192:ILE:O	2.08	0.54
1:C:309:LEU:H	1:C:309:LEU:CD1	2.19	0.54
2:S:22:LEU:HD13	2:S:81:MET:HE3	1.88	0.54
2:S:25:THR:HA	2:S:28:LYS:HD2	1.89	0.54
2:D:26:ALA:HB2	2:D:44:LEU:HD12	1.89	0.54
1:C:4:ILE:O	1:C:4:ILE:HG13	2.07	0.54
1:C:133:VAL:HG21	1:C:152:GLN:HG3	1.90	0.54
1:C:133:VAL:CG2	1:C:152:GLN:HG3	2.38	0.54
1:C:158:VAL:HG22	1:C:320:VAL:HB	1.90	0.54
1:C:233:HIS:O	1:C:236:SER:HB2	2.07	0.54
2:D:7:LYS:O	2:D:87:GLY:HA2	2.07	0.54
4:B:712:DT:H2''	4:B:713:DC:O5'	2.07	0.54
2:S:2:ALA:CB	2:S:74:LEU:HD13	2.38	0.54
1:C:84:GLU:HA	1:C:94:ILE:HD12	1.89	0.54
2:D:42:VAL:CG1	2:D:53:LEU:HD11	2.37	0.53
2:S:19:ALA:O	2:S:23:VAL:HG23	2.08	0.53
1:C:7:TYR:CE1	1:C:17:MET:SD	2.99	0.53
1:C:75:PHE:HE2	1:C:295:THR:OG1	1.91	0.53
1:C:123:PHE:HB3	1:C:145:LEU:HD23	1.90	0.53
2:D:8:VAL:HG21	2:D:56:ALA:O	2.08	0.53
1:A:263:GLY:O	1:A:264:LEU:C	2.52	0.53
1:C:311:ASN:O	1:C:313:GLU:N	2.40	0.53
1:C:277:ASN:N	1:C:290:THR:HG21	2.23	0.53
1:A:115:GLY:C	1:A:117:GLN:H	2.17	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:O	1:A:77:SER:HB3	2.09	0.53
1:A:245:LEU:HD13	1:A:273:ILE:HB	1.91	0.53
2:S:63:ILE:O	2:S:74:LEU:HD11	2.09	0.53
1:A:216:PHE:CE2	1:A:241:PRO:HG3	2.44	0.52
1:A:267:PRO:O	1:A:333:LYS:HE3	2.08	0.52
3:E:704:DA:H2''	3:E:705:DA:OP2	2.09	0.52
1:A:81:ARG:HD2	1:A:85:ASP:OD1	2.09	0.52
1:C:118:VAL:O	1:C:141:VAL:HG11	2.09	0.52
3:E:709:DG:H5'	3:E:709:DG:C8	2.45	0.52
1:C:161:ASP:OD1	1:C:164:GLN:HB2	2.09	0.52
2:D:14:ILE:HD13	2:D:55:ILE:HG21	1.91	0.52
1:A:71:ILE:N	1:A:98:ASN:ND2	2.49	0.52
1:A:124:MET:CG	1:A:146:ALA:HB3	2.40	0.52
1:C:102:ASN:ND2	1:C:105:LYS:HB2	2.25	0.51
1:A:248:THR:HG22	1:A:250:GLU:H	1.75	0.51
1:C:161:ASP:CG	1:C:164:GLN:HB2	2.36	0.51
1:A:228:LEU:HA	1:A:258:ALA:HB2	1.91	0.51
1:C:247:ALA:O	1:C:275:PHE:HB3	2.10	0.51
2:D:8:VAL:HG23	2:D:8:VAL:O	2.10	0.51
2:S:23:VAL:HG21	2:S:47:ILE:HD13	1.92	0.51
2:S:26:ALA:HB2	2:S:44:LEU:HD22	1.93	0.51
2:S:25:THR:O	2:S:28:LYS:HG3	2.10	0.51
1:C:252:ALA:HB3	1:C:288:LEU:HD21	1.92	0.51
1:A:68:ILE:CG1	1:A:69:PRO:HD2	2.41	0.51
1:C:311:ASN:C	1:C:313:GLU:N	2.69	0.51
1:A:83:ILE:CD1	1:A:122:VAL:HG11	2.37	0.50
1:C:62:THR:N	1:C:119:ASP:OD1	2.44	0.50
1:C:275:PHE:O	1:C:276:ASP:HB2	2.11	0.50
2:S:53:LEU:HB3	2:S:55:ILE:HG13	1.91	0.50
1:C:70:ASP:HA	1:C:98:ASN:HD22	1.75	0.50
2:D:14:ILE:HG13	2:D:86:LEU:HD22	1.93	0.50
1:A:81:ARG:HG3	1:A:296:TYR:CE1	2.45	0.50
1:C:81:ARG:NH1	1:C:85:ASP:OD2	2.44	0.50
2:S:69:ASP:HB2	2:S:72:ASP:OD1	2.11	0.50
1:C:101:GLN:HE22	1:C:126:GLY:H	1.56	0.50
1:C:277:ASN:H	1:C:290:THR:HG21	1.76	0.50
2:S:26:ALA:C	2:S:45:LYS:HG2	2.37	0.50
1:C:286:PRO:HB2	1:C:330:LYS:CB	2.41	0.50
1:A:258:ALA:O	1:A:262:GLN:HG3	2.11	0.49
1:A:290:THR:HG22	1:A:291:VAL:N	2.27	0.49
2:S:65:ALA:O	2:S:70:GLU:HB2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ILE:HD11	1:C:272:ILE:HB	1.94	0.49
1:A:54:ARG:HD3	3:E:710:DT:OP1	2.12	0.49
1:A:307:THR:HA	1:A:310:MET:HE3	1.95	0.49
3:E:713:DC:C2'	3:E:714:DA:H5''	2.41	0.49
4:B:703:DG:H1'	4:B:704:DT:H5'	1.94	0.49
1:A:245:LEU:HD12	1:A:273:ILE:O	2.12	0.49
1:C:115:GLY:C	1:C:117:GLN:H	2.20	0.49
1:A:275:PHE:HA	1:A:290:THR:HG23	1.93	0.49
1:A:311:ASN:O	1:A:313:GLU:N	2.44	0.49
1:C:99:SER:HB2	1:C:106:GLU:HG2	1.95	0.49
1:A:266:ILE:HG22	1:A:286:PRO:HG3	1.93	0.49
1:A:305:LEU:HD12	1:A:305:LEU:O	2.12	0.49
1:A:102:ASN:HD22	1:A:105:LYS:CB	2.14	0.49
1:A:176:LYS:HE3	1:A:332:THR:CG2	2.42	0.49
2:S:3:GLN:H	2:S:74:LEU:HD21	1.77	0.49
4:B:706:DC:H4'	4:B:706:DC:OP1	2.11	0.49
1:A:172:LEU:HD11	1:A:328:LEU:HD21	1.94	0.49
1:A:178:HIS:NE2	1:A:271:ASP:OD2	2.46	0.49
1:C:150:GLU:CG	1:C:152:GLN:HG2	2.42	0.49
1:A:66:VAL:HB	1:A:96:LEU:HD22	1.94	0.49
1:A:152:GLN:H	1:A:152:GLN:NE2	2.11	0.49
1:A:275:PHE:CA	1:A:290:THR:HG23	2.43	0.49
1:A:284:VAL:HG12	1:A:285:ARG:N	2.27	0.49
1:C:102:ASN:HD22	1:C:105:LYS:HB2	1.78	0.49
2:D:67:GLY:C	2:D:69:ASP:H	2.21	0.49
1:A:131:GLU:O	1:A:132:HIS:C	2.54	0.49
1:A:233:HIS:ND1	1:A:233:HIS:C	2.70	0.48
1:C:19:THR:HG22	1:C:22:ARG:NH1	2.28	0.48
1:C:95:ILE:O	1:C:113:MET:HE1	2.13	0.48
2:S:3:GLN:N	2:S:74:LEU:HD21	2.28	0.48
1:C:231:LEU:HD12	1:C:255:ILE:HG23	1.94	0.48
1:A:160:ILE:CD1	1:A:293:GLN:HG3	2.36	0.48
1:C:23:VAL:HG11	1:C:38:VAL:CG1	2.43	0.48
1:A:16:SER:O	1:A:20:VAL:HG23	2.13	0.48
1:C:259:ALA:HB1	1:C:264:LEU:HB2	1.94	0.48
1:C:286:PRO:HB2	1:C:330:LYS:HB2	1.95	0.48
1:A:99:SER:HB2	1:A:106:GLU:HG2	1.95	0.48
1:A:256:ILE:HD13	1:A:272:ILE:CD1	2.44	0.48
1:C:185:SER:HA	1:C:247:ALA:HB2	1.95	0.48
2:D:17:ARG:O	2:D:20:THR:HB	2.14	0.48
1:A:81:ARG:HD2	1:A:85:ASP:CG	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:5:THR:HA	2:S:61:ILE:O	2.14	0.48
2:S:34:ASN:HB2	2:S:64:SER:OG	2.14	0.48
4:B:705:DA:H2''	4:B:706:DC:O4'	2.14	0.48
1:C:183:PHE:CE1	1:C:185:SER:HB3	2.48	0.48
1:C:305:LEU:O	1:C:309:LEU:HD13	2.14	0.48
1:A:228:LEU:HA	1:A:258:ALA:CB	2.44	0.47
1:A:81:ARG:NH1	1:A:85:ASP:OD1	2.31	0.47
1:A:69:PRO:HG3	1:A:76:TYR:CZ	2.50	0.47
1:A:75:PHE:CE1	1:A:79:LEU:HD12	2.48	0.47
1:C:114:LEU:HD22	1:C:140:PRO:HD2	1.97	0.47
1:A:2:MET:HE3	1:A:3:ASN:OD1	2.15	0.47
1:C:101:GLN:HA	1:C:101:GLN:NE2	2.26	0.47
1:C:222:TYR:HA	1:C:251:MET:HG3	1.95	0.47
2:D:3:GLN:NE2	2:D:3:GLN:N	2.62	0.47
2:D:8:VAL:HG22	2:D:59:ALA:O	2.15	0.47
1:A:70:ASP:HA	1:A:98:ASN:ND2	2.26	0.47
1:C:80:ALA:O	1:C:84:GLU:HB3	2.14	0.47
2:S:36:GLU:HA	2:S:41:THR:HA	1.97	0.47
1:C:259:ALA:O	1:C:264:LEU:HG	2.14	0.47
1:A:161:ASP:OD2	1:A:161:ASP:C	2.57	0.46
1:C:155:THR:HG23	1:C:156:PRO:HD2	1.97	0.46
1:A:152:GLN:O	1:A:153:GLU:C	2.58	0.46
1:C:23:VAL:HG21	1:C:38:VAL:CG1	2.29	0.46
1:C:311:ASN:HB3	1:C:313:GLU:HG2	1.98	0.46
1:A:103:MET:HG3	1:A:132:HIS:CE1	2.50	0.46
2:S:29:TYR:HB3	2:S:69:ASP:OD1	2.16	0.46
4:B:707:DC:H6	4:B:707:DC:H2'	1.63	0.46
1:A:166:ILE:HG12	1:A:197:LYS:HG2	1.98	0.46
1:A:309:LEU:CD1	1:A:309:LEU:N	2.79	0.46
1:C:19:THR:HG22	1:C:22:ARG:HH11	1.81	0.46
1:C:304:ARG:HG2	2:D:48:MET:HG3	1.97	0.46
1:A:6:ILE:CG2	1:A:7:TYR:N	2.77	0.46
1:A:228:LEU:CD2	1:A:258:ALA:HB2	2.42	0.46
1:A:279:ARG:HG2	1:A:279:ARG:HH21	1.81	0.46
1:C:101:GLN:HE21	1:C:101:GLN:CA	2.19	0.46
1:C:152:GLN:O	1:C:153:GLU:HB2	2.16	0.46
1:C:105:LYS:O	1:C:109:LEU:HG	2.15	0.46
1:A:150:GLU:CG	1:A:152:GLN:HG2	2.43	0.46
1:C:86:ILE:HG22	1:C:303:MET:CG	2.46	0.46
1:A:228:LEU:HA	1:A:254:GLY:O	2.16	0.45
1:C:235:MET:CE	1:C:241:PRO:HD2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:ASN:OD1	2:D:45:LYS:HB2	2.16	0.45
2:S:14:ILE:HB	2:S:55:ILE:HB	1.97	0.45
1:C:20:VAL:O	1:C:24:VAL:HG23	2.16	0.45
1:C:90:TYR:CD1	1:C:307:THR:HG21	2.51	0.45
1:C:297:ASP:OD2	2:D:51:MET:HG2	2.16	0.45
1:A:78:GLU:OE1	1:A:296:TYR:HB2	2.17	0.45
1:C:282:LEU:HD13	1:C:329:ARG:NE	2.31	0.45
1:A:165:ALA:HB1	1:A:291:VAL:HG11	1.98	0.45
1:A:215:GLN:HE21	1:A:237:LEU:HD22	1.81	0.45
2:S:17:ARG:HB2	2:S:18:PRO:CD	2.42	0.45
2:D:34:ASN:OD1	2:D:41:THR:HG22	2.17	0.45
1:A:330:LYS:C	1:A:332:THR:H	2.24	0.45
2:D:78:GLU:O	2:D:79:GLU:C	2.59	0.45
1:A:36:LYS:O	1:A:40:GLU:HG3	2.16	0.45
2:D:79:GLU:OE2	2:D:83:SER:OG	2.34	0.45
3:E:706:DG:H4'	3:E:706:DG:OP1	2.17	0.45
2:S:2:ALA:HB1	2:S:74:LEU:CD2	2.39	0.45
1:C:166:ILE:HG13	1:C:197:LYS:HA	1.97	0.45
1:C:266:ILE:HD12	1:C:272:ILE:HD13	1.99	0.45
1:C:267:PRO:O	1:C:333:LYS:NZ	2.36	0.45
1:A:13:ALA:O	1:A:37:LYS:HD2	2.17	0.44
1:A:330:LYS:HE2	1:A:330:LYS:N	2.32	0.44
1:C:164:GLN:O	1:C:168:ASP:OD1	2.35	0.44
1:A:42:ILE:HG23	1:A:47:TYR:HB3	1.99	0.44
1:A:152:GLN:H	1:A:152:GLN:CD	2.25	0.44
1:A:159:ALA:O	1:A:321:GLU:HA	2.17	0.44
2:S:6:PHE:CE1	2:S:63:ILE:HD12	2.53	0.44
2:D:25:THR:O	2:D:28:LYS:HB2	2.18	0.44
2:D:46:SEP:O	2:D:47:ILE:C	2.60	0.44
1:A:223:THR:HB	1:A:226:SER:H	1.83	0.44
1:A:231:LEU:CD1	1:A:259:ALA:HB2	2.46	0.44
1:A:322:LEU:HB3	1:A:323:PRO:HD2	1.99	0.44
2:S:10:ALA:HB2	2:S:85:GLY:O	2.17	0.44
1:A:102:ASN:HD21	1:A:104:GLU:HB3	1.83	0.44
1:C:79:LEU:HG	1:C:295:THR:HG23	1.98	0.44
2:D:44:LEU:HD13	2:D:44:LEU:O	2.18	0.44
1:A:54:ARG:NH1	3:E:710:DT:OP1	2.49	0.44
1:C:166:ILE:O	1:C:170:VAL:HG23	2.18	0.44
1:A:75:PHE:CE2	1:A:295:THR:HG23	2.53	0.44
1:C:10:ALA:HB2	1:C:17:MET:HA	2.00	0.44
1:A:228:LEU:HD23	1:A:258:ALA:CA	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PHE:CZ	1:A:79:LEU:HD12	2.53	0.44
1:A:178:HIS:CE1	1:A:243:ALA:HB2	2.52	0.44
1:A:248:THR:HG22	1:A:249:ASP:N	2.33	0.44
2:S:7:LYS:HA	2:S:59:ALA:O	2.18	0.44
1:C:35:ARG:O	1:C:38:VAL:HG12	2.18	0.44
1:C:293:GLN:O	1:C:295:THR:N	2.48	0.44
2:S:3:GLN:O	2:S:4:LYS:HB2	2.18	0.43
2:S:31:ALA:O	2:S:33:VAL:HG23	2.17	0.43
2:D:18:PRO:O	2:D:21:VAL:HB	2.17	0.43
1:A:80:ALA:O	1:A:81:ARG:C	2.60	0.43
1:C:83:ILE:HG23	1:C:303:MET:HE2	2.00	0.43
2:D:9:THR:CG2	2:D:87:GLY:H	2.26	0.43
1:A:145:LEU:HB2	1:A:157:SER:CB	2.48	0.43
1:C:11:ARG:C	1:C:13:ALA:H	2.25	0.43
2:D:5:THR:HG22	2:D:6:PHE:N	2.34	0.43
4:B:703:DG:H2''	4:B:704:DT:O5'	2.19	0.43
1:A:101:GLN:OE1	1:A:126:GLY:HA3	2.19	0.43
1:A:221:ASP:CG	1:A:223:THR:HG1	2.23	0.43
1:C:129:THR:HG23	1:C:132:HIS:CE1	2.52	0.43
2:S:20:THR:O	2:S:24:GLN:HG3	2.18	0.43
1:C:228:LEU:HA	1:C:258:ALA:HB2	2.01	0.43
1:A:89:MET:HG2	1:A:90:TYR:CD2	2.53	0.43
1:A:161:ASP:CG	1:A:164:GLN:HB2	2.43	0.43
1:A:287:GLN:CB	1:A:329:ARG:HB3	2.45	0.43
1:C:151:GLU:O	1:C:153:GLU:HG2	2.18	0.43
1:A:95:ILE:N	1:A:95:ILE:CD1	2.82	0.43
1:A:95:ILE:O	1:A:113:MET:HE1	2.18	0.43
1:C:124:MET:CG	1:C:146:ALA:HB3	2.43	0.43
2:D:49:GLY:O	2:D:52:SER:OG	2.36	0.43
1:C:19:THR:HA	1:C:22:ARG:HG3	2.01	0.43
1:C:234:LEU:C	1:C:236:SER:H	2.27	0.43
2:D:9:THR:HG23	2:D:85:GLY:O	2.19	0.43
2:D:49:GLY:O	2:D:53:LEU:HD13	2.19	0.43
1:A:188:MET:O	1:A:189:ALA:C	2.62	0.43
1:C:213:ASN:C	1:C:215:GLN:H	2.27	0.43
1:C:248:THR:HA	1:C:275:PHE:HB3	2.01	0.43
3:E:709:DG:H1	4:B:706:DC:H42	1.66	0.43
1:A:110:LEU:HD12	1:A:135:GLU:HG2	2.01	0.42
1:A:128:ILE:H	1:A:128:ILE:CD1	2.31	0.42
1:C:165:ALA:HA	1:C:324:HIS:CD2	2.53	0.42
1:A:50:ASN:C	1:A:50:ASN:OD1	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ILE:HD13	1:C:45:LEU:HB3	2.00	0.42
1:C:81:ARG:O	1:C:85:ASP:HB2	2.18	0.42
1:C:165:ALA:HA	1:C:324:HIS:NE2	2.34	0.42
3:E:708:DG:C1'	3:E:709:DG:H5''	2.45	0.42
1:A:231:LEU:HD22	1:A:258:ALA:C	2.44	0.42
1:C:253:LEU:HD21	1:C:284:VAL:HG22	2.01	0.42
1:A:221:ASP:O	1:A:222:TYR:CB	2.67	0.42
1:A:221:ASP:OD1	1:A:221:ASP:C	2.62	0.42
1:C:110:LEU:HD11	1:C:136:PHE:CD2	2.54	0.42
1:C:185:SER:OG	1:C:188:MET:HE3	2.19	0.42
2:D:75:ASN:O	2:D:78:GLU:HB2	2.20	0.42
1:A:64:VAL:CG2	1:A:303:MET:HE1	2.40	0.42
1:A:166:ILE:HG13	1:A:197:LYS:HG2	2.02	0.42
1:A:294:PRO:O	1:A:298:ILE:HG13	2.19	0.42
1:A:97:SER:OG	1:A:109:LEU:HD22	2.20	0.42
1:A:288:LEU:O	1:A:329:ARG:HG3	2.19	0.42
1:C:129:THR:O	1:C:133:VAL:HG23	2.20	0.42
1:A:94:ILE:O	1:C:95:ILE:HA	2.20	0.42
1:A:103:MET:HE2	1:A:132:HIS:HE1	1.84	0.42
2:D:33:VAL:HG11	2:D:77:LEU:HD11	2.00	0.42
1:A:283:MET:HG2	1:C:224:TYR:CD2	2.54	0.42
1:C:252:ALA:HB1	1:C:288:LEU:HD11	2.01	0.42
2:D:9:THR:N	2:D:87:GLY:HA2	2.32	0.42
1:A:263:GLY:O	1:A:264:LEU:O	2.37	0.42
1:C:231:LEU:HD13	1:C:255:ILE:O	2.20	0.42
1:C:294:PRO:O	1:C:295:THR:C	2.61	0.42
1:A:71:ILE:HG13	1:A:71:ILE:O	2.20	0.42
1:A:103:MET:HE1	1:A:129:THR:HG21	2.02	0.42
1:C:95:ILE:HG22	1:C:113:MET:CE	2.50	0.42
2:D:40:LYS:HE3	2:D:40:LYS:HB2	1.89	0.42
1:C:102:ASN:O	1:C:106:GLU:HG3	2.20	0.41
1:A:90:TYR:CE1	1:A:304:ARG:NH2	2.88	0.41
1:A:280:LEU:O	1:A:281:SER:C	2.63	0.41
2:S:36:GLU:HB2	2:S:41:THR:HG23	2.02	0.41
1:C:4:ILE:CD1	1:C:45:LEU:HB3	2.50	0.41
1:C:53:ALA:CB	4:B:709:DC:H5'	2.50	0.41
1:C:222:TYR:O	1:C:250:GLU:HB3	2.20	0.41
2:D:63:ILE:HG21	2:D:77:LEU:HD13	2.02	0.41
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.89	0.41
2:D:80:THR:HA	2:D:83:SER:HB2	2.02	0.41
1:A:89:MET:HE2	1:A:90:TYR:HE2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:ARG:NH2	2:D:17:ARG:HG3	2.34	0.41
2:D:74:LEU:O	2:D:78:GLU:HG3	2.20	0.41
1:A:6:ILE:HG23	1:A:17:MET:HG2	2.02	0.41
1:A:68:ILE:HG12	1:A:69:PRO:HD2	2.02	0.41
1:A:95:ILE:HA	1:C:94:ILE:O	2.20	0.41
1:A:280:LEU:O	1:A:284:VAL:HG23	2.20	0.41
1:C:275:PHE:CA	1:C:290:THR:HG23	2.47	0.41
2:D:17:ARG:CG	2:D:17:ARG:HH21	2.33	0.41
2:S:35:LEU:HD21	2:S:55:ILE:CD1	2.50	0.41
1:C:306:LEU:HG	1:C:310:MET:HE2	2.02	0.41
1:A:23:VAL:HG13	1:A:35:ARG:HG3	2.03	0.41
1:A:138:ARG:O	1:A:138:ARG:HG3	2.20	0.41
1:A:231:LEU:HD22	1:A:258:ALA:HB3	2.02	0.41
1:C:79:LEU:HG	1:C:295:THR:CG2	2.51	0.41
1:A:172:LEU:HD23	1:A:172:LEU:O	2.21	0.41
1:A:219:GLU:O	1:A:219:GLU:HG2	2.21	0.41
1:A:257:HIS:HB3	1:C:285:ARG:NH1	2.36	0.41
2:S:6:PHE:HA	2:S:88:GLU:OXT	2.21	0.41
2:S:8:VAL:HG21	2:S:56:ALA:O	2.21	0.41
2:S:54:GLY:O	2:S:56:ALA:N	2.54	0.41
1:C:179:THR:HG23	1:C:210:LEU:CD2	2.48	0.41
2:D:37:TYR:CD1	2:D:37:TYR:C	2.99	0.41
1:C:50:ASN:OD1	1:C:50:ASN:C	2.63	0.41
2:D:22:LEU:CD2	2:D:81:MET:HE3	2.47	0.40
2:D:23:VAL:HA	2:D:44:LEU:O	2.20	0.40
2:D:79:GLU:O	2:D:82:LYS:HG3	2.22	0.40
1:A:95:ILE:CG2	1:A:113:MET:HE2	2.51	0.40
1:A:100:ASP:C	1:A:102:ASN:N	2.78	0.40
1:C:185:SER:O	1:C:251:MET:HE1	2.21	0.40
1:A:309:LEU:N	1:A:309:LEU:HD13	2.37	0.40
1:A:311:ASN:C	1:A:313:GLU:N	2.79	0.40
1:C:23:VAL:O	1:C:24:VAL:C	2.64	0.40
1:C:171:LYS:O	1:C:172:LEU:C	2.64	0.40
1:C:305:LEU:HD11	1:C:315:VAL:HG11	2.02	0.40
1:C:173:LEU:HD13	1:C:181:ILE:HG21	2.04	0.40
1:C:231:LEU:CD1	1:C:255:ILE:HG23	2.51	0.40
4:B:713:DC:H1'	4:B:714:DA:H5''	2.03	0.40

There are no symmetry-related clashes.

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	330/339 (97%)	292 (88%)	29 (9%)	9 (3%)	4	22
1	C	330/339 (97%)	285 (86%)	36 (11%)	9 (3%)	4	22
2	D	84/87 (97%)	71 (84%)	8 (10%)	5 (6%)	1	9
2	S	84/87 (97%)	69 (82%)	11 (13%)	4 (5%)	2	12
All	All	828/852 (97%)	717 (87%)	84 (10%)	27 (3%)	3	19

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	LYS
2	S	55	ILE
2	S	68	ALA
2	D	8	VAL
1	A	264	LEU
1	A	276	ASP
1	C	29	ASN
1	C	282	LEU
1	C	312	LYS
1	C	317	GLU
2	D	16	ALA
2	D	59	ALA
1	A	153	GLU
1	A	317	GLU
2	S	16	ALA
1	C	214	GLU
1	A	15	VAL
1	A	268	GLU
1	A	281	SER
2	S	4	LYS
1	C	12	GLU
1	C	175	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	35	ARG
2	D	4	LYS
2	D	65	ALA
1	A	4	ILE
1	C	187	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/293 (98%)	264 (92%)	22 (8%)	12	37
1	C	286/293 (98%)	264 (92%)	22 (8%)	12	37
2	D	66/66 (100%)	60 (91%)	6 (9%)	9	31
2	S	66/66 (100%)	56 (85%)	10 (15%)	3	13
All	All	704/718 (98%)	644 (92%)	60 (8%)	10	33

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	32	PRO
1	A	35	ARG
1	A	56	LEU
1	A	74	ILE
1	A	79	LEU
1	A	93	ASN
1	A	94	ILE
1	A	96	LEU
1	A	105	LYS
1	A	110	LEU
1	A	113	MET
1	A	151	GLU
1	A	152	GLN
1	A	164	GLN
1	A	206	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	231	LEU
1	A	235	MET
1	A	242	THR
1	A	309	LEU
1	A	318	HIS
1	A	319	ILE
2	S	4	LYS
2	S	27	SER
2	S	28	LYS
2	S	32	ASP
2	S	40	LYS
2	S	53	LEU
2	S	62	THR
2	S	72	ASP
2	S	74	LEU
2	S	84	GLU
1	C	2	MET
1	C	11	ARG
1	C	12	GLU
1	C	17	MET
1	C	34	THR
1	C	56	LEU
1	C	71	ILE
1	C	79	LEU
1	C	96	LEU
1	C	101	GLN
1	C	110	LEU
1	C	152	GLN
1	C	164	GLN
1	C	180	ASP
1	C	228	LEU
1	C	244	ILE
1	C	264	LEU
1	C	268	GLU
1	C	284	VAL
1	C	285	ARG
1	C	309	LEU
1	C	325	ARG
2	D	3	GLN
2	D	17	ARG
2	D	34	ASN
2	D	44	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	53	LEU
2	D	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	102	ASN
1	A	117	GLN
1	A	193	ASN
1	A	213	ASN
1	A	215	GLN
1	A	232	GLN
1	A	257	HIS
1	A	262	GLN
1	A	277	ASN
1	A	287	GLN
2	S	75	ASN
1	C	98	ASN
1	C	101	GLN
1	C	102	ASN
1	C	117	GLN
1	C	193	ASN
1	C	209	ASN
1	C	232	GLN
2	D	3	GLN
2	D	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	SEP	S	46	2	8,9,10	1.02	0	7,12,14	1.79	2 (28%)
2	SEP	D	46	2	8,9,10	1.03	0	7,12,14	1.56	2 (28%)

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	SEP	S	46	2	-	6/6/8/10	-
2	SEP	D	46	2	-	6/6/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	S	46	SEP	O3P-P-O1P	2.94	122.31	110.83
2	D	46	SEP	O3P-P-O1P	2.83	121.87	110.83
2	S	46	SEP	OG-CB-CA	2.80	110.87	108.14
2	D	46	SEP	OG-CB-CA	2.21	110.29	108.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	46	SEP	C-CA-CB-OG
2	S	46	SEP	CA-CB-OG-P
2	S	46	SEP	CB-OG-P-O1P
2	S	46	SEP	CB-OG-P-O2P
2	S	46	SEP	CB-OG-P-O3P
2	D	46	SEP	C-CA-CB-OG
2	D	46	SEP	CB-OG-P-O2P
2	D	46	SEP	CB-OG-P-O3P
2	D	46	SEP	CA-CB-OG-P
2	S	46	SEP	N-CA-CB-OG
2	D	46	SEP	N-CA-CB-OG
2	D	46	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	46	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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(Å ²)	Q<0.9
1	A	332/339 (97%)	-0.13	3 (0%) 81 65	49, 75, 98, 117	0
1	C	332/339 (97%)	-0.06	2 (0%) 85 73	51, 92, 121, 133	0
2	D	86/87 (98%)	0.11	0 100 100	72, 109, 127, 128	0
2	S	86/87 (98%)	0.17	1 (1%) 76 58	77, 113, 133, 141	0
3	E	16/16 (100%)	0.03	0 100 100	60, 93, 109, 110	0
4	B	16/16 (100%)	-0.02	0 100 100	70, 91, 106, 108	0
All	All	868/884 (98%)	-0.05	6 (0%) 84 70	49, 87, 123, 141	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	87	GLY	3.7
1	A	2	MET	3.1
1	A	3	ASN	2.4
1	A	7	TYR	2.3
1	C	281	SER	2.1
1	C	51	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SEP	D	46	10/11	0.93	0.07	84,87,90,92	0
2	SEP	S	46	10/11	0.97	0.06	83,87,89,90	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.