



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2014 – 03:27 AM EDT

PDB ID : 4D0L
Title : Phosphatidylinositol 4-kinase III beta-PIK93 in a complex with Rab11a- GTP gammaS
Authors : Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.
Deposited on : 2014-04-29
Resolution : 2.94 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

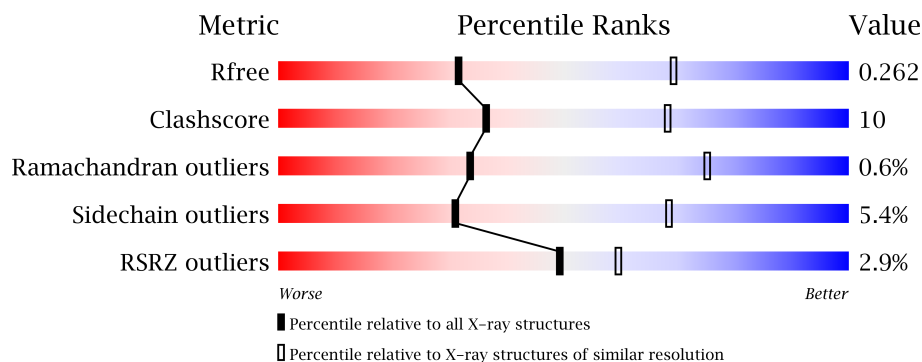
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.94 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}	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	566	
1	C	566	
1	E	566	
2	B	219	
2	D	219	
2	F	219	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15864 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	C	476	Total	C	N	O	S	0	0	0
			3833	2456	660	693	24			
1	E	479	Total	C	N	O	S	0	0	0
			3859	2473	666	696	24			

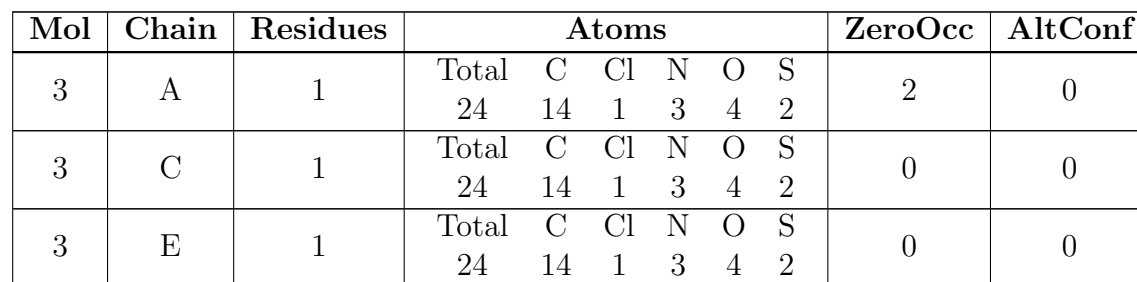
- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	D	177	Total	C	N	O	S	0	0	0
			1409	891	244	272	2			
2	F	177	Total	C	N	O	S	0	0	0
			1409	891	244	272	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
D	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
F	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491

- Molecule 3 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)-PHENYLTHIAZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).



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- The chemical structure of GSP (Guanosine 3'-phosphate) is shown. It consists of a guanine base (a purine ring system with an amino group at position 2 and a carbonyl group at position 6) linked to a ribose sugar (a five-membered ring with hydroxyl groups at positions 2' and 3'). The ribose sugar is linked to a pyrophosphate group (two phosphate groups connected by an oxygen atom). The pyrophosphate group is further linked to a sulfur atom (S) via a phosphorothioate bond. The structure is labeled with various atoms and bonds, including N1, N2, N3, N4, N5, N6, N7, N8, N9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O80

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

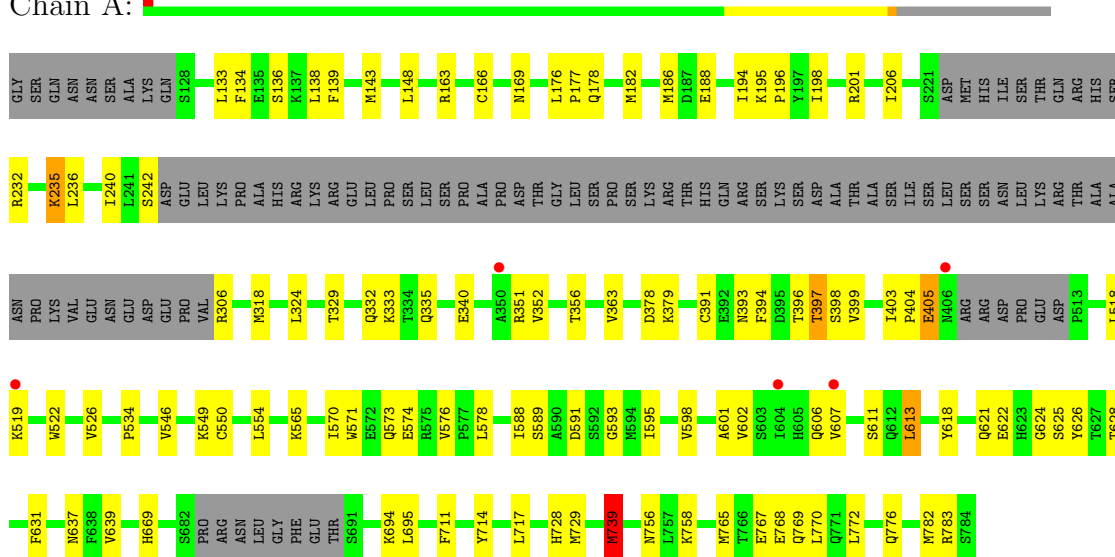
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		
6	E	4	Total	O	0	0
			4	4		
6	F	3	Total	O	0	0
			3	3		

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.

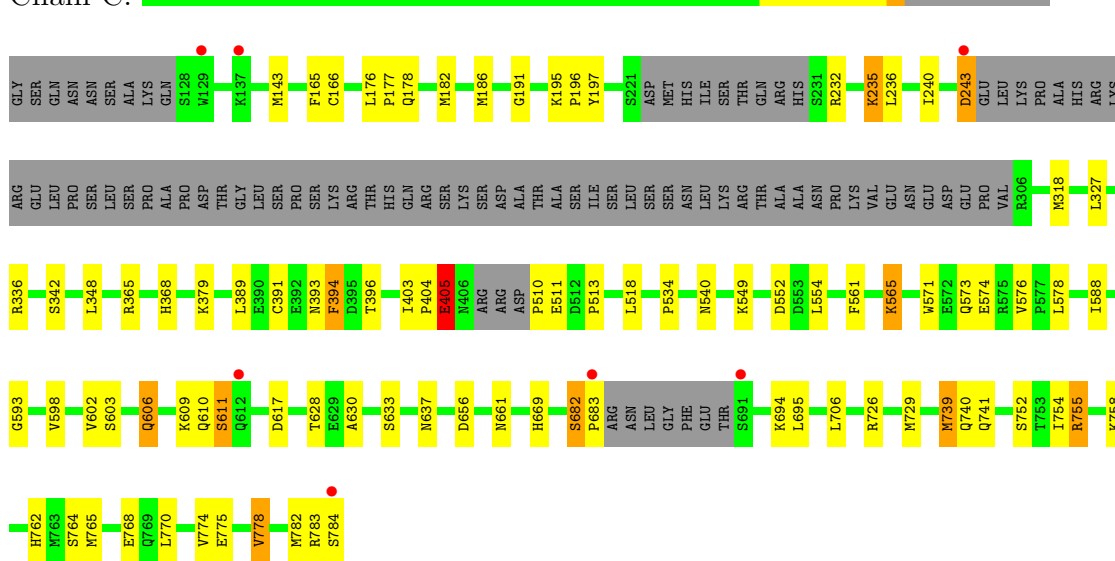
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain A:



• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

Chain C:



• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.80Å 146.93Å 188.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.84 – 2.94 49.58 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (115.84-2.94) 99.7 (49.58-2.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.216 , 0.259 0.218 , 0.262	Depositor DCC
R_{free} test set	3095 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61151 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15864	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, MG, 093

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	0.53	0/3866	0.75	1/5219 (0.0%)
1	C	0.53	0/3913	0.76	2/5285 (0.0%)
1	E	0.53	0/3940	0.75	2/5322 (0.0%)
2	B	0.50	0/1399	0.79	1/1892 (0.1%)
2	D	0.50	0/1431	0.70	0/1933
2	F	0.52	0/1431	0.74	0/1933
All	All	0.53	0/15980	0.75	6/21584 (0.0%)

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	1
1	C	0	1
1	E	0	2
2	F	0	1
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	657	ARG	NE-CZ-NH1	6.79	123.70	120.30
2	B	88	LEU	CB-CG-CD1	6.40	121.89	111.00
1	E	348	LEU	C-N-CA	-5.49	98.94	122.00
1	C	143	MET	CG-SD-CE	5.17	108.48	100.20
1	A	739	MET	CG-SD-CE	-5.12	92.01	100.20
1	C	611	SER	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	403	ILE	Peptide
1	E	348	LEU	Peptide
1	E	750	GLY	Peptide
2	F	110	ARG	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3788	0	3839	77	1
1	C	3833	0	3870	57	0
1	E	3859	0	3895	106	0
2	B	1377	0	1370	32	0
2	D	1409	0	1405	25	0
2	F	1409	0	1407	23	0
3	A	24	0	16	7	0
3	C	24	0	16	5	0
3	E	24	0	16	7	0
4	B	32	0	12	3	0
4	D	32	0	12	2	0
4	F	32	0	12	3	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	8	0	0	0	0
6	B	2	0	0	1	0
6	C	1	0	0	0	0
6	E	4	0	0	1	0
6	F	3	0	0	0	0
All	All	15864	0	15870	328	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (328) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:56:ASP:OD2	2:B:174:ARG:NH1	1.72	1.20
1:C:240:ILE:O	1:C:243:ASP:OD1	1.75	1.04
1:E:323:ARG:NH1	1:E:340:GLU:OE2	1.90	1.03
1:E:686:LEU:HD22	1:E:688:PHE:CE2	1.98	0.98
1:C:694:LYS:HD3	1:C:784:SER:HA	1.46	0.95
1:A:232:ARG:O	1:A:235:LYS:NZ	1.99	0.94
1:A:549:LYS:NZ	3:A:2002:093:OAM	2.02	0.93
1:E:511:GLU:N	1:E:511:GLU:OE1	2.01	0.92
1:E:598:VAL:H	3:E:2002:093:HAK	1.18	0.92
1:E:686:LEU:HD13	1:E:688:PHE:CD2	2.04	0.91
1:E:686:LEU:HD13	1:E:688:PHE:CG	2.05	0.90
1:A:178:GLN:HA	1:A:739:MET:HE1	1.56	0.88
1:E:686:LEU:HB3	1:E:688:PHE:CE1	2.09	0.88
1:A:163:ARG:O	1:A:166:CYS:SG	2.33	0.86
2:B:95:LYS:O	2:B:98:THR:HG22	1.75	0.85
1:C:404:PRO:O	1:C:405:GLU:HB2	1.76	0.85
1:C:177:PRO:HB2	1:C:739:MET:HE1	1.58	0.84
1:E:344:LEU:O	1:E:348:LEU:HG	1.78	0.84
2:B:54:GLN:HG3	1:C:783:ARG:HD2	1.63	0.80
1:E:520:GLU:OE1	1:E:528:ARG:NH2	2.14	0.80
1:E:566:GLN:HE21	1:E:731:LYS:HB3	1.46	0.79
1:E:684:ARG:HA	1:E:684:ARG:CZ	2.12	0.79
1:E:686:LEU:HB3	1:E:688:PHE:CD1	2.19	0.78
2:D:181:MET:HA	2:D:181:MET:CE	2.14	0.78
1:E:607:VAL:O	1:E:611:SER:HB3	1.85	0.77
1:E:682:SER:CB	1:E:684:ARG:HB2	2.15	0.77
1:A:139:PHE:HA	1:A:143:MET:HE2	1.67	0.76
1:A:602:VAL:HG23	1:A:607:VAL:HG23	1.66	0.76
3:E:2002:093:HAE2	3:E:2002:093:HAD	1.69	0.75
2:F:110:ARG:HD3	2:F:114:ASP:O	1.88	0.74
3:C:2002:093:HAE2	3:C:2002:093:HAD	1.70	0.73
1:A:393:ASN:O	1:A:397:THR:OG1	2.06	0.72
1:A:178:GLN:CD	1:A:739:MET:CE	2.58	0.72
1:A:611:SER:HB2	1:A:613:LEU:HD22	1.70	0.72
1:E:520:GLU:OE2	1:E:524:GLU:HB3	1.89	0.72
1:C:365:ARG:NH2	1:C:405:GLU:OE2	2.22	0.72
1:E:684:ARG:NE	1:E:684:ARG:HA	2.03	0.71
2:D:110:ARG:NH1	2:D:114:ASP:O	2.24	0.71
1:C:232:ARG:O	1:C:235:LYS:HD2	1.92	0.70
1:E:682:SER:HB2	1:E:684:ARG:HB2	1.74	0.69
1:E:232:ARG:O	1:E:235:LYS:HD2	1.92	0.69
3:C:2002:093:CAE	3:C:2002:093:HAD	2.22	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:598:VAL:H	3:C:2002:093:HAK	1.39	0.69
1:E:726:ARG:CA	1:E:763:MET:HE1	2.22	0.69
3:A:2002:093:HAD	3:A:2002:093:HAE2	1.74	0.69
1:E:139:PHE:HA	1:E:143:MET:HE2	1.76	0.68
1:E:726:ARG:HA	1:E:763:MET:HE1	1.75	0.68
1:E:686:LEU:HB2	1:E:688:PHE:N	2.09	0.67
2:F:106:LEU:O	2:F:109:LEU:HB3	1.94	0.67
1:A:518:LEU:HG	1:A:519:LYS:H	1.60	0.67
1:E:682:SER:OG	1:E:684:ARG:NH1	2.28	0.66
1:A:618:TYR:CZ	1:A:622:GLU:HG3	2.30	0.66
1:E:607:VAL:O	1:E:611:SER:CB	2.43	0.66
2:F:81:TYR:HB3	2:F:113:ALA:HB2	1.77	0.66
2:B:81:TYR:HB3	2:B:113:ALA:HB2	1.78	0.65
2:B:120:MET:HE1	2:B:164:ALA:HB1	1.78	0.65
1:E:628:THR:HG23	1:E:631:PHE:H	1.61	0.65
1:A:611:SER:HB2	1:A:613:LEU:CD2	2.25	0.65
2:D:81:TYR:HB3	2:D:113:ALA:HB2	1.77	0.65
1:A:206:ILE:HD11	1:A:394:PHE:HE2	1.62	0.65
1:A:765:MET:HA	1:A:769:GLN:OE1	1.97	0.65
1:E:682:SER:HB3	1:E:684:ARG:N	2.12	0.65
3:A:2002:093:CAE	3:A:2002:093:HAD	2.28	0.63
1:E:232:ARG:O	1:E:235:LYS:CD	2.46	0.63
1:A:178:GLN:CA	1:A:739:MET:HE1	2.25	0.63
1:E:238:LYS:O	1:E:242:SER:HB3	1.97	0.63
1:C:232:ARG:O	1:C:235:LYS:CD	2.46	0.63
3:E:2002:093:CAE	3:E:2002:093:HAD	2.29	0.62
1:E:752:SER:HB2	1:E:755:ARG:CZ	2.29	0.62
1:A:628:THR:HG23	1:A:631:PHE:H	1.64	0.62
2:B:45:GLY:O	2:B:67:THR:O	2.18	0.62
1:C:694:LYS:HD3	1:C:784:SER:CA	2.24	0.62
1:A:637:ASN:HB3	1:A:669:HIS:CD2	2.35	0.61
2:F:110:ARG:HD2	2:F:115:SER:HA	1.80	0.61
2:B:67:THR:O	2:B:68:ALA:HB3	2.00	0.60
1:C:404:PRO:O	1:C:405:GLU:CB	2.45	0.60
1:E:686:LEU:HD22	1:E:688:PHE:CZ	2.36	0.60
1:E:682:SER:N	1:E:683:PRO:HA	2.16	0.60
1:E:783:ARG:O	1:E:784:SER:OG	2.16	0.60
1:C:740:GLN:OE1	1:C:754:ILE:HD13	2.01	0.60
1:E:212:CYS:O	1:E:216:LEU:HD12	2.03	0.59
1:A:767:GLU:HA	1:A:770:LEU:HD12	1.84	0.59
1:A:134:PHE:O	1:A:163:ARG:NH1	2.36	0.59
1:C:637:ASN:HB3	1:C:669:HIS:CD2	2.38	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:352:VAL:HG12	1:E:363:VAL:HG11	1.84	0.59
2:B:8:TYR:CE2	2:B:11:LEU:HB2	2.38	0.59
2:D:38:LEU:HA	4:D:2000:GSP:O2'	2.03	0.59
4:F:2000:GSP:O2B	4:F:2000:GSP:O3G	2.20	0.59
1:A:602:VAL:HG23	1:A:607:VAL:CG2	2.34	0.58
2:B:92:ASP:H	2:B:98:THR:HG21	1.68	0.58
1:C:510:PRO:O	1:C:511:GLU:HB2	2.03	0.58
1:A:598:VAL:H	3:A:2002:093:HAK	1.51	0.58
1:E:607:VAL:O	1:E:611:SER:N	2.37	0.58
1:E:682:SER:HB3	1:E:684:ARG:HB2	1.85	0.58
1:C:774:VAL:O	1:C:778:VAL:HG12	2.04	0.58
1:A:242:SER:O	1:A:306:ARG:HD3	2.04	0.57
2:D:85:VAL:HG13	2:D:172:ILE:HD13	1.87	0.57
1:A:518:LEU:HG	1:A:519:LYS:N	2.19	0.57
1:E:637:ASN:HB3	1:E:669:HIS:CD2	2.40	0.57
1:E:686:LEU:HD13	1:E:688:PHE:CB	2.34	0.56
2:B:28:LEU:HD22	2:B:66:ASP:HB2	1.87	0.56
1:A:570:ILE:HG23	1:A:728:HIS:HD2	1.71	0.56
1:E:686:LEU:CB	1:E:688:PHE:CD1	2.87	0.56
1:C:628:THR:HG22	1:C:630:ALA:N	2.21	0.56
2:F:28:LEU:HD22	2:F:66:ASP:HB2	1.88	0.56
1:A:188:GLU:HG3	1:A:232:ARG:HH12	1.71	0.55
1:A:306:ARG:O	1:A:351:ARG:NH1	2.40	0.55
1:E:682:SER:N	1:E:683:PRO:CA	2.68	0.55
2:F:170:THR:O	2:F:174:ARG:HG3	2.07	0.55
2:B:8:TYR:HA	2:B:59:THR:OG1	2.06	0.55
1:E:139:PHE:HD1	1:E:143:MET:HE2	1.71	0.55
2:D:28:LEU:HD22	2:D:66:ASP:HB2	1.88	0.55
2:F:110:ARG:HE	2:F:117:ILE:HG22	1.72	0.55
1:C:182:MET:HA	1:C:186:MET:HG3	1.89	0.55
2:D:8:TYR:CE2	2:D:11:LEU:HB2	2.43	0.54
1:E:686:LEU:HB2	1:E:687:GLY:CA	2.37	0.54
1:E:598:VAL:O	3:E:2002:093:NAR	2.40	0.54
1:E:686:LEU:HD13	1:E:688:PHE:HB2	1.90	0.54
1:A:403:ILE:HG22	1:A:534:PRO:HB3	1.90	0.54
4:B:2000:GSP:O2B	4:B:2000:GSP:O3G	2.26	0.54
1:E:139:PHE:HD1	1:E:143:MET:CE	2.21	0.54
1:A:178:GLN:CD	1:A:739:MET:HE3	2.27	0.54
1:E:512:ASP:N	1:E:513:PRO:HD3	2.22	0.54
2:B:144:GLU:HA	2:B:144:GLU:OE1	2.07	0.54
1:A:182:MET:HA	1:A:186:MET:HG3	1.90	0.53
1:E:598:VAL:N	3:E:2002:093:HAK	1.98	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:LYS:HD2	1:A:550:CYS:SG	2.49	0.53
2:B:67:THR:O	2:B:68:ALA:CB	2.55	0.53
1:E:361:HIS:HB2	1:E:388:VAL:HG13	1.90	0.53
1:A:139:PHE:HD1	1:A:143:MET:CE	2.20	0.53
1:E:730:ASP:O	1:E:734:GLN:HB2	2.09	0.53
1:A:139:PHE:HD1	1:A:143:MET:HE2	1.73	0.52
1:C:554:LEU:HD13	1:C:593:GLY:HA3	1.90	0.52
1:E:571:TRP:CE2	1:E:578:LEU:HD12	2.45	0.52
1:E:683:PRO:O	1:E:684:ARG:HB3	2.08	0.52
2:D:181:MET:HA	2:D:181:MET:HE3	1.92	0.52
2:F:8:TYR:HA	2:F:59:THR:OG1	2.10	0.52
1:A:329:THR:HG23	1:A:332:GLN:H	1.73	0.52
1:E:603:SER:OG	1:E:606:GLN:HB2	2.10	0.52
1:E:588:ILE:HD12	1:E:593:GLY:HA2	1.91	0.51
1:E:243:ASP:OD1	1:E:243:ASP:N	2.43	0.51
1:A:625:SER:O	1:A:628:THR:HG22	2.11	0.51
1:A:598:VAL:N	3:A:2002:093:HAK	2.08	0.51
1:A:570:ILE:HG23	1:A:728:HIS:CD2	2.46	0.51
2:F:173:TYR:O	2:F:173:TYR:CG	2.63	0.51
2:F:110:ARG:CD	2:F:115:SER:HA	2.41	0.51
1:E:182:MET:HA	1:E:186:MET:HG3	1.92	0.51
2:B:24:LYS:HE2	6:B:3001:HOH:O	2.09	0.51
1:C:178:GLN:CD	1:C:739:MET:HE2	2.31	0.51
2:B:56:ASP:OD2	2:B:174:ARG:CZ	2.55	0.50
1:A:178:GLN:CG	1:A:739:MET:CE	2.90	0.50
1:A:768:GLU:H	1:A:768:GLU:CD	2.13	0.50
1:C:588:ILE:HD12	1:C:593:GLY:HA2	1.93	0.50
1:A:404:PRO:O	1:A:405:GLU:CB	2.59	0.50
1:E:395:ASP:N	6:E:3002:HOH:O	2.44	0.50
2:B:6:ASP:O	1:E:628:THR:HA	2.11	0.50
1:C:774:VAL:O	1:C:778:VAL:CG1	2.60	0.50
1:E:657:ARG:HD2	1:E:672:HIS:CE1	2.47	0.50
1:A:169:ASN:OD1	1:A:201:ARG:CZ	2.59	0.49
1:A:195:LYS:HB3	1:A:196:PRO:HD3	1.94	0.49
1:A:626:TYR:HA	1:A:631:PHE:CD2	2.47	0.49
1:E:216:LEU:O	1:E:220:SER:HB2	2.12	0.49
2:F:106:LEU:HA	2:F:109:LEU:HB2	1.95	0.49
1:E:625:SER:O	1:E:628:THR:HG22	2.12	0.49
1:E:613:LEU:HG	1:E:617:ASP:HB3	1.94	0.49
1:A:324:LEU:O	1:A:333:LYS:HE3	2.12	0.49
1:A:588:ILE:HD12	1:A:593:GLY:HA2	1.94	0.49
1:A:571:TRP:CE2	1:A:578:LEU:HD12	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:ILE:HD11	1:A:394:PHE:CE2	2.45	0.48
1:C:571:TRP:CE2	1:C:578:LEU:HD12	2.48	0.48
1:C:195:LYS:HB3	1:C:196:PRO:HD3	1.95	0.48
1:C:740:GLN:OE1	1:C:754:ILE:CD1	2.61	0.48
1:A:549:LYS:HD3	1:A:554:LEU:HD21	1.95	0.48
2:D:58:LYS:HE3	2:D:173:TYR:OH	2.13	0.48
1:C:561:PHE:CZ	1:C:565:LYS:HD3	2.48	0.48
1:E:655:LYS:HA	1:E:691:SER:O	2.14	0.48
2:F:120:MET:CB	2:F:168:ILE:HD12	2.44	0.48
1:C:602:VAL:CG1	1:C:606:GLN:HG2	2.43	0.48
1:C:694:LYS:HD3	1:C:784:SER:CB	2.44	0.48
1:E:351:ARG:HG3	1:E:399:VAL:CG1	2.43	0.48
1:E:195:LYS:HB3	1:E:196:PRO:HD3	1.95	0.48
1:E:686:LEU:H	1:E:687:GLY:HA2	1.78	0.48
1:A:571:TRP:CD2	1:A:578:LEU:HD12	2.49	0.47
1:C:628:THR:HG22	1:C:630:ALA:H	1.79	0.47
1:A:621:GLN:NE2	1:A:622:GLU:OE2	2.46	0.47
2:B:173:TYR:CG	2:B:173:TYR:O	2.67	0.47
2:B:28:LEU:HD11	2:B:49:ALA:HB3	1.96	0.47
1:A:695:LEU:HD23	1:A:782:MET:HE2	1.96	0.47
1:C:571:TRP:CD2	1:C:578:LEU:HD12	2.49	0.47
1:A:356:THR:HG21	1:A:546:VAL:HG12	1.95	0.47
2:B:99:TYR:O	2:B:102:VAL:HG22	2.15	0.47
1:E:694:LYS:HD3	1:E:784:SER:HB2	1.96	0.47
1:E:571:TRP:CD2	1:E:578:LEU:HD12	2.49	0.47
1:E:684:ARG:NE	1:E:684:ARG:CA	2.74	0.47
1:C:405:GLU:HG3	1:C:534:PRO:HG3	1.97	0.47
1:E:746:PRO:O	1:E:749:HIS:HB2	2.15	0.47
2:D:28:LEU:HD11	2:D:49:ALA:HB3	1.96	0.47
3:C:2002:093:CAE	3:C:2002:093:CAD	2.91	0.47
2:B:38:LEU:HA	4:B:2000:GSP:O2'	2.15	0.46
1:E:657:ARG:HD3	1:E:657:ARG:HA	1.59	0.46
1:E:680:SER:HB2	1:E:747:CYS:O	2.15	0.46
2:B:17:ILE:HD13	2:B:109:LEU:HD11	1.97	0.46
2:B:91:TYR:HB2	2:B:98:THR:HG23	1.96	0.46
1:E:236:LEU:O	1:E:240:ILE:HG13	2.16	0.46
1:E:686:LEU:HB2	1:E:687:GLY:C	2.35	0.46
1:A:729:MET:CE	1:A:758:LYS:HA	2.45	0.46
2:F:28:LEU:HD11	2:F:49:ALA:HB3	1.96	0.46
1:C:191:GLY:HA3	1:C:232:ARG:HH21	1.80	0.46
2:B:120:MET:HB2	2:B:168:ILE:HD12	1.97	0.46
1:C:394:PHE:O	1:C:396:THR:N	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:177:PRO:CB	1:C:739:MET:HE1	2.40	0.46
1:E:684:ARG:HG3	1:E:684:ARG:O	2.16	0.46
1:E:752:SER:HB3	1:E:755:ARG:NH2	2.30	0.46
1:C:729:MET:CE	1:C:758:LYS:HA	2.46	0.46
1:E:523:GLN:HA	1:E:526:VAL:HG12	1.98	0.46
1:E:715:LYS:NZ	1:E:775:GLU:OE2	2.42	0.46
1:C:236:LEU:O	1:C:240:ILE:HG13	2.16	0.46
2:D:173:TYR:CG	2:D:173:TYR:O	2.69	0.46
2:D:86:GLY:HA3	2:D:172:ILE:HD11	1.98	0.45
1:A:178:GLN:NE2	1:A:739:MET:CE	2.79	0.45
1:A:178:GLN:HG3	1:A:739:MET:CE	2.47	0.45
1:A:178:GLN:NE2	1:A:739:MET:HE2	2.31	0.45
1:A:236:LEU:O	1:A:240:ILE:HG13	2.16	0.45
3:E:2002:093:CAE	3:E:2002:093:CAD	2.93	0.45
1:E:386:VAL:O	1:E:543:LEU:CD2	2.64	0.45
1:C:778:VAL:HG23	1:C:782:MET:CE	2.46	0.45
1:E:352:VAL:CG1	1:E:363:VAL:HG11	2.46	0.45
1:E:624:GLY:HA3	1:E:628:THR:HG21	1.99	0.45
2:F:109:LEU:HG	2:F:110:ARG:HG2	1.99	0.45
3:A:2002:093:CAE	3:A:2002:093:CAD	2.95	0.45
1:E:779:ASP:HB3	1:E:783:ARG:NH2	2.32	0.45
2:B:92:ASP:HB3	2:B:98:THR:HG21	2.00	0.44
1:C:682:SER:HB3	1:C:683:PRO:HD3	1.98	0.44
1:A:133:LEU:O	1:A:136:SER:OG	2.28	0.44
2:D:31:PHE:O	2:D:51:ARG:NH1	2.44	0.44
1:A:756:ASN:OD1	2:F:34:ASN:ND2	2.50	0.44
1:E:686:LEU:HB2	1:E:687:GLY:HA2	1.99	0.44
1:C:549:LYS:HE3	1:C:552:ASP:OD2	2.17	0.44
1:E:752:SER:CB	1:E:755:ARG:CZ	2.95	0.44
1:C:726:ARG:NH2	1:C:762:HIS:O	2.50	0.44
2:D:21:GLY:O	4:D:2000:GSP:H5'1	2.17	0.44
1:E:726:ARG:HA	1:E:763:MET:CE	2.45	0.44
1:E:176:LEU:N	1:E:177:PRO:CD	2.81	0.44
2:F:178:GLN:O	2:F:182:SER:N	2.51	0.44
1:C:342:SER:OG	1:C:368:HIS:CD2	2.71	0.44
2:D:181:MET:HA	2:D:181:MET:HE2	1.97	0.44
2:F:174:ARG:O	2:F:178:GLN:NE2	2.51	0.43
1:A:235:LYS:HG2	1:A:236:LEU:N	2.33	0.43
2:F:86:GLY:HA3	2:F:172:ILE:HD11	2.01	0.43
1:A:783:ARG:HD3	2:F:170:THR:HG21	1.99	0.43
1:A:176:LEU:N	1:A:177:PRO:CD	2.81	0.43
2:B:92:ASP:H	2:B:98:THR:CG2	2.30	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:176:LEU:N	1:C:177:PRO:CD	2.82	0.43
2:B:125:LYS:HG2	4:B:2000:GSP:C6	2.53	0.43
1:E:682:SER:CB	1:E:684:ARG:NH1	2.82	0.43
1:A:352:VAL:HG23	1:A:363:VAL:HB	2.00	0.43
1:A:576:VAL:HG12	1:A:578:LEU:HG	2.01	0.43
1:E:512:ASP:OD1	1:E:512:ASP:N	2.52	0.43
2:D:110:ARG:NH1	2:D:117:ILE:HG22	2.34	0.43
2:D:170:THR:O	2:D:174:ARG:HG3	2.19	0.43
1:E:639:VAL:HG13	1:E:714:TYR:HB2	2.01	0.43
2:F:38:LEU:HA	4:F:2000:GSP:O2'	2.19	0.43
1:E:139:PHE:CD1	1:E:143:MET:HE2	2.52	0.42
1:A:624:GLY:HA3	1:A:628:THR:HG21	2.00	0.42
2:B:88:LEU:HD21	2:B:120:MET:HE2	2.01	0.42
2:F:23:GLY:HA2	4:F:2000:GSP:O1A	2.18	0.42
1:A:589:SER:OG	1:A:591:ASP:HB2	2.19	0.42
1:A:772:LEU:HG	1:A:776:GLN:NE2	2.35	0.42
1:E:686:LEU:HB2	1:E:688:PHE:H	1.81	0.42
1:C:598:VAL:N	3:C:2002:093:HAK	2.11	0.42
1:C:394:PHE:C	1:C:396:THR:H	2.23	0.42
1:E:686:LEU:CD1	1:E:688:PHE:CD2	2.91	0.42
1:C:576:VAL:HG12	1:C:578:LEU:HG	2.01	0.42
1:C:755:ARG:HD2	1:C:755:ARG:HA	1.82	0.42
2:D:120:MET:HB2	2:D:168:ILE:HD12	2.01	0.42
1:E:683:PRO:O	1:E:684:ARG:CB	2.68	0.42
1:C:552:ASP:O	1:C:554:LEU:HD12	2.20	0.42
2:D:110:ARG:NH2	2:D:117:ILE:HG22	2.35	0.42
1:E:232:ARG:O	1:E:235:LYS:HG3	2.19	0.42
2:B:86:GLY:HA3	2:B:172:ILE:HD11	2.01	0.42
1:C:765:MET:HB3	1:C:770:LEU:HD12	2.02	0.42
1:A:711:PHE:CZ	1:A:782:MET:HE1	2.54	0.42
1:E:729:MET:HG3	1:E:761:PHE:CG	2.54	0.42
1:A:573:GLN:C	1:A:574:GLU:O	2.58	0.41
2:D:58:LYS:CE	2:D:173:TYR:OH	2.68	0.41
1:E:232:ARG:O	1:E:235:LYS:CG	2.68	0.41
2:F:120:MET:HB3	2:F:168:ILE:HD12	2.01	0.41
2:B:28:LEU:CD2	2:B:66:ASP:HB2	2.50	0.41
1:C:695:LEU:HA	1:C:695:LEU:HD12	1.94	0.41
3:E:2002:093:OAL	3:E:2002:093:SAP	2.78	0.41
1:E:386:VAL:O	1:E:543:LEU:HD23	2.20	0.41
1:A:405:GLU:HG3	1:A:534:PRO:HG3	2.02	0.41
1:A:695:LEU:HA	1:A:695:LEU:HD12	1.95	0.41
2:B:120:MET:HE1	2:B:164:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:639:VAL:HG13	1:A:714:TYR:HB2	2.03	0.41
1:E:513:PRO:CG	1:E:514:SER:H	2.33	0.41
1:E:394:PHE:O	1:E:395:ASP:CB	2.69	0.41
1:E:576:VAL:HG12	1:E:578:LEU:HG	2.02	0.41
1:A:578:LEU:CD2	1:A:717:LEU:HB3	2.51	0.41
2:F:8:TYR:HE1	2:F:52:SER:HB2	1.86	0.41
2:B:178:GLN:NE2	2:B:178:GLN:HA	2.36	0.41
1:C:365:ARG:NE	1:C:405:GLU:OE2	2.52	0.41
1:C:393:ASN:C	1:C:394:PHE:O	2.57	0.40
1:C:573:GLN:C	1:C:574:GLU:O	2.57	0.40
1:E:191:GLY:HA3	1:E:232:ARG:HH21	1.86	0.40
1:A:601:ALA:O	3:A:2002:093:HAT2	2.21	0.40
1:A:549:LYS:HD2	1:A:595:ILE:HD12	2.03	0.40
2:B:176:VAL:HG23	2:B:177:SER:N	2.35	0.40
1:C:165:PHE:CZ	1:C:197:TYR:HA	2.56	0.40
1:C:389:LEU:HD22	1:C:540:ASN:HB3	2.03	0.40
1:C:656:ASP:O	1:C:661:ASN:ND2	2.53	0.40
2:D:114:ASP:OD1	2:D:115:SER:N	2.54	0.40
2:D:10:TYR:HE2	2:D:58:LYS:HZ2	1.68	0.40
1:E:686:LEU:N	1:E:687:GLY:HA2	2.34	0.40
2:D:175:ILE:O	2:D:179:LYS:HG2	2.21	0.40
2:D:28:LEU:CD2	2:D:66:ASP:HB2	2.51	0.40
1:E:511:GLU:N	1:E:513:PRO:HD3	2.36	0.40
1:E:578:LEU:CD2	1:E:717:LEU:HB3	2.52	0.40
1:E:773:LEU:HG	1:E:777:MET:HE3	2.03	0.40
1:A:393:ASN:ND2	1:A:396:THR:HG22	2.36	0.40
1:A:522:TRP:O	1:A:526:VAL:HG23	2.22	0.40
1:C:694:LYS:HD3	1:C:784:SER:HB2	2.02	0.40
1:C:778:VAL:HG23	1:C:782:MET:HE3	2.02	0.40
2:D:137:ASP:OD1	2:D:140:ARG:NH2	2.47	0.40
1:E:686:LEU:HD22	1:E:688:PHE:CD2	2.54	0.40
1:A:194:ILE:HG22	1:A:198:ILE:HD12	2.03	0.40
1:C:327:LEU:HD21	1:C:336:ARG:NH2	2.37	0.40
1:E:394:PHE:O	1:E:395:ASP:HB2	2.21	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:340:GLU:OE1	1:A:626:TYR:OH[4_595]	2.16	0.04

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	460/566 (81%)	445 (97%)	13 (3%)	2 (0%)	43	82
1	C	466/566 (82%)	445 (96%)	16 (3%)	5 (1%)	21	60
1	E	471/566 (83%)	446 (95%)	22 (5%)	3 (1%)	33	75
2	B	171/219 (78%)	164 (96%)	6 (4%)	1 (1%)	33	75
2	D	175/219 (80%)	170 (97%)	5 (3%)	0	100	100
2	F	175/219 (80%)	168 (96%)	7 (4%)	0	100	100
All	All	1918/2355 (81%)	1838 (96%)	69 (4%)	11 (1%)	33	75

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	513	PRO
1	E	513	PRO
1	C	405	GLU
2	B	68	ALA
1	C	682	SER
1	A	405	GLU
1	C	394	PHE
1	C	741	GLN
1	A	399	VAL
1	E	348	LEU
1	E	349	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	422/508 (83%)	409 (97%)	13 (3%)	52	87
1	C	428/508 (84%)	403 (94%)	25 (6%)	28	64
1	E	429/508 (84%)	398 (93%)	31 (7%)	21	51
2	B	147/191 (77%)	139 (95%)	8 (5%)	31	68
2	D	151/191 (79%)	142 (94%)	9 (6%)	27	63
2	F	151/191 (79%)	144 (95%)	7 (5%)	37	75
All	All	1728/2097 (82%)	1635 (95%)	93 (5%)	31	68

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	148	LEU
1	A	235	LYS
1	A	318	MET
1	A	335	GLN
1	A	378	ASP
1	A	391	CYS
1	A	397	THR
1	A	565	LYS
1	A	606	GLN
1	A	613	LEU
1	A	694	LYS
1	A	739	MET
2	B	7	GLU
2	B	11	LEU
2	B	20	SER
2	B	33	ARG
2	B	46	VAL
2	B	54	GLN
2	B	55	VAL
2	B	174	ARG
1	C	166	CYS
1	C	235	LYS
1	C	243	ASP
1	C	318	MET
1	C	348	LEU
1	C	379	LYS
1	C	391	CYS
1	C	405	GLU
1	C	518	LEU

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Mol	Chain	Res	Type
1	C	565	LYS
1	C	603	SER
1	C	606	GLN
1	C	609	LYS
1	C	610	GLN
1	C	611	SER
1	C	617	ASP
1	C	633	SER
1	C	706	LEU
1	C	739	MET
1	C	752	SER
1	C	755	ARG
1	C	764	SER
1	C	768	GLU
1	C	775	GLU
1	C	778	VAL
2	D	7	GLU
2	D	11	LEU
2	D	20	SER
2	D	46	VAL
2	D	95	LYS
2	D	162	GLU
2	D	177	SER
2	D	181	MET
2	D	182	SER
1	E	137	LYS
1	E	145	ILE
1	E	166	CYS
1	E	216	LEU
1	E	220	SER
1	E	221	SER
1	E	235	LYS
1	E	243	ASP
1	E	318	MET
1	E	339	SER
1	E	379	LYS
1	E	391	CYS
1	E	392	GLU
1	E	512	ASP
1	E	543	LEU
1	E	565	LYS
1	E	598	VAL

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Mol	Chain	Res	Type
1	E	606	GLN
1	E	609	LYS
1	E	612	GLN
1	E	613	LEU
1	E	633	SER
1	E	680	SER
1	E	682	SER
1	E	684	ARG
1	E	685	ASN
1	E	737	GLU
1	E	739	MET
1	E	744	GLN
1	E	775	GLU
1	E	776	GLN
2	F	20	SER
2	F	46	VAL
2	F	95	LYS
2	F	104	ARG
2	F	162	GLU
2	F	174	ARG
2	F	177	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	ASN
1	A	540	ASN
1	A	606	GLN
1	A	776	GLN
2	B	178	GLN
1	C	185	HIS
1	C	540	ASN
1	C	612	GLN
1	E	150	ASN
1	E	185	HIS
1	E	204	GLN
1	E	335	GLN
1	E	368	HIS
1	E	540	ASN
1	E	566	GLN
1	E	728	HIS
2	F	34	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	093	A	2002	-	25,25,25	4.23	9 (36%)	33,36,36	4.74	16 (48%)
4	GSP	B	2000	5	34,34,34	1.55	7 (20%)	52,54,54	3.47	13 (25%)
3	093	C	2002	1	25,25,25	3.72	7 (28%)	33,36,36	5.13	17 (51%)
4	GSP	D	2000	5	34,34,34	1.51	7 (20%)	52,54,54	3.24	18 (34%)
3	093	E	2002	-	25,25,25	3.69	9 (36%)	33,36,36	6.58	11 (33%)
4	GSP	F	2000	5	34,34,34	1.59	6 (17%)	52,54,54	3.40	17 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	093	A	2002	-	-	0/17/19/19	0/2/2/2
4	GSP	B	2000	5	-	0/21/38/38	0/3/3/3
3	093	C	2002	1	-	0/17/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GSP	D	2000	5	-	0/21/38/38	0/3/3/3
3	093	E	2002	-	-	0/17/19/19	0/2/2/2
4	GSP	F	2000	5	-	0/21/38/38	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	093	CAI-SAP	-15.65	1.55	1.75
3	C	2002	093	CAI-SAP	-12.96	1.58	1.75
3	E	2002	093	CAI-SAP	-12.45	1.59	1.75
3	A	2002	093	CAQ-SAP	-7.70	1.60	1.73
3	C	2002	093	CAQ-SAP	-7.62	1.60	1.73
3	C	2002	093	CAJ-NAK	7.58	1.47	1.38
3	E	2002	093	CAJ-NAK	7.49	1.47	1.38
3	A	2002	093	CAJ-NAK	7.42	1.47	1.38
3	E	2002	093	CAQ-SAP	-6.31	1.62	1.73
3	E	2002	093	CAH-CAI	4.62	1.52	1.48
3	A	2002	093	SAN-NAU	4.39	1.67	1.61
4	F	2000	GSP	C5-N7	-4.34	1.32	1.38
3	A	2002	093	CAQ-NAR	4.31	1.45	1.32
3	E	2002	093	CAQ-NAR	4.10	1.45	1.32
3	C	2002	093	CAQ-NAR	3.85	1.44	1.32
4	B	2000	GSP	C4-N9	-3.73	1.32	1.37
4	F	2000	GSP	C4-N9	-3.52	1.32	1.37
4	D	2000	GSP	C5-N7	-3.36	1.34	1.38
4	D	2000	GSP	C4-N9	-3.32	1.32	1.37
3	E	2002	093	CAS-NAR	3.29	1.44	1.38
3	C	2002	093	CAS-NAR	3.24	1.44	1.38
4	B	2000	GSP	C5-N7	-3.22	1.34	1.38
3	A	2002	093	CAV-CAW	-3.19	1.38	1.50
4	F	2000	GSP	O4'-C1'	3.11	1.45	1.41
4	D	2000	GSP	C5-C4	3.04	1.47	1.40
3	A	2002	093	CAS-NAR	3.01	1.44	1.38
3	C	2002	093	CAH-CAI	2.96	1.51	1.48
3	A	2002	093	CAT-CAS	2.93	1.53	1.49
4	F	2000	GSP	C2-N2	2.90	1.36	1.32
4	B	2000	GSP	C6-N1	-2.79	1.32	1.36
4	B	2000	GSP	C5-C4	2.71	1.46	1.40
3	E	2002	093	CAT-CAS	2.62	1.53	1.49
3	C	2002	093	CAT-CAS	2.57	1.52	1.49
4	D	2000	GSP	C2-N2	2.51	1.36	1.32
3	E	2002	093	OAM-SAN	-2.41	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2000	GSP	C2-N3	2.40	1.36	1.33
4	D	2000	GSP	C2-N3	2.32	1.36	1.33
4	D	2000	GSP	PG-O3G	2.31	1.63	1.55
4	F	2000	GSP	PG-O3G	2.26	1.63	1.55
4	D	2000	GSP	PG-S1G	2.25	1.95	1.90
3	A	2002	093	OAM-SAN	-2.24	1.41	1.43
4	B	2000	GSP	PG-S1G	2.19	1.95	1.90
4	B	2000	GSP	PG-O3G	2.09	1.62	1.55
4	B	2000	GSP	C2-N3	2.06	1.36	1.33
3	E	2002	093	CAB-CAF	2.03	1.43	1.40

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2002	093	CAQ-NAK-CAJ	-30.61	109.56	112.36
3	A	2002	093	OAO-SAN-OAM	-19.44	93.89	119.55
4	B	2000	GSP	C6-C5-N7	19.23	136.73	134.14
4	F	2000	GSP	O3B-PG-S1G	-18.42	106.36	114.53
3	C	2002	093	CAQ-NAK-CAJ	-18.36	110.68	112.36
3	C	2002	093	OAO-SAN-OAM	-16.71	97.50	119.55
3	E	2002	093	OAO-SAN-OAM	-15.72	98.81	119.55
4	D	2000	GSP	C6-C5-N7	13.63	135.98	134.14
4	D	2000	GSP	O2G-PG-S1G	-11.29	100.83	112.73
3	A	2002	093	CAQ-NAK-CAJ	-10.14	111.43	112.36
3	E	2002	093	CAI-CAJ-NAK	7.73	110.28	106.87
3	A	2002	093	CAE-CAJ-CAI	-7.25	125.60	131.22
4	B	2000	GSP	O2G-PG-S1G	-7.07	105.28	112.73
3	A	2002	093	CAT-CAS-NAR	6.46	121.08	114.80
3	E	2002	093	CAE-CAJ-CAI	-6.07	126.51	131.22
4	D	2000	GSP	C5-C4-N3	-6.06	119.09	126.07
4	B	2000	GSP	C5-C4-N3	-6.04	119.11	126.07
3	C	2002	093	CAE-CAJ-CAI	-5.80	126.72	131.22
4	F	2000	GSP	N3-C4-N9	5.75	135.34	126.91
4	F	2000	GSP	C5-C4-N3	-5.56	119.66	126.07
3	C	2002	093	OAM-SAN-CAF	5.49	116.47	107.68
3	E	2002	093	OAO-SAN-NAU	5.46	116.21	107.06
4	B	2000	GSP	PB-O3B-PG	-5.26	114.00	132.05
4	D	2000	GSP	N3-C4-N9	5.25	134.61	126.91
3	C	2002	093	OAO-SAN-NAU	5.12	115.65	107.06
4	B	2000	GSP	N3-C4-N9	5.06	134.34	126.91
4	D	2000	GSP	O3B-PG-S1G	4.92	116.71	114.53
3	C	2002	093	CAI-CAJ-NAK	4.87	109.02	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2002	093	CAH-CAI-SAP	4.80	125.70	116.31
3	A	2002	093	OAO-SAN-NAU	4.74	115.01	107.06
3	E	2002	093	CAT-CAS-NAR	4.61	119.28	114.80
3	A	2002	093	CAI-CAJ-NAK	4.59	108.89	106.87
3	A	2002	093	OAM-SAN-NAU	4.56	114.70	107.06
4	D	2000	GSP	PA-O3A-PB	-4.46	119.58	131.93
4	F	2000	GSP	PA-O3A-PB	-4.39	119.79	131.93
4	D	2000	GSP	C2-N3-C4	4.34	120.50	115.30
4	F	2000	GSP	C8-N9-C4	4.33	110.48	106.96
3	A	2002	093	OAO-SAN-CAF	4.31	114.58	107.68
3	C	2002	093	CAT-CAS-NAR	4.17	118.85	114.80
3	C	2002	093	OAO-SAN-CAF	4.15	114.32	107.68
3	C	2002	093	CAB-CAF-SAN	-4.14	120.71	123.39
4	B	2000	GSP	C2-N3-C4	4.08	120.19	115.30
4	F	2000	GSP	O2G-PG-S1G	-3.93	108.58	112.73
4	F	2000	GSP	C2-N3-C4	3.93	120.01	115.30
4	F	2000	GSP	C6-N1-C2	3.90	122.40	120.20
4	F	2000	GSP	O3G-PG-O2G	3.76	113.50	105.97
4	B	2000	GSP	O3B-PG-S1G	-3.75	112.86	114.53
3	C	2002	093	CAH-CAI-SAP	3.72	123.59	116.31
4	D	2000	GSP	C6-N1-C2	3.61	122.24	120.20
4	F	2000	GSP	PB-O3B-PG	-3.59	119.73	132.05
3	A	2002	093	OAM-SAN-CAF	3.42	113.16	107.68
3	A	2002	093	OAX-CAW-CAV	-3.41	98.72	111.69
3	E	2002	093	CAF-CAB-CL	3.41	124.27	121.60
4	B	2000	GSP	PA-O3A-PB	-3.41	122.49	131.93
3	E	2002	093	CAD-CAH-CAI	-3.39	118.33	120.94
3	E	2002	093	OAM-SAN-CAF	3.36	113.06	107.68
3	C	2002	093	CAC-CAB-CAF	3.29	122.01	120.09
4	D	2000	GSP	C4-C5-N7	-3.15	106.36	109.41
4	F	2000	GSP	C6-C5-N7	3.15	134.56	134.14
4	F	2000	GSP	O3A-PB-O3B	-3.15	95.27	101.66
4	B	2000	GSP	O3A-PB-O3B	3.12	108.00	101.66
3	C	2002	093	CAF-SAN-NAU	-3.10	103.89	107.79
3	C	2002	093	CAG-CAH-CAI	-3.07	118.58	120.94
4	D	2000	GSP	PB-O3B-PG	-3.05	121.58	132.05
4	D	2000	GSP	C3'-C2'-C1'	3.05	105.70	100.92
3	A	2002	093	CAH-CAI-SAP	3.02	122.22	116.31
3	C	2002	093	CAF-CAB-CL	-2.96	119.27	121.60
4	F	2000	GSP	C2'-C1'-N9	-2.95	105.30	113.35
4	F	2000	GSP	O4'-C1'-N9	2.94	114.50	108.10
4	B	2000	GSP	C4-C5-N7	-2.94	106.57	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	093	CAD-CAH-CAG	2.82	122.03	118.19
3	A	2002	093	OAL-CAS-NAR	-2.82	118.52	123.61
3	A	2002	093	CAD-CAH-CAG	2.80	121.99	118.19
4	B	2000	GSP	C8-N9-C4	2.79	109.23	106.96
3	E	2002	093	OAQ-SAN-CAF	2.78	112.13	107.68
4	D	2000	GSP	C8-N9-C4	2.64	109.10	106.96
4	D	2000	GSP	N2-C2-N3	-2.61	116.89	120.28
4	F	2000	GSP	C4'-O4'-C1'	-2.58	106.88	109.72
3	A	2002	093	CAG-CAH-CAI	-2.57	118.96	120.94
3	A	2002	093	CAD-CAH-CAI	-2.56	118.97	120.94
4	B	2000	GSP	O3G-PG-S1G	-2.56	110.03	112.73
4	D	2000	GSP	O3G-PG-S1G	-2.54	110.05	112.73
3	A	2002	093	CAE-CAJ-NAK	2.43	125.50	122.64
4	D	2000	GSP	C4'-O4'-C1'	2.42	112.38	109.72
4	D	2000	GSP	C2'-C3'-C4'	2.38	107.39	102.64
3	C	2002	093	CAQ-NAR-CAS	2.29	122.79	116.09
4	F	2000	GSP	C4-C5-N7	-2.25	107.24	109.41
4	D	2000	GSP	N2-C2-N1	2.23	120.21	117.82
4	F	2000	GSP	O3'-C3'-C2'	-2.21	104.69	111.83
4	B	2000	GSP	C6-N1-C2	2.15	121.42	120.20
4	D	2000	GSP	O3G-PG-O2G	2.07	110.12	105.97
3	C	2002	093	CAD-CAH-CAI	-2.04	119.37	120.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å ²)	Q<0.9
1	A	470/566 (83%)	0.10	5 (1%) 77 85	39, 61, 99, 117	0
1	C	476/566 (84%)	0.07	7 (1%) 70 81	38, 61, 98, 146	0
1	E	479/566 (84%)	0.20	24 (5%) 28 35	42, 67, 110, 171	0
2	B	173/219 (78%)	0.28	4 (2%) 57 68	53, 82, 113, 139	0
2	D	177/219 (80%)	0.34	12 (6%) 17 22	45, 65, 106, 149	0
2	F	177/219 (80%)	0.18	4 (2%) 57 68	41, 65, 109, 136	0
All	All	1952/2355 (82%)	0.16	56 (2%) 49 59	38, 65, 106, 171	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	686	LEU	5.0
1	E	401	ALA	4.0
1	E	687	GLY	3.8
1	C	683	PRO	3.7
1	E	615	LEU	3.3
1	E	688	PHE	3.2
2	D	181	MET	3.1
2	B	99	TYR	3.1
2	D	104	ARG	3.0
1	E	403	ILE	3.0
1	E	682	SER	2.9
2	D	102	VAL	2.9
2	D	179	LYS	2.9
1	E	784	SER	2.8
2	D	182	SER	2.8
1	E	137	LYS	2.7
2	D	175	ILE	2.7
1	E	685	ASN	2.7
1	E	404	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	346	HIS	2.7
1	E	402	ARG	2.6
1	C	243	ASP	2.6
1	E	626	TYR	2.5
2	D	142	PHE	2.5
2	B	119	ILE	2.5
2	D	116	ASN	2.5
2	D	103	GLU	2.4
2	F	180	GLN	2.4
1	E	684	ARG	2.4
1	C	129	TRP	2.4
1	C	137	LYS	2.3
1	E	350	ALA	2.3
1	A	607	VAL	2.3
1	E	398	SER	2.3
1	E	348	LEU	2.3
1	A	604	ILE	2.3
2	D	180	GLN	2.2
1	E	351	ARG	2.2
1	E	619	PHE	2.2
2	B	80	TYR	2.2
2	B	105	TRP	2.2
1	C	612	GLN	2.2
1	E	396	THR	2.2
1	A	406	ASN	2.2
1	C	784	SER	2.1
2	D	140	ARG	2.1
1	E	537	HIS	2.1
1	A	350	ALA	2.1
1	C	691	SER	2.1
2	D	119	ILE	2.1
1	E	236	LEU	2.1
1	A	519	LYS	2.0
2	F	115	SER	2.0
2	F	141	ALA	2.0
2	F	111	ASP	2.0
1	E	693	PHE	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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	093	E	2002	24/24	0.21	1.04	65,72,83,124	0
3	093	A	2002	24/24	0.23	0.72	57,75,105,130	2
3	093	C	2002	24/24	0.20	0.50	57,66,75,123	0
4	GSP	D	2000	32/32	0.16	-0.31	46,55,65,72	0
4	GSP	B	2000	32/32	0.13	-1.09	47,58,76,86	0
4	GSP	F	2000	32/32	0.13	-1.25	43,47,58,61	0
5	MG	F	2001	1/1	0.12	-1.31	59,59,59,59	0
5	MG	D	2001	1/1	0.11	-2.88	72,72,72,72	0
5	MG	B	2001	1/1	0.04	-4.62	87,87,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.