Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:37 PM GMT

PDB ID	:	4FIR
Title	:	Crystal structure of pyridoxal biosynthesis lyase PdxS from Pyrococcus
Authors	:	Matsuura, A.; Yoon, J.Y.; Yoon, H.J.; Lee, H.H.; Suh, S.W.
Deposited on	:	2012-06-11
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

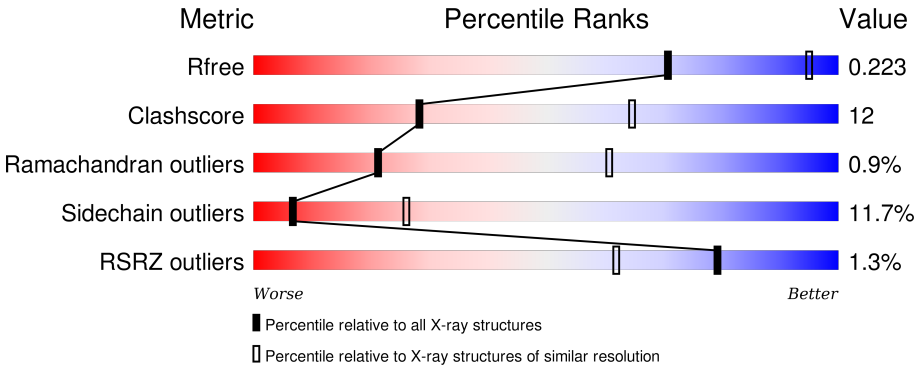
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	335	72% 23%
1	B	335	70% 24% 5%
1	C	335	71% 24% 5%
1	D	335	72% 23%
1	E	335	72% 23%

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Mol	Chain	Length	Quality of chain
1	F	335	2% 71% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	R5P	F	401	-	-	X	-

2 Entry composition

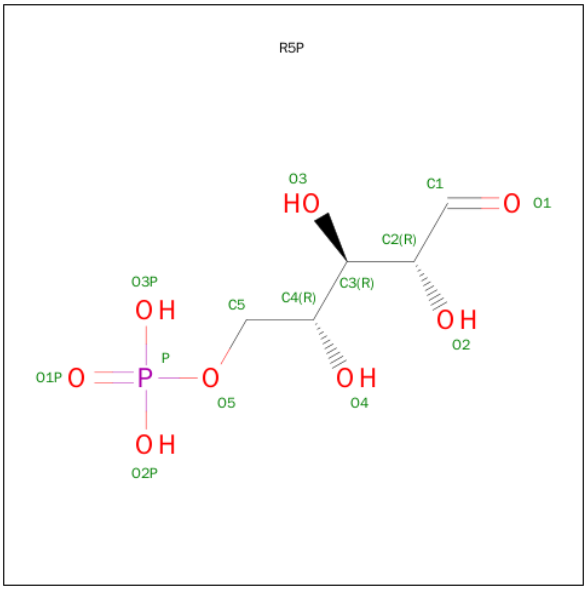
There are 3 unique types of molecules in this entry. The entry contains 15269 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyridoxal biosynthesis lyase pdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2520	1600	442	460	18			
1	B	333	Total	C	N	O	S	0	0	0
			2519	1599	442	460	18			
1	C	333	Total	C	N	O	S	0	0	0
			2520	1600	442	460	18			
1	D	333	Total	C	N	O	S	0	0	0
			2520	1600	442	460	18			
1	E	333	Total	C	N	O	S	0	0	0
			2520	1600	442	460	18			
1	F	333	Total	C	N	O	S	0	0	0
			2520	1600	442	460	18			

- Molecule 2 is SUGAR (RIBOSE-5-PHOSPHATE) (three-letter code: R5P) (formula: $C_5H_{11}O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 13 5 7 1	0	0
2	B	1	Total C O P 13 5 7 1	0	0
2	C	1	Total C O P 13 5 7 1	0	0
2	D	1	Total C O P 13 5 7 1	0	0
2	E	1	Total C O P 13 5 7 1	0	0
2	F	1	Total C O P 13 5 7 1	0	0

- Molecule 3 is water.

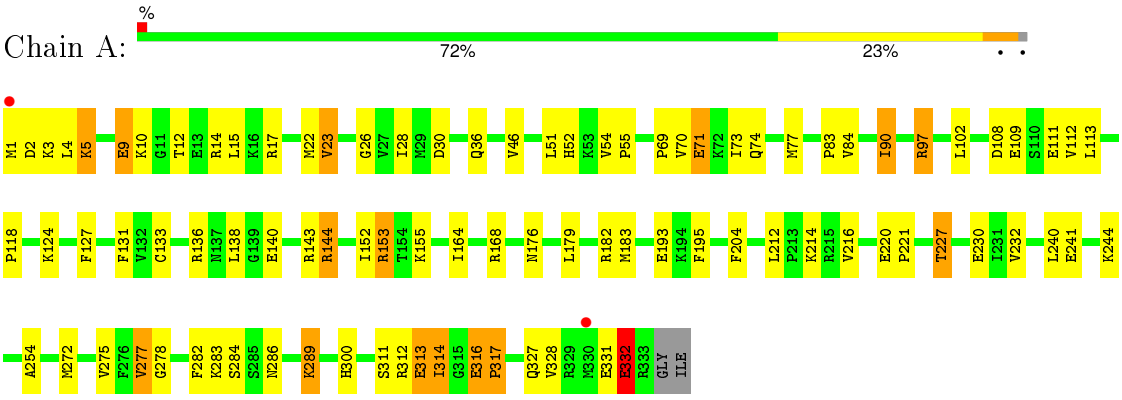
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total O 14 14	0	0
3	B	7	Total O 7 7	0	0
3	C	8	Total O 8 8	0	0
3	D	13	Total O 13 13	0	0
3	E	14	Total O 14 14	0	0
3	F	16	Total O 16 16	0	0

3 Residue-property plots (i)

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.

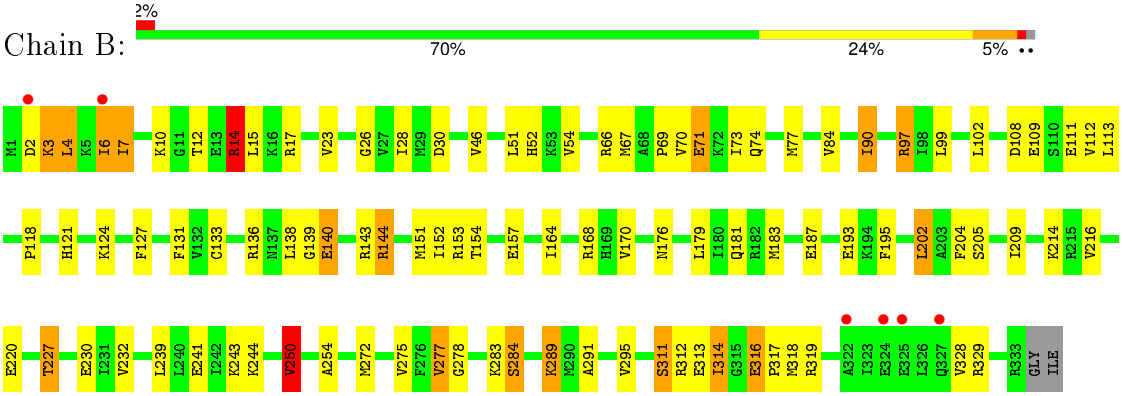
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain A:



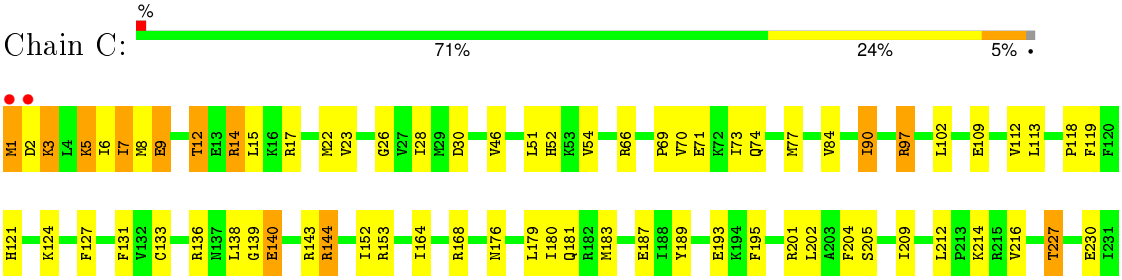
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

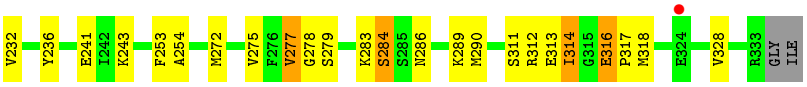
Chain B:



- Molecule 1: Pyridoxal biosynthesis lyase pdxS

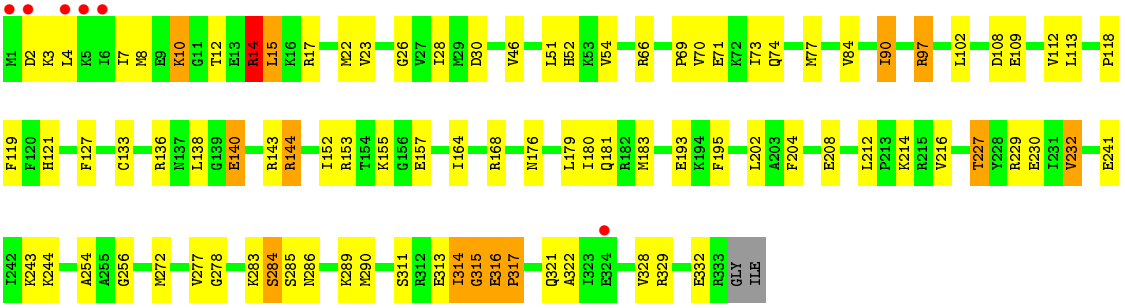
Chain C:





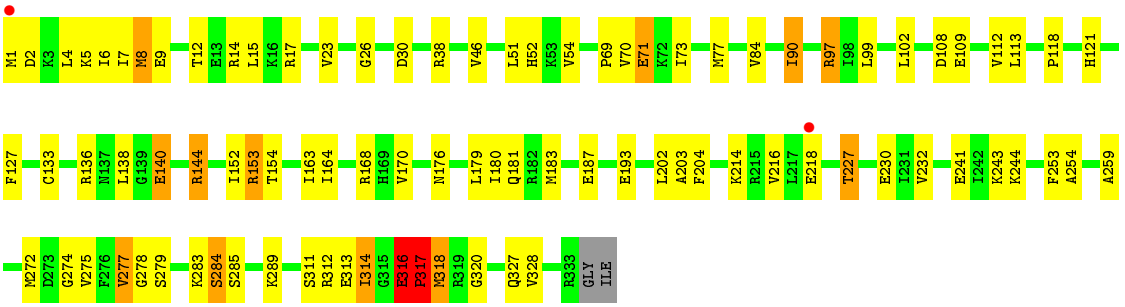
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain D:



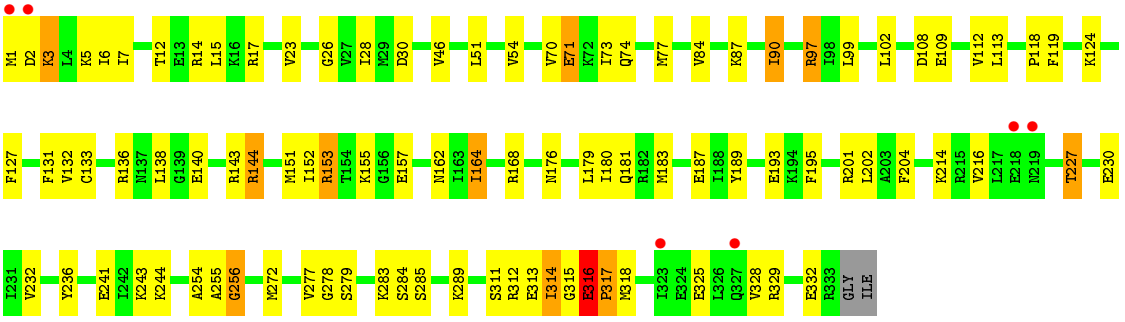
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain E:



• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.16Å 179.06Å 109.36Å 90.00° 102.53° 90.00°	Depositor
Resolution (Å)	29.84 – 3.10 29.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.84-3.10) 98.1 (29.84-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.77 (at 3.11Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.185 , 0.227 0.184 , 0.223	Depositor DCC
R_{free} test set	1983 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 39506 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15269	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R5P

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	0.61	1/2559 (0.0%)	0.76	0/3450
1	B	0.61	0/2558	0.80	5/3448 (0.1%)
1	C	0.59	0/2559	0.78	2/3450 (0.1%)
1	D	0.61	0/2559	0.83	4/3450 (0.1%)
1	E	0.65	1/2559 (0.0%)	0.79	1/3450 (0.0%)
1	F	0.61	2/2559 (0.1%)	0.79	3/3450 (0.1%)
All	All	0.61	4/15353 (0.0%)	0.79	15/20698 (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	4
1	B	0	2
1	D	0	4
1	E	0	3
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	317	PRO	CA-CB	-7.17	1.39	1.53
1	A	313	GLU	CB-CG	5.51	1.62	1.52
1	F	316	GLU	CB-CG	5.30	1.62	1.52
1	F	316	GLU	CG-CD	5.20	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	14	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	C	317	PRO	N-CA-CB	8.21	113.15	103.30
1	F	317	PRO	N-CA-CB	7.89	112.77	103.30
1	D	14	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	B	317	PRO	N-CA-CB	7.23	111.97	103.30
1	B	250	VAL	CG1-CB-CG2	6.97	122.05	110.90
1	E	317	PRO	N-CA-CB	6.13	110.65	103.30
1	C	14	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	15	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	F	318	MET	C-N-CA	-5.34	108.36	121.70
1	F	256	GLY	N-CA-C	5.25	126.22	113.10
1	B	202	LEU	CB-CG-CD2	5.20	119.84	111.00
1	B	14	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	317	PRO	N-CA-CB	5.13	109.46	103.30
1	B	311	SER	N-CA-CB	-5.06	102.92	110.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	HIS	Mainchain
1	A	327	GLN	Mainchain
1	A	331	GLU	Mainchain
1	A	332	GLU	Mainchain
1	B	319	ARG	Peptide
1	B	66	ARG	Peptide
1	D	315	GLY	Mainchain,Peptide
1	D	316	GLU	Peptide
1	D	321	GLN	Peptide
1	E	316	GLU	Peptide
1	E	318	MET	Peptide
1	E	327	GLN	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	2520	0	2551	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2519	0	2550	69	0
1	C	2520	0	2552	66	0
1	D	2520	0	2551	65	0
1	E	2520	0	2552	51	1
1	F	2520	0	2553	63	0
2	A	13	0	8	1	0
2	B	13	0	8	1	0
2	C	13	0	8	1	0
2	D	13	0	8	1	0
2	E	13	0	8	1	0
2	F	13	0	8	7	0
3	A	14	0	0	0	0
3	B	7	0	0	0	0
3	C	8	0	0	1	0
3	D	13	0	0	0	0
3	E	14	0	0	0	0
3	F	16	0	0	3	0
All	All	15269	0	15357	353	1

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 12.

All (353) 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:D:286:ASN:N	1:D:316:GLU:OE1	1.91	1.02
1:C:1:MET:SD	1:C:2:ASP:N	2.43	0.92
1:D:138:LEU:HB3	1:D:176:ASN:HD22	1.34	0.91
1:B:138:LEU:HB3	1:B:176:ASN:HD22	1.37	0.89
1:D:14:ARG:HG2	1:D:14:ARG:HH11	1.40	0.87
1:A:138:LEU:HB3	1:A:176:ASN:HD22	1.41	0.85
1:D:285:SER:H	1:D:316:GLU:HG2	1.40	0.84
1:B:14:ARG:HG2	1:B:14:ARG:HH11	1.39	0.84
1:A:227:THR:HG22	1:A:230:GLU:H	1.46	0.81
1:B:227:THR:HG22	1:B:230:GLU:H	1.44	0.80
1:E:227:THR:HG22	1:E:230:GLU:H	1.48	0.78
1:E:14:ARG:HG2	1:E:14:ARG:HH11	1.48	0.78
1:D:227:THR:HG22	1:D:230:GLU:H	1.50	0.77
1:F:14:ARG:HH11	1:F:14:ARG:HG2	1.48	0.77
1:F:227:THR:HG22	1:F:230:GLU:H	1.50	0.77
1:B:318:MET:CB	1:C:66:ARG:HH22	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:GLY:HA2	2:F:401:R5P:H51	1.65	0.76
1:B:121:HIS:CD2	1:B:144:ARG:NH1	2.54	0.75
1:C:70:VAL:HG13	1:C:102:LEU:HD21	1.69	0.74
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.52	0.74
1:C:316:GLU:HG2	3:C:507:HOH:O	1.88	0.73
1:D:70:VAL:HG13	1:D:102:LEU:HD21	1.71	0.73
1:C:227:THR:HG22	1:C:230:GLU:H	1.52	0.72
1:C:14:ARG:HH11	1:C:14:ARG:HG2	1.54	0.72
1:B:121:HIS:HD2	1:B:144:ARG:NH1	1.88	0.72
1:B:70:VAL:HG13	1:B:102:LEU:HD21	1.73	0.70
1:A:204:PHE:HB3	1:A:214:LYS:HD3	1.74	0.69
1:F:70:VAL:HG13	1:F:102:LEU:HD21	1.75	0.69
1:C:8:MET:O	1:C:12:THR:OG1	2.11	0.68
1:D:168:ARG:HB2	1:E:118:PRO:HG3	1.74	0.67
1:D:315:GLY:N	1:D:316:GLU:HG3	2.09	0.67
1:A:138:LEU:HB3	1:A:176:ASN:ND2	2.09	0.67
1:A:168:ARG:HB2	1:B:118:PRO:HG3	1.75	0.67
1:E:70:VAL:HG13	1:E:102:LEU:HD21	1.76	0.67
1:E:138:LEU:HB3	1:E:176:ASN:HD22	1.60	0.66
1:E:204:PHE:HB3	1:E:214:LYS:HD3	1.76	0.66
1:B:168:ARG:HB2	1:C:118:PRO:HG3	1.77	0.66
1:B:204:PHE:HB3	1:B:214:LYS:HD3	1.77	0.66
1:D:138:LEU:HB3	1:D:176:ASN:ND2	2.10	0.65
1:A:70:VAL:HG13	1:A:102:LEU:HD21	1.78	0.65
1:C:97:ARG:HG2	1:C:127:PHE:CE1	2.32	0.65
1:F:183:MET:HE2	1:F:187:GLU:HB3	1.77	0.65
1:B:23:VAL:HG22	1:B:46:VAL:HG23	1.80	0.64
1:F:138:LEU:HB3	1:F:176:ASN:HD22	1.63	0.63
1:E:313:GLU:O	1:E:314:ILE:HG23	1.97	0.63
1:A:118:PRO:HG3	1:F:168:ARG:HB2	1.80	0.63
1:D:285:SER:N	1:D:316:GLU:HG2	2.13	0.63
1:C:168:ARG:HB2	1:D:118:PRO:HG3	1.79	0.63
1:B:138:LEU:HB3	1:B:176:ASN:ND2	2.11	0.62
1:F:204:PHE:HB3	1:F:214:LYS:HD3	1.81	0.62
1:B:30:ASP:HB2	1:B:278:GLY:HA2	1.79	0.62
1:D:204:PHE:HB3	1:D:214:LYS:HD3	1.81	0.62
1:D:315:GLY:C	1:D:316:GLU:HG3	2.19	0.62
1:F:254:ALA:HB2	1:F:272:MET:HG3	1.80	0.62
1:E:259:ALA:HB1	1:E:317:PRO:CB	2.29	0.62
1:C:183:MET:HE2	1:C:187:GLU:HB3	1.81	0.62
1:B:97:ARG:HG2	1:B:127:PHE:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:SER:HB2	1:D:316:GLU:HB3	1.81	0.61
1:B:73:ILE:O	1:B:77:MET:HG3	2.00	0.61
1:F:73:ILE:O	1:F:77:MET:HG3	2.00	0.61
1:A:23:VAL:HG22	1:A:46:VAL:HG23	1.82	0.61
1:C:23:VAL:HG22	1:C:46:VAL:HG23	1.82	0.61
1:E:97:ARG:HG2	1:E:127:PHE:CE1	2.36	0.60
1:F:87:LYS:NZ	2:F:401:R5P:O2	2.33	0.60
1:A:254:ALA:HB2	1:A:272:MET:HG3	1.83	0.60
1:D:73:ILE:O	1:D:77:MET:HG3	2.01	0.60
1:B:121:HIS:CD2	1:B:144:ARG:CZ	2.85	0.60
1:A:26:GLY:HA3	1:A:46:VAL:HG11	1.84	0.60
1:C:138:LEU:HB3	1:C:176:ASN:HD22	1.67	0.59
1:B:90:ILE:HG23	1:B:121:HIS:ND1	2.17	0.59
1:D:23:VAL:HG22	1:D:46:VAL:HG23	1.84	0.59
1:C:316:GLU:N	1:C:316:GLU:OE1	2.35	0.59
1:E:285:SER:H	1:E:316:GLU:HB2	1.68	0.59
1:E:30:ASP:HB2	1:E:278:GLY:HA2	1.84	0.59
1:C:284:SER:HB2	1:C:316:GLU:HB2	1.83	0.58
1:D:30:ASP:HB2	1:D:278:GLY:HA2	1.84	0.58
1:D:290:MET:HB2	1:D:316:GLU:OE2	2.04	0.58
1:A:14:ARG:HG2	1:A:14:ARG:NH1	2.19	0.58
1:F:136:ARG:NH1	1:F:140:GLU:OE2	2.37	0.58
1:C:204:PHE:HB3	1:C:214:LYS:HD3	1.86	0.58
1:F:157:GLU:OE2	1:F:329:ARG:N	2.36	0.57
1:E:8:MET:SD	1:E:8:MET:N	2.77	0.57
1:A:30:ASP:HB2	1:A:278:GLY:HA2	1.85	0.57
1:E:254:ALA:HB2	1:E:272:MET:HG3	1.86	0.57
1:A:179:LEU:O	1:A:183:MET:HG3	2.04	0.57
1:E:73:ILE:O	1:E:77:MET:HG3	2.04	0.57
1:B:124:LYS:HG2	1:B:131:PHE:CD2	2.39	0.57
1:A:136:ARG:NH1	1:A:140:GLU:OE2	2.38	0.57
1:E:136:ARG:NH1	1:E:140:GLU:OE2	2.38	0.57
1:D:14:ARG:NH1	1:D:14:ARG:HG2	2.10	0.56
1:E:168:ARG:HB2	1:F:118:PRO:HG3	1.86	0.56
1:C:73:ILE:O	1:C:77:MET:HG3	2.06	0.56
1:C:133:CYS:HB3	1:C:144:ARG:HG3	1.87	0.56
1:F:97:ARG:HG2	1:F:127:PHE:CE1	2.41	0.56
1:A:73:ILE:O	1:A:77:MET:HG3	2.04	0.56
1:B:313:GLU:O	1:B:314:ILE:HG23	2.05	0.56
1:D:313:GLU:O	1:D:314:ILE:HG23	2.06	0.56
1:E:14:ARG:HG2	1:E:14:ARG:NH1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:NH1	1:C:140:GLU:OE2	2.39	0.56
1:C:30:ASP:HB2	1:C:278:GLY:HA2	1.88	0.56
1:C:313:GLU:O	1:C:314:ILE:HG23	2.06	0.55
1:D:179:LEU:O	1:D:183:MET:HG3	2.06	0.55
1:C:254:ALA:HB2	1:C:272:MET:HG3	1.88	0.55
1:B:179:LEU:O	1:B:183:MET:HG3	2.07	0.55
1:B:151:MET:HA	1:B:250:VAL:HG13	1.88	0.55
1:B:193:GLU:HA	1:B:232:VAL:HG22	1.88	0.55
1:A:55:PRO:HG2	2:A:401:R5P:H51	1.88	0.55
1:F:313:GLU:O	1:F:314:ILE:HG23	2.07	0.55
1:E:133:CYS:HB3	1:E:144:ARG:HG3	1.89	0.54
1:A:97:ARG:HG2	1:A:127:PHE:CE1	2.42	0.54
1:C:133:CYS:CB	1:C:144:ARG:HG3	2.37	0.54
1:F:279:SER:N	2:F:401:R5P:O2P	2.36	0.54
1:C:290:MET:HE3	1:C:316:GLU:HB3	1.90	0.54
1:A:77:MET:HA	1:A:84:VAL:HG21	1.89	0.54
1:B:136:ARG:NH1	1:B:140:GLU:OE2	2.41	0.54
1:C:318:MET:CB	1:D:66:ARG:HH22	2.21	0.54
1:B:157:GLU:OE2	1:B:329:ARG:N	2.39	0.54
1:D:77:MET:HA	1:D:84:VAL:HG21	1.90	0.54
1:A:133:CYS:HB3	1:A:144:ARG:HG3	1.90	0.54
1:B:254:ALA:HB2	1:B:272:MET:HG3	1.89	0.53
1:B:30:ASP:HB2	1:B:278:GLY:CA	2.37	0.53
1:D:2:ASP:HB3	1:D:4:LEU:H	1.72	0.53
1:E:193:GLU:HA	1:E:232:VAL:HG22	1.90	0.53
1:B:133:CYS:CB	1:B:144:ARG:HG3	2.39	0.53
1:B:183:MET:HE2	1:B:187:GLU:HB3	1.90	0.53
1:C:77:MET:HA	1:C:84:VAL:HG21	1.90	0.53
1:D:254:ALA:HB2	1:D:272:MET:HG3	1.90	0.53
1:B:14:ARG:HG2	1:B:14:ARG:NH1	2.16	0.53
1:C:138:LEU:HB3	1:C:176:ASN:ND2	2.24	0.53
1:C:193:GLU:HA	1:C:232:VAL:HG22	1.90	0.53
1:E:77:MET:HA	1:E:84:VAL:HG21	1.91	0.52
1:D:133:CYS:HB3	1:D:144:ARG:HG3	1.92	0.52
1:B:316:GLU:OE2	1:B:316:GLU:N	2.40	0.52
1:F:14:ARG:HG2	1:F:14:ARG:NH1	2.17	0.52
1:E:23:VAL:HG22	1:E:46:VAL:HG23	1.92	0.52
1:F:133:CYS:HB3	1:F:144:ARG:HG3	1.92	0.52
1:F:26:GLY:HA3	1:F:46:VAL:HG11	1.92	0.52
1:A:133:CYS:CB	1:A:144:ARG:HG3	2.38	0.52
1:D:133:CYS:CB	1:D:144:ARG:HG3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:SER:OG	1:D:316:GLU:CD	2.49	0.52
1:F:23:VAL:HG11	1:F:28:ILE:HD11	1.92	0.52
1:F:87:LYS:HZ1	2:F:401:R5P:C2	2.23	0.51
1:F:77:MET:HA	1:F:84:VAL:HG21	1.92	0.51
1:D:256:GLY:HA2	2:D:401:R5P:H51	1.92	0.51
1:D:97:ARG:HG2	1:D:127:PHE:CE1	2.45	0.51
1:F:193:GLU:HA	1:F:232:VAL:HG22	1.92	0.51
1:F:23:VAL:HG22	1:F:46:VAL:HG23	1.91	0.51
1:F:30:ASP:HB2	1:F:278:GLY:HA2	1.91	0.51
1:D:26:GLY:HA3	1:D:46:VAL:HG11	1.91	0.51
1:D:4:LEU:O	1:D:8:MET:HB3	2.10	0.51
1:A:1:MET:O	1:A:5:LYS:HB2	2.10	0.51
1:E:183:MET:HE2	1:E:187:GLU:HB3	1.93	0.51
1:D:315:GLY:C	1:D:316:GLU:CG	2.78	0.51
1:E:26:GLY:HA3	1:E:46:VAL:HG11	1.92	0.51
1:C:284:SER:HB2	1:C:316:GLU:CB	2.41	0.50
1:F:133:CYS:CB	1:F:144:ARG:HG3	2.41	0.50
1:D:157:GLU:OE2	1:D:329:ARG:N	2.44	0.50
1:E:138:LEU:HB3	1:E:176:ASN:ND2	2.24	0.50
1:D:136:ARG:NH1	1:D:140:GLU:OE2	2.44	0.50
1:D:193:GLU:HA	1:D:232:VAL:HG22	1.93	0.50
1:A:26:GLY:HA3	1:A:46:VAL:CG1	2.40	0.50
1:A:124:LYS:HG2	1:A:131:PHE:CD2	2.47	0.50
1:F:325:GLU:O	3:F:511:HOH:O	2.18	0.50
1:D:315:GLY:H	1:D:316:GLU:HG3	1.76	0.50
1:E:30:ASP:HB2	1:E:278:GLY:CA	2.42	0.50
1:B:3:LYS:HG3	1:B:4:LEU:HD22	1.93	0.50
1:A:313:GLU:O	1:A:314:ILE:HG23	2.11	0.49
1:F:138:LEU:HB3	1:F:176:ASN:ND2	2.25	0.49
1:C:2:ASP:O	1:C:6:ILE:HG12	2.12	0.49
1:E:179:LEU:O	1:E:183:MET:HG3	2.13	0.49
1:B:133:CYS:HB3	1:B:144:ARG:HG3	1.93	0.49
1:C:9:GLU:HA	1:C:12:THR:OG1	2.13	0.49
1:B:284:SER:HA	1:B:316:GLU:HB2	1.94	0.49
1:F:256:GLY:CA	2:F:401:R5P:H51	2.37	0.49
1:B:14:ARG:CG	1:B:14:ARG:HH11	2.19	0.49
1:C:26:GLY:HA3	1:C:46:VAL:HG11	1.95	0.49
1:C:181:GLN:HA	1:C:243:LYS:HG3	1.95	0.49
1:C:183:MET:HE3	1:D:212:LEU:HD11	1.95	0.49
1:D:30:ASP:HB2	1:D:278:GLY:CA	2.43	0.49
1:E:133:CYS:CB	1:E:144:ARG:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLN:HA	1:D:243:LYS:HG3	1.94	0.48
1:C:97:ARG:HG2	1:C:127:PHE:CZ	2.47	0.48
1:B:23:VAL:HG11	1:B:28:ILE:HD11	1.96	0.48
1:F:124:LYS:HG2	1:F:131:PHE:CD2	2.49	0.48
1:F:176:ASN:ND2	3:F:516:HOH:O	2.45	0.48
1:A:30:ASP:HB2	1:A:278:GLY:CA	2.44	0.48
1:F:285:SER:H	1:F:316:GLU:HB2	1.79	0.48
1:D:155:LYS:HZ3	1:D:332:GLU:CB	2.27	0.48
1:C:3:LYS:O	1:C:7:ILE:HD13	2.13	0.48
1:D:284:SER:HB2	1:D:316:GLU:CB	2.43	0.48
1:B:77:MET:HA	1:B:84:VAL:HG21	1.93	0.48
1:D:315:GLY:CA	1:D:316:GLU:HG3	2.44	0.48
1:E:202:LEU:O	1:E:203:ALA:C	2.50	0.48
1:C:124:LYS:HG2	1:C:131:PHE:CD2	2.48	0.48
1:A:52:HIS:HD2	1:A:69:PRO:HD3	1.78	0.48
1:F:181:GLN:HA	1:F:243:LYS:HG3	1.95	0.48
1:C:14:ARG:HG2	1:C:14:ARG:NH1	2.25	0.48
1:C:179:LEU:O	1:C:183:MET:HG3	2.14	0.48
1:A:212:LEU:HD11	1:F:183:MET:HE3	1.95	0.47
1:C:30:ASP:HB2	1:C:278:GLY:CA	2.44	0.47
1:B:30:ASP:CG	2:B:401:R5P:HO3	2.16	0.47
1:D:10:LYS:O	1:D:10:LYS:HD3	2.14	0.47
1:F:26:GLY:HA3	1:F:46:VAL:CG1	2.44	0.47
1:D:290:MET:HE2	1:D:316:GLU:OE2	2.15	0.47
1:D:283:LYS:HD3	1:D:283:LYS:HA	1.66	0.47
1:E:2:ASP:N	1:E:2:ASP:OD2	2.47	0.47
1:B:284:SER:HB2	1:B:316:GLU:HB2	1.97	0.47
1:C:121:HIS:CD2	1:C:144:ARG:HD2	2.49	0.47
1:B:283:LYS:HA	1:B:283:LYS:HD3	1.63	0.47
1:E:313:GLU:O	1:E:314:ILE:HD13	2.14	0.47
1:B:275:VAL:HG12	1:B:277:VAL:HG12	1.97	0.47
1:E:26:GLY:HA3	1:E:46:VAL:CG1	2.45	0.47
1:B:144:ARG:HA	1:B:144:ARG:HD3	1.59	0.46
1:A:5:LYS:HE2	1:A:9:GLU:OE2	2.15	0.46
1:E:181:GLN:HA	1:E:243:LYS:HG3	1.97	0.46
1:E:180:ILE:HD13	1:E:180:ILE:HA	1.71	0.46
1:E:4:LEU:HG	1:E:8:MET:CE	2.45	0.46
1:B:26:GLY:HA3	1:B:46:VAL:HG11	1.97	0.46
1:F:30:ASP:HB2	1:F:278:GLY:CA	2.46	0.46
1:E:99:LEU:HA	1:E:99:LEU:HD23	1.79	0.46
1:F:155:LYS:HZ3	1:F:332:GLU:CB	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ARG:HA	1:D:144:ARG:HD3	1.55	0.46
1:F:313:GLU:O	1:F:314:ILE:HD13	2.16	0.46
1:A:193:GLU:HA	1:A:232:VAL:HG22	1.98	0.46
1:B:312:ARG:HH12	1:C:74:GLN:HG2	1.81	0.46
1:A:155:LYS:HZ1	1:A:332:GLU:CB	2.29	0.46
1:F:144:ARG:HA	1:F:144:ARG:HD3	1.50	0.46
1:C:5:LYS:HA	1:C:5:LYS:HD3	1.62	0.46
1:B:52:HIS:HD2	1:B:69:PRO:HD3	1.81	0.46
1:B:313:GLU:O	1:B:314:ILE:HD13	2.16	0.45
1:B:139:GLY:HA2	1:B:195:PHE:CD2	2.51	0.45
1:B:181:GLN:HA	1:B:243:LYS:HG3	1.98	0.45
1:D:26:GLY:HA3	1:D:46:VAL:CG1	2.47	0.45
1:B:183:MET:HE3	1:C:212:LEU:HD11	1.98	0.45
1:C:119:PHE:CD2	1:C:202:LEU:HB2	2.51	0.45
1:D:108:ASP:OD1	1:D:153:ARG:NH1	2.48	0.45
1:B:71:GLU:H	1:B:71:GLU:HG3	1.50	0.45
1:C:283:LYS:HA	1:C:283:LYS:HD3	1.68	0.45
1:B:108:ASP:OD1	1:B:153:ARG:NH1	2.47	0.45
1:D:52:HIS:HD2	1:D:69:PRO:HD3	1.82	0.45
1:E:90:ILE:HA	1:E:109:GLU:HG2	1.99	0.45
1:A:312:ARG:HH12	1:B:74:GLN:HG2	1.81	0.45
1:C:275:VAL:HG12	1:C:277:VAL:HG12	1.99	0.45
1:B:26:GLY:HA3	1:B:46:VAL:CG1	2.46	0.45
1:B:97:ARG:HG2	1:B:127:PHE:CZ	2.51	0.45
1:F:179:LEU:O	1:F:183:MET:HG3	2.17	0.44
1:B:143:ARG:HD3	1:B:195:PHE:O	2.17	0.44
1:C:52:HIS:HD2	1:C:69:PRO:HD3	1.82	0.44
1:F:71:GLU:HG3	1:F:71:GLU:H	1.42	0.44
1:A:97:ARG:NH2	1:A:127:PHE:HA	2.32	0.44
1:A:275:VAL:HG12	1:A:277:VAL:HG12	1.99	0.44
1:A:71:GLU:HG3	1:A:71:GLU:H	1.47	0.44
1:B:97:ARG:NH2	1:B:127:PHE:HA	2.33	0.44
1:D:119:PHE:CD2	1:D:202:LEU:HB2	2.52	0.44
1:C:26:GLY:HA3	1:C:46:VAL:CG1	2.47	0.44
1:A:289:LYS:HE3	1:A:313:GLU:OE1	2.18	0.44
1:E:283:LYS:HD3	1:E:283:LYS:HA	1.65	0.44
1:E:71:GLU:HG3	1:E:71:GLU:H	1.48	0.44
1:C:180:ILE:HA	1:C:180:ILE:HD13	1.76	0.44
1:F:255:ALA:HB1	2:F:401:R5P:HC4	1.99	0.44
1:C:90:ILE:HA	1:C:109:GLU:HG2	2.00	0.44
1:A:182:ARG:NH1	1:B:220:GLU:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:HB3	1:A:314:ILE:HG22	2.00	0.44
1:B:3:LYS:O	1:B:6:ILE:HG13	2.18	0.44
1:A:283:LYS:HA	1:A:283:LYS:HD3	1.66	0.44
1:A:90:ILE:HA	1:A:109:GLU:HG2	2.00	0.43
1:D:23:VAL:HG11	1:D:28:ILE:HD11	1.99	0.43
1:E:284:SER:HA	1:E:316:GLU:CB	2.48	0.43
1:D:90:ILE:HA	1:D:109:GLU:HG2	2.00	0.43
1:C:312:ARG:HH12	1:D:74:GLN:HG2	1.84	0.43
1:E:144:ARG:HA	1:E:144:ARG:HD3	1.50	0.43
1:F:108:ASP:OD1	1:F:153:ARG:NH1	2.48	0.43
1:C:23:VAL:HG11	1:C:28:ILE:HD11	2.00	0.43
1:B:99:LEU:HD23	1:B:99:LEU:HA	1.80	0.43
1:B:23:VAL:HG22	1:B:46:VAL:CG2	2.47	0.43
1:C:139:GLY:HA2	1:C:195:PHE:CD2	2.54	0.43
1:A:111:GLU:OE1	1:A:153:ARG:NH2	2.52	0.43
1:F:201:ARG:HD3	1:F:201:ARG:HH11	1.61	0.43
1:F:119:PHE:CD2	1:F:202:LEU:HB2	2.54	0.43
1:D:227:THR:HG23	1:D:229:ARG:H	1.84	0.42
1:F:283:LYS:HD3	1:F:283:LYS:HA	1.68	0.42
1:A:144:ARG:HA	1:A:144:ARG:HD3	1.55	0.42
1:D:193:GLU:HA	1:D:232:VAL:CG2	2.49	0.42
1:E:2:ASP:O	1:E:6:ILE:HG13	2.20	0.42
1:D:97:ARG:HG2	1:D:127:PHE:CZ	2.54	0.42
1:F:279:SER:O	1:F:283:LYS:HB2	2.19	0.42
1:B:154:THR:HG21	1:B:170:VAL:HG23	2.00	0.42
1:F:87:LYS:CE	2:F:401:R5P:O2	2.67	0.42
1:A:23:VAL:HG11	1:A:28:ILE:HD11	2.01	0.42
1:A:143:ARG:HD3	1:A:195:PHE:O	2.20	0.42
1:D:180:ILE:HD13	1:D:180:ILE:HA	1.77	0.42
1:B:291:ALA:O	1:B:295:VAL:HG23	2.19	0.42
1:D:208:GLU:HB2	1:D:214:LYS:HE3	2.01	0.42
1:E:52:HIS:HD2	1:E:69:PRO:HD3	1.83	0.42
1:D:284:SER:CB	1:D:316:GLU:HB3	2.49	0.42
1:E:121:HIS:CD2	1:E:144:ARG:HD2	2.55	0.42
1:E:275:VAL:HG12	1:E:277:VAL:HG12	2.02	0.42
1:C:23:VAL:HG22	1:C:46:VAL:CG2	2.48	0.42
1:E:284:SER:HA	1:E:316:GLU:HB3	2.02	0.42
1:B:7:ILE:H	1:B:7:ILE:HG12	1.61	0.42
1:C:286:ASN:HB3	1:C:314:ILE:HG22	2.01	0.42
1:E:154:THR:HG21	1:E:170:VAL:HG23	2.01	0.42
1:F:1:MET:H1	1:F:5:LYS:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:ARG:HD3	1:F:195:PHE:O	2.20	0.41
1:F:189:TYR:HA	1:F:236:TYR:CD1	2.55	0.41
1:E:279:SER:N	2:E:401:R5P:O1P	2.52	0.41
1:F:90:ILE:HA	1:F:109:GLU:HG2	2.02	0.41
1:C:189:TYR:HA	1:C:236:TYR:CD1	2.55	0.41
1:F:180:ILE:HA	1:F:180:ILE:HD13	1.76	0.41
1:D:121:HIS:CD2	1:D:144:ARG:HD2	2.55	0.41
1:B:239:LEU:HA	1:B:239:LEU:HD23	1.87	0.41
1:C:143:ARG:HD3	1:C:195:PHE:O	2.20	0.41
1:F:227:THR:HG21	3:F:503:HOH:O	2.20	0.41
1:A:46:VAL:O	1:A:83:PRO:HD2	2.21	0.41
1:C:144:ARG:HA	1:C:144:ARG:HD3	1.53	0.41
1:D:22:MET:HB3	1:D:22:MET:HE3	1.86	0.41
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.84	0.41
1:A:316:GLU:H	1:A:317:PRO:HA	1.85	0.41
1:D:286:ASN:HB3	1:D:314:ILE:HG22	2.02	0.41
1:B:227:THR:HG22	1:B:230:GLU:HG3	2.03	0.41
1:B:90:ILE:HA	1:B:109:GLU:HG2	2.03	0.41
1:B:289:LYS:HG2	1:B:313:GLU:O	2.21	0.41
1:B:205:SER:O	1:B:209:ILE:HG13	2.21	0.41
1:A:22:MET:HE3	1:A:22:MET:HB3	1.86	0.41
1:A:74:GLN:HG2	1:F:312:ARG:HH12	1.86	0.41
1:D:143:ARG:HD3	1:D:195:PHE:O	2.21	0.41
1:E:253:PHE:CZ	1:E:274:GLY:HA3	2.56	0.41
1:B:193:GLU:HA	1:B:232:VAL:CG2	2.50	0.41
1:A:289:LYS:HG2	1:A:313:GLU:O	2.21	0.41
1:F:1:MET:N	1:F:5:LYS:HD3	2.36	0.41
1:C:153:ARG:HA	1:C:253:PHE:O	2.21	0.41
1:F:132:VAL:HA	1:F:151:MET:O	2.21	0.41
1:A:23:VAL:HG22	1:A:46:VAL:CG2	2.49	0.40
1:C:140:GLU:HG2	1:C:143:ARG:NH2	2.37	0.40
1:A:313:GLU:C	1:A:314:ILE:HD13	2.42	0.40
1:A:36:GLN:HG2	1:A:282:PHE:CE1	2.55	0.40
1:A:313:GLU:O	1:A:314:ILE:HD13	2.20	0.40
1:F:2:ASP:HB3	1:F:3:LYS:H	1.68	0.40
1:E:163:ILE:HD12	1:E:163:ILE:HA	1.97	0.40
1:E:312:ARG:HH12	1:F:74:GLN:HG2	1.86	0.40
1:C:205:SER:O	1:C:209:ILE:HG13	2.22	0.40
1:B:111:GLU:OE1	1:B:153:ARG:NH2	2.54	0.40
1:C:189:TYR:HA	1:C:236:TYR:HD1	1.87	0.40
1:C:279:SER:N	2:C:401:R5P:O1P	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:MET:HE3	1:D:316:GLU:HB2	2.03	0.40
1:F:315:GLY:O	1:F:316:GLU:CB	2.70	0.40
1:A:108:ASP:OD1	1:A:153:ARG:NH1	2.52	0.40
1:F:99:LEU:HD23	1:F:99:LEU:HA	1.76	0.40
1:C:201:ARG:HD3	1:C:201:ARG:HH11	1.65	0.40
1:C:22:MET:HB3	1:C:22:MET:HE3	1.88	0.40
1:A:220:GLU:HA	1:A:221:PRO:HD3	1.91	0.40
1:F:162:ASN:OD1	1:F:164:ILE:HG22	2.21	0.40
1:E:108:ASP:OD1	1:E:153:ARG:NH1	2.48	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	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ARG:NH1	1:E:218:GLU:OE1[1_655]	2.17	0.03

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	331/335 (99%)	318 (96%)	9 (3%)	4 (1%)	16	52
1	B	331/335 (99%)	321 (97%)	8 (2%)	2 (1%)	30	68
1	C	331/335 (99%)	320 (97%)	10 (3%)	1 (0%)	46	80
1	D	331/335 (99%)	314 (95%)	14 (4%)	3 (1%)	21	61
1	E	331/335 (99%)	314 (95%)	13 (4%)	4 (1%)	16	52
1	F	331/335 (99%)	319 (96%)	9 (3%)	3 (1%)	21	61
All	All	1986/2010 (99%)	1906 (96%)	63 (3%)	17 (1%)	21	61

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	MET
1	D	317	PRO
1	D	322	ALA
1	E	317	PRO
1	F	316	GLU
1	F	317	PRO
1	A	317	PRO
1	A	332	GLU
1	E	318	MET
1	A	316	GLU
1	B	328	VAL
1	C	328	VAL
1	D	328	VAL
1	F	328	VAL
1	E	320	GLY
1	A	328	VAL
1	E	328	VAL

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	251/267 (94%)	221 (88%)	30 (12%)	6 24
1	B	251/267 (94%)	218 (87%)	33 (13%)	5 21
1	C	251/267 (94%)	223 (89%)	28 (11%)	7 29
1	D	251/267 (94%)	223 (89%)	28 (11%)	7 29
1	E	251/267 (94%)	221 (88%)	30 (12%)	6 24
1	F	251/267 (94%)	224 (89%)	27 (11%)	8 30
All	All	1506/1602 (94%)	1330 (88%)	176 (12%)	7 26

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LYS
1	A	9	GLU
1	A	10	LYS
1	A	12	THR
1	A	15	LEU
1	A	17	ARG
1	A	23	VAL
1	A	51	LEU
1	A	54	VAL
1	A	71	GLU
1	A	90	ILE
1	A	97	ARG
1	A	112	VAL
1	A	113	LEU
1	A	144	ARG
1	A	152	ILE
1	A	153	ARG
1	A	164	ILE
1	A	216	VAL
1	A	227	THR
1	A	241	GLU
1	A	244	LYS
1	A	277	VAL
1	A	284	SER
1	A	289	LYS
1	A	311	SER
1	A	314	ILE
1	B	2	ASP
1	B	3	LYS
1	B	4	LEU
1	B	6	ILE
1	B	7	ILE
1	B	10	LYS
1	B	12	THR
1	B	14	ARG
1	B	15	LEU
1	B	17	ARG
1	B	51	LEU
1	B	54	VAL
1	B	71	GLU
1	B	90	ILE

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Mol	Chain	Res	Type
1	B	97	ARG
1	B	112	VAL
1	B	113	LEU
1	B	140	GLU
1	B	144	ARG
1	B	152	ILE
1	B	164	ILE
1	B	202	LEU
1	B	216	VAL
1	B	227	THR
1	B	241	GLU
1	B	244	LYS
1	B	250	VAL
1	B	277	VAL
1	B	284	SER
1	B	289	LYS
1	B	311	SER
1	B	314	ILE
1	B	316	GLU
1	C	1	MET
1	C	3	LYS
1	C	5	LYS
1	C	7	ILE
1	C	9	GLU
1	C	12	THR
1	C	15	LEU
1	C	17	ARG
1	C	51	LEU
1	C	54	VAL
1	C	71	GLU
1	C	90	ILE
1	C	97	ARG
1	C	112	VAL
1	C	113	LEU
1	C	140	GLU
1	C	144	ARG
1	C	152	ILE
1	C	164	ILE
1	C	216	VAL
1	C	227	THR
1	C	241	GLU
1	C	277	VAL

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Mol	Chain	Res	Type
1	C	284	SER
1	C	289	LYS
1	C	311	SER
1	C	314	ILE
1	C	316	GLU
1	D	3	LYS
1	D	7	ILE
1	D	10	LYS
1	D	12	THR
1	D	14	ARG
1	D	15	LEU
1	D	17	ARG
1	D	51	LEU
1	D	54	VAL
1	D	71	GLU
1	D	90	ILE
1	D	97	ARG
1	D	112	VAL
1	D	113	LEU
1	D	140	GLU
1	D	144	ARG
1	D	152	ILE
1	D	164	ILE
1	D	216	VAL
1	D	227	THR
1	D	232	VAL
1	D	241	GLU
1	D	244	LYS
1	D	277	VAL
1	D	284	SER
1	D	289	LYS
1	D	311	SER
1	D	314	ILE
1	E	1	MET
1	E	5	LYS
1	E	7	ILE
1	E	8	MET
1	E	9	GLU
1	E	12	THR
1	E	15	LEU
1	E	17	ARG
1	E	51	LEU

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Mol	Chain	Res	Type
1	E	54	VAL
1	E	71	GLU
1	E	90	ILE
1	E	97	ARG
1	E	112	VAL
1	E	113	LEU
1	E	140	GLU
1	E	144	ARG
1	E	152	ILE
1	E	153	ARG
1	E	164	ILE
1	E	216	VAL
1	E	227	THR
1	E	241	GLU
1	E	244	LYS
1	E	277	VAL
1	E	284	SER
1	E	289	LYS
1	E	311	SER
1	E	314	ILE
1	E	316	GLU
1	F	3	LYS
1	F	6	ILE
1	F	7	ILE
1	F	12	THR
1	F	15	LEU
1	F	17	ARG
1	F	51	LEU
1	F	54	VAL
1	F	71	GLU
1	F	90	ILE
1	F	97	ARG
1	F	112	VAL
1	F	113	LEU
1	F	144	ARG
1	F	152	ILE
1	F	153	ARG
1	F	164	ILE
1	F	216	VAL
1	F	227	THR
1	F	241	GLU
1	F	244	LYS

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Mol	Chain	Res	Type
1	F	277	VAL
1	F	284	SER
1	F	289	LYS
1	F	311	SER
1	F	314	ILE
1	F	316	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	B	121	HIS
1	B	176	ASN
1	C	176	ASN
1	D	176	ASN
1	E	176	ASN
1	F	176	ASN

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

6 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	R5P	A	401	1	11,12,13	0.54	0	11,17,18	1.69	4 (36%)
2	R5P	B	401	1	11,12,13	0.53	0	11,17,18	1.72	2 (18%)
2	R5P	C	401	1	11,12,13	0.76	0	11,17,18	1.12	0
2	R5P	D	401	1	11,12,13	0.63	0	11,17,18	1.63	2 (18%)
2	R5P	E	401	1	11,12,13	0.64	0	11,17,18	1.43	2 (18%)
2	R5P	F	401	-	11,12,13	0.81	0	11,17,18	1.77	2 (18%)

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	R5P	A	401	1	-	0/14/14/16	0/0/0/0
2	R5P	B	401	1	-	0/14/14/16	0/0/0/0
2	R5P	C	401	1	-	0/14/14/16	0/0/0/0
2	R5P	D	401	1	-	0/14/14/16	0/0/0/0
2	R5P	E	401	1	-	0/14/14/16	0/0/0/0
2	R5P	F	401	-	-	0/14/14/16	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	R5P	C4-C3-C2	-3.01	107.56	112.47
2	A	401	R5P	O3P-P-O5	-2.88	98.28	106.56
2	F	401	R5P	O2P-P-O5	-2.80	98.50	106.56
2	F	401	R5P	C4-C3-C2	-2.76	107.98	112.47
2	B	401	R5P	O5-P-O1P	-2.69	100.29	107.14
2	D	401	R5P	O5-P-O1P	-2.48	100.84	107.14
2	E	401	R5P	O5-P-O1P	-2.44	100.92	107.14
2	A	401	R5P	C4-C3-C2	2.05	115.81	112.47
2	E	401	R5P	O4-C4-C5	2.18	114.94	110.19
2	A	401	R5P	O4-C4-C3	2.22	114.61	109.02
2	A	401	R5P	O3P-P-O2P	2.41	116.57	107.38
2	B	401	R5P	C4-C3-C2	2.74	116.94	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	R5P	1	0
2	B	401	R5P	1	0
2	C	401	R5P	1	0
2	D	401	R5P	1	0
2	E	401	R5P	1	0
2	F	401	R5P	7	0

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, 95^{th} 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	333/335 (99%)	-0.53	2 (0%)	90	80	30, 49, 83, 121	0
1	B	333/335 (99%)	-0.38	6 (1%)	71	50	31, 51, 94, 148	0
1	C	333/335 (99%)	-0.35	3 (0%)	85	72	31, 52, 85, 118	0
1	D	333/335 (99%)	-0.31	6 (1%)	71	50	30, 49, 87, 147	0
1	E	333/335 (99%)	-0.48	2 (0%)	90	80	28, 46, 79, 116	0
1	F	333/335 (99%)	-0.47	6 (1%)	71	50	30, 48, 86, 144	0
All	All	1998/2010 (99%)	-0.42	25 (1%)	79	62	28, 49, 85, 148	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.6
1	B	2	ASP	5.5
1	D	2	ASP	5.3
1	D	6	ILE	4.1
1	F	1	MET	3.8
1	C	1	MET	3.6
1	F	2	ASP	3.4
1	A	1	MET	3.1
1	D	324	GLU	2.8
1	B	6	ILE	2.6
1	B	327	GLN	2.6
1	F	327	GLN	2.4
1	C	324	GLU	2.4
1	D	5	LYS	2.4
1	B	324	GLU	2.3
1	E	1	MET	2.3
1	D	4	LEU	2.3
1	B	325	GLU	2.2
1	B	322	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	218	GLU	2.2
1	F	218	GLU	2.2
1	F	323	ILE	2.1
1	F	219	ASN	2.0
1	C	2	ASP	2.0
1	A	330	MET	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, 95^{th} 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	R5P	B	401	13/14	0.97	0.23	1.27	44,57,65,68	0
2	R5P	C	401	13/14	0.97	0.22	0.63	49,66,75,75	0
2	R5P	D	401	13/14	0.96	0.23	0.53	32,51,77,77	0
2	R5P	A	401	13/14	0.97	0.20	0.40	41,50,66,71	0
2	R5P	F	401	13/14	0.96	0.19	0.22	28,48,61,63	0
2	R5P	E	401	13/14	0.97	0.18	-0.09	35,53,62,83	0

6.5 Other polymers (i)

There are no such residues in this entry.