Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:08 AM GMT

PDB ID	:	3H9K
Title	:	Structures of Thymidylate Synthase R163K with Substrates and Inhibitors Show Subunit Asymmetry
Authors	:	Gibson, L.M.; Lovelace, L.L.; Lebioda, L.
Deposited on	:	2009-04-30
Resolution	:	2.65 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:

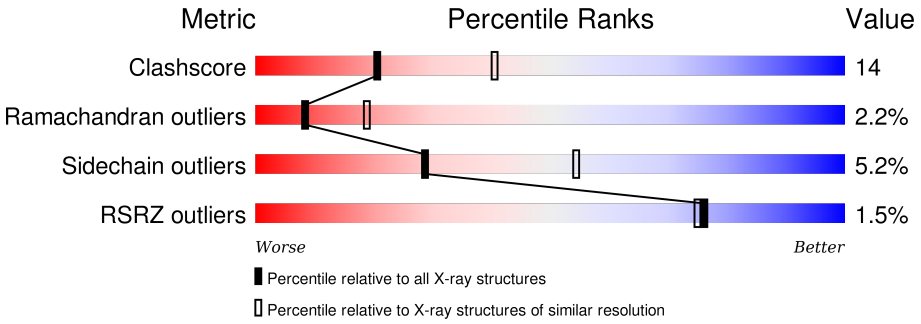
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 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))
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	313	70% 19% • 10%
1	B	313	2% 66% 22% • 10%
1	C	313	64% 24% • 10%
1	D	313	3% 47% 37% 5% 11%
1	E	313	% 64% 23% • 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UFP	A	400	-	-	-	X
2	UFP	B	400	-	-	-	X
2	UFP	D	565	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11468 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.

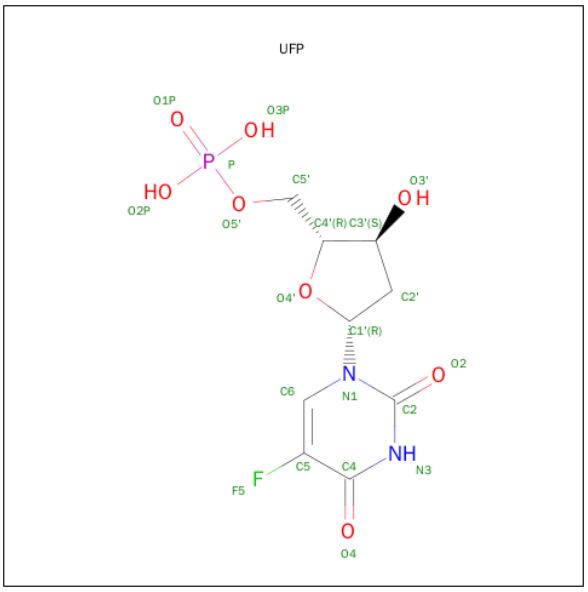
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	B	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	C	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	D	280	Total	C	N	O	S	0	0	0
			2261	1446	394	410	11			
1	E	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			

There are 5 discrepancies between the modelled and reference sequences:

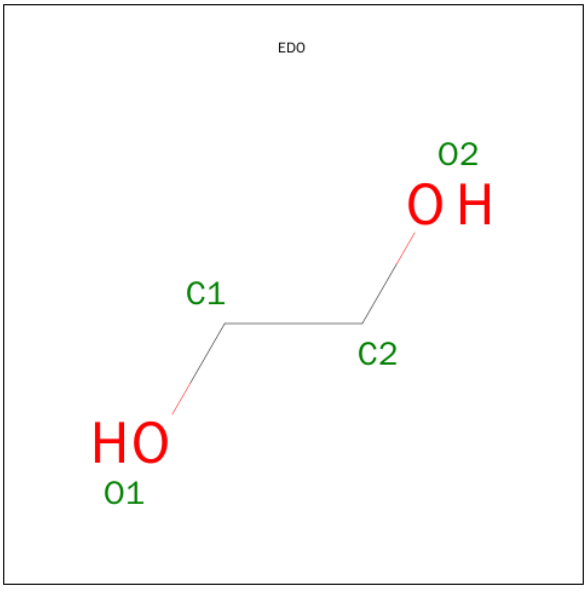
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LYS	ARG	ENGINEERED	UNP P04818
B	163	LYS	ARG	ENGINEERED	UNP P04818
C	163	LYS	ARG	ENGINEERED	UNP P04818
D	163	LYS	ARG	ENGINEERED	UNP P04818
E	163	LYS	ARG	ENGINEERED	UNP P04818

- Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
2	B	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
2	D	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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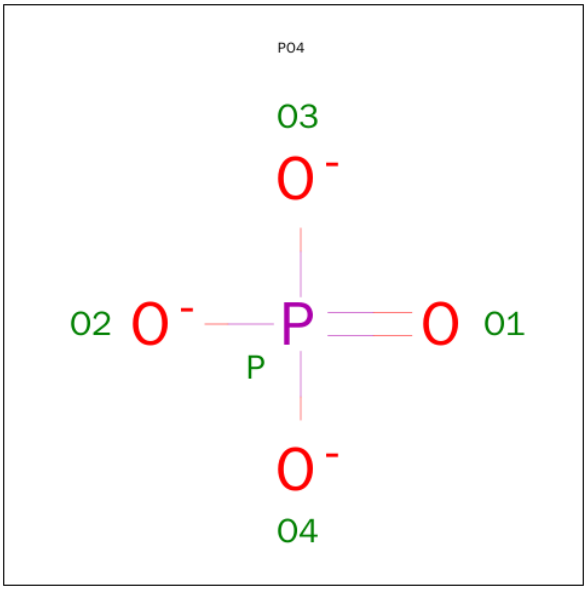
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

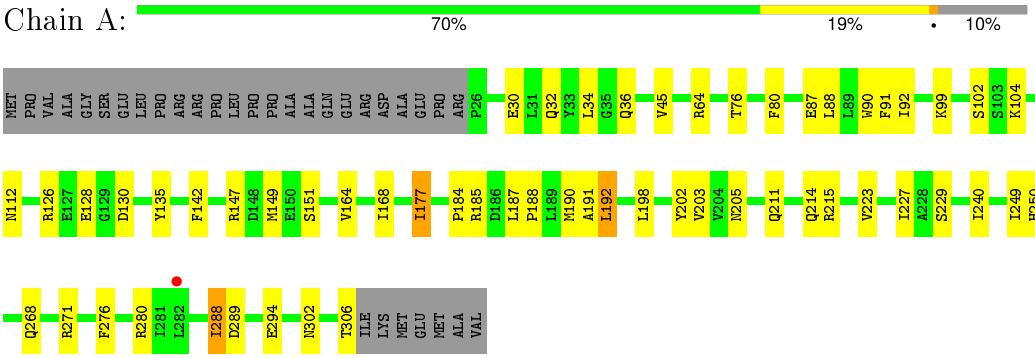
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	10	Total O 10 10	0	0
5	C	12	Total O 12 12	0	0
5	D	6	Total O 6 6	0	0
5	E	14	Total O 14 14	0	0

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.

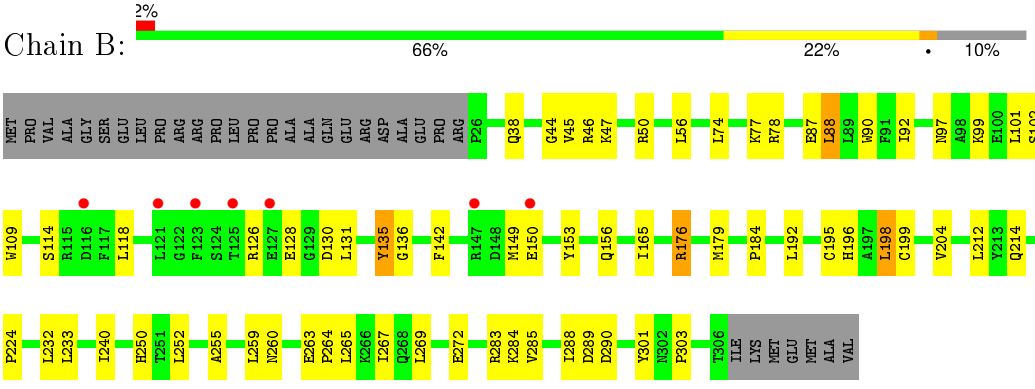
- Molecule 1: Thymidylate synthase

Chain A:



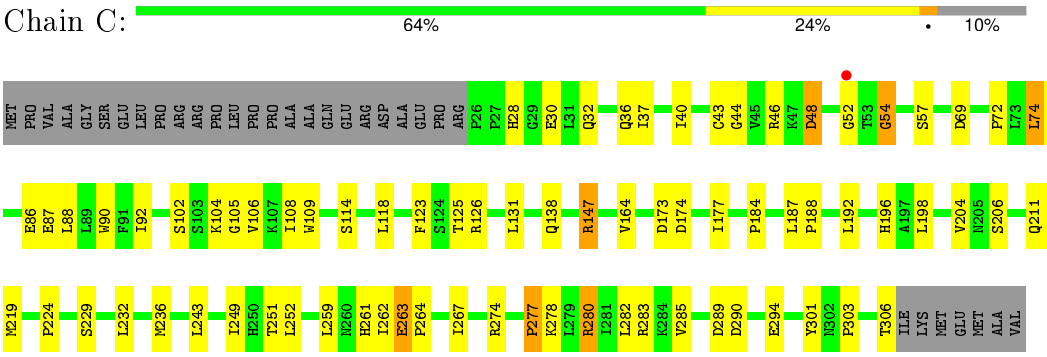
- Molecule 1: Thymidylate synthase

Chain B:



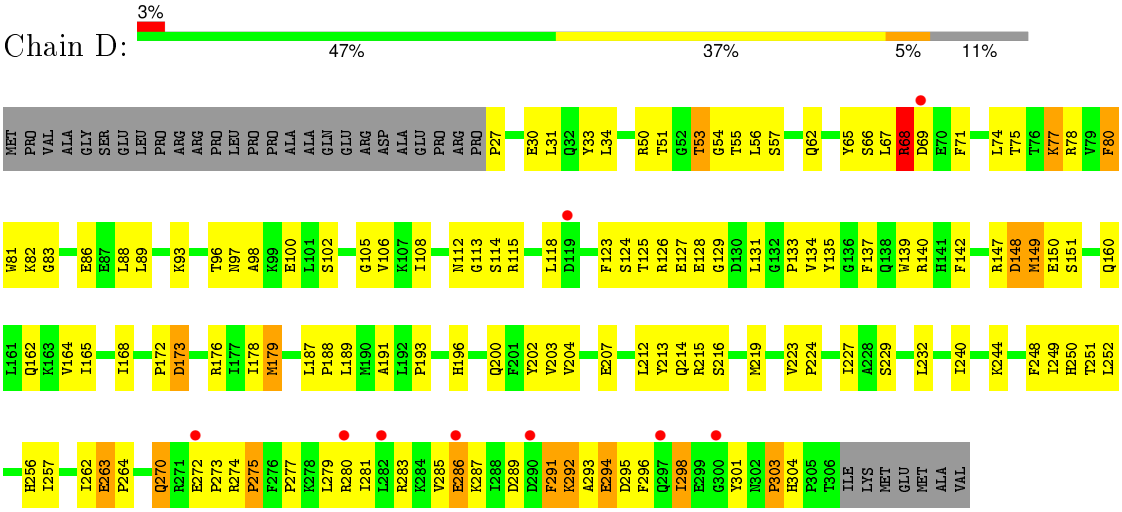
- Molecule 1: Thymidylate synthase

Chain C:



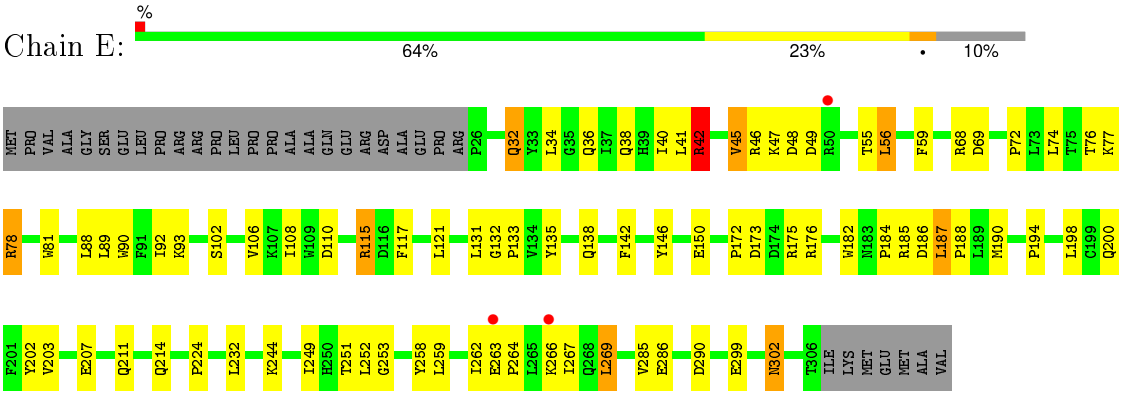
• Molecule 1: Thymidylate synthase

Chain D:



• Molecule 1: Thymidylate synthase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.28Å 122.19Å 99.83Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 49.49 – 2.62	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-2.65) 92.7 (49.49-2.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.260 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 64151 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11468	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.82% 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: UFP, PO4, EDO

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	0.46	0/2328	0.66	0/3150
1	B	0.41	0/2328	0.61	0/3150
1	C	0.43	0/2328	0.63	0/3150
1	D	0.37	0/2320	0.57	0/3138
1	E	0.42	0/2328	0.58	0/3150
All	All	0.42	0/11632	0.61	0/15738

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	C	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	213	TYR	Sidechain
1	E	202	TYR	Sidechain

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	2268	0	2235	52	0
1	B	2268	0	2235	58	0
1	C	2268	0	2235	65	0
1	D	2261	0	2228	111	0
1	E	2268	0	2235	59	0
2	A	21	0	10	1	0
2	B	21	0	10	0	0
2	D	21	0	10	2	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	12	0	0	0	0
5	B	10	0	0	0	0
5	C	12	0	0	1	0
5	D	6	0	0	0	0
5	E	14	0	0	0	0
All	All	11468	0	11210	327	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 14.

All (327) 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:C:263:GLU:HG2	1:C:264:PRO:HD3	1.39	1.05
1:C:280:ARG:HB3	1:C:280:ARG:HH11	1.29	0.94
1:B:165:ILE:HD12	1:B:240:ILE:HD11	1.50	0.92
1:D:298:ILE:H	1:D:298:ILE:HD12	1.34	0.91
1:D:123:PHE:HB3	1:D:126:ARG:HD2	1.61	0.82
1:A:271:ARG:HH22	1:A:306:THR:HB	1.45	0.81
1:C:88:LEU:HD23	1:C:236:MET:HE3	1.63	0.81
1:B:50:ARG:HB2	1:B:50:ARG:HH11	1.47	0.80
1:E:55:THR:HG22	1:E:258:TYR:HA	1.63	0.80
1:C:88:LEU:HD23	1:C:236:MET:CE	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:GLN:O	1:D:164:VAL:HG23	1.85	0.77
1:D:33:TYR:HD1	1:D:34:LEU:HD12	1.49	0.77
1:D:204:VAL:HG21	1:E:45:VAL:HG21	1.68	0.75
1:C:263:GLU:CG	1:C:264:PRO:HD3	2.16	0.74
1:A:126:ARG:HG2	1:A:130:ASP:HB3	1.69	0.74
1:D:280:ARG:HB3	1:D:280:ARG:NH1	2.04	0.73
1:D:279:LEU:HD11	1:D:296:PHE:HB3	1.71	0.73
1:C:285:VAL:HG13	1:C:290:ASP:HB2	1.69	0.73
1:D:270:GLN:HE21	1:D:270:GLN:HA	1.54	0.73
1:A:168:ILE:HD13	1:A:177:ILE:HD13	1.70	0.72
1:C:102:SER:HA	1:C:106:VAL:O	1.90	0.72
1:D:214:GLN:HB3	1:D:252:LEU:HD23	1.70	0.72
1:D:53:THR:HG22	1:D:54:GLY:N	2.03	0.71
1:A:32:GLN:NE2	1:A:64:ARG:H	1.88	0.70
1:E:36:GLN:O	1:E:40:ILE:HG12	1.93	0.69
1:C:294:GLU:H	1:C:294:GLU:CD	1.95	0.69
1:E:259:LEU:HA	1:E:262:ILE:HG12	1.76	0.68
1:B:153:TYR:HA	1:B:156:GLN:NE2	2.09	0.68
1:B:88:LEU:HD12	1:B:232:LEU:HD23	1.76	0.67
1:C:263:GLU:HG2	1:C:264:PRO:CD	2.23	0.66
1:C:196:HIS:HB3	1:C:212:LEU:HD11	1.77	0.66
1:D:285:VAL:HG12	1:D:286:GLU:H	1.61	0.65
1:A:91:PHE:CE1	1:A:135:TYR:HB2	2.31	0.65
1:C:174:ASP:HB3	1:C:177:ILE:HD11	1.79	0.65
1:D:298:ILE:HD12	1:D:298:ILE:N	2.10	0.65
1:A:147:ARG:HB3	1:A:151:SER:OG	1.98	0.64
1:C:232:LEU:HG	1:C:236:MET:HE3	1.80	0.64
1:D:115:ARG:NH2	1:D:127:GLU:HA	2.12	0.63
1:D:74:LEU:HD22	1:D:74:LEU:H	1.64	0.63
1:B:252:LEU:HD13	1:B:255:ALA:HB2	1.81	0.62
1:B:223:VAL:HG13	1:B:250:HIS:HE1	1.64	0.62
1:A:187:LEU:HB2	1:A:188:PRO:HD3	1.80	0.62
1:B:196:HIS:HB3	1:B:212:LEU:HD11	1.82	0.62
1:D:200:GLN:HE22	1:E:253:GLY:HA3	1.65	0.62
2:D:565:UFP:H5'2	1:E:175:ARG:HH21	1.65	0.61
1:B:50:ARG:NH1	1:B:50:ARG:HB2	2.15	0.61
1:E:102:SER:HA	1:E:106:VAL:O	2.00	0.61
1:E:88:LEU:O	1:E:92:ILE:HG12	2.01	0.61
1:C:214:GLN:HB3	1:C:252:LEU:HD23	1.82	0.61
1:B:214:GLN:HB3	1:B:252:LEU:HD23	1.83	0.60
1:D:57:SER:HB3	1:D:256:HIS:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:O	1:A:90:TRP:HB3	2.00	0.60
1:A:102:SER:HB2	1:A:110:ASP:OD1	2.02	0.60
1:B:88:LEU:O	1:B:92:ILE:HG12	2.02	0.60
1:B:285:VAL:HG13	1:B:290:ASP:HB2	1.83	0.60
1:D:112:ASN:HB3	1:D:191:ALA:HB1	1.84	0.60
1:A:257:ILE:HD13	1:A:265:LEU:HD13	1.83	0.60
1:C:48:ASP:HA	1:C:54:GLY:HA2	1.83	0.60
1:C:277:PRO:HG2	1:C:301:TYR:CD1	2.37	0.59
1:A:30:GLU:OE1	1:A:76:THR:HG23	2.02	0.59
1:A:192:LEU:HD22	1:A:192:LEU:O	2.02	0.59
1:D:62:GLN:HA	1:D:250:HIS:O	2.03	0.59
1:D:81:TRP:NE1	1:D:298:ILE:HD11	2.18	0.58
1:B:285:VAL:CG1	1:B:290:ASP:HB2	2.33	0.58
2:A:400:UFP:O2P	1:B:176:ARG:NH2	2.35	0.58
1:C:108:ILE:HG13	1:C:109:TRP:CD1	2.39	0.58
1:C:277:PRO:HG3	1:C:301:TYR:HA	1.85	0.58
1:B:78:ARG:HE	1:B:303:PRO:HG2	1.68	0.58
1:C:74:LEU:HD12	1:C:224:PRO:HB3	1.85	0.58
1:E:182:TRP:CZ2	1:E:187:LEU:HD11	2.38	0.58
1:B:126:ARG:HG2	1:B:130:ASP:HB3	1.85	0.57
1:E:214:GLN:HB3	1:E:252:LEU:HD23	1.87	0.57
1:A:99:LYS:HZ1	1:A:128:GLU:HG3	1.68	0.57
1:D:88:LEU:HD23	1:D:232:LEU:HD23	1.84	0.57
1:D:98:ALA:HB3	1:D:129:GLY:HA2	1.86	0.57
1:A:99:LYS:NZ	1:A:128:GLU:HG3	2.18	0.57
1:E:266:LYS:HB3	1:E:266:LYS:NZ	2.20	0.57
1:C:108:ILE:HG13	1:C:109:TRP:HD1	1.69	0.56
1:D:80:PHE:CE1	1:D:82:LYS:HB3	2.40	0.56
1:D:207:GLU:HA	1:D:244:LYS:O	2.05	0.56
1:D:68:ARG:HD2	1:D:207:GLU:OE1	2.05	0.56
1:C:173:ASP:HB2	5:C:315:HOH:O	2.05	0.56
1:C:187:LEU:N	1:C:188:PRO:HD2	2.20	0.56
1:B:301:TYR:CZ	1:B:303:PRO:HG3	2.40	0.56
1:A:202:TYR:CE1	1:B:47:LYS:HE3	2.41	0.56
1:C:277:PRO:HG2	1:C:301:TYR:HD1	1.71	0.56
1:A:88:LEU:O	1:A:92:ILE:HG12	2.06	0.56
1:A:192:LEU:HD13	1:A:192:LEU:N	2.20	0.55
1:D:142:PHE:CE2	1:E:184:PRO:HD2	2.42	0.55
1:A:168:ILE:HG23	1:A:203:VAL:HG21	1.88	0.55
1:B:301:TYR:O	1:B:303:PRO:HD3	2.06	0.55
1:E:285:VAL:CG1	1:E:290:ASP:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:O	1:D:93:LYS:HG3	2.06	0.55
1:B:264:PRO:O	1:B:267:ILE:HG13	2.07	0.55
1:D:123:PHE:HB3	1:D:126:ARG:CD	2.36	0.55
1:A:271:ARG:NH2	1:A:306:THR:HB	2.20	0.54
1:D:97:ASN:OD1	1:D:149:MET:HG3	2.07	0.54
1:B:109:TRP:CZ3	1:B:192:LEU:HD21	2.42	0.54
1:E:249:ILE:N	1:E:249:ILE:HD12	2.22	0.54
1:C:123:PHE:HB3	1:C:126:ARG:HG3	1.88	0.54
1:D:294:GLU:H	1:D:294:GLU:CD	2.11	0.54
1:D:178:ILE:HG12	1:D:200:GLN:HG3	1.89	0.54
1:A:280:ARG:HG2	1:A:280:ARG:HH11	1.72	0.54
1:C:280:ARG:NH1	1:C:280:ARG:HB3	2.10	0.54
1:E:32:GLN:O	1:E:36:GLN:HG3	2.08	0.54
1:E:285:VAL:HG13	1:E:290:ASP:HB2	1.90	0.54
1:B:192:LEU:HD23	1:B:192:LEU:N	2.23	0.54
1:E:74:LEU:HD12	1:E:224:PRO:HB3	1.90	0.54
1:B:223:VAL:HB	1:B:224:PRO:HD3	1.89	0.54
1:E:133:PRO:HD3	1:E:146:TYR:CD2	2.42	0.54
1:D:74:LEU:CD2	1:D:74:LEU:H	2.20	0.54
1:B:223:VAL:HG13	1:B:250:HIS:CE1	2.42	0.53
1:C:30:GLU:HG3	1:C:74:LEU:HD22	1.90	0.53
1:D:65:TYR:CE2	1:D:227:ILE:HD13	2.43	0.53
1:D:298:ILE:H	1:D:298:ILE:CD1	2.12	0.53
1:E:41:LEU:HA	1:E:56:LEU:HD23	1.89	0.53
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.72	0.53
1:E:106:VAL:HG12	1:E:108:ILE:HG12	1.89	0.53
1:C:88:LEU:O	1:C:92:ILE:HG13	2.09	0.53
1:C:86:GLU:HB2	1:C:106:VAL:HG21	1.90	0.53
1:E:46:ARG:NH1	1:E:259:LEU:HD11	2.24	0.53
1:D:56:LEU:HD22	1:D:262:ILE:HD11	1.90	0.53
1:C:206:SER:HA	1:C:243:LEU:HD22	1.89	0.53
1:E:38:GLN:HB3	1:E:269:LEU:HD11	1.91	0.53
1:D:280:ARG:HH11	1:D:280:ARG:HB3	1.70	0.53
1:A:130:ASP:HB2	1:A:149:MET:HE2	1.90	0.53
1:B:198:LEU:C	1:B:198:LEU:HD12	2.29	0.53
1:B:283:ARG:HG2	1:B:284:LYS:H	1.73	0.53
1:D:196:HIS:HB3	1:D:212:LEU:HD11	1.90	0.52
1:E:187:LEU:N	1:E:188:PRO:HD2	2.24	0.52
1:D:223:VAL:HB	1:D:224:PRO:HD3	1.91	0.52
1:E:38:GLN:HG3	1:E:42:ARG:HH11	1.73	0.52
1:E:117:PHE:CE1	1:E:121:LEU:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LEU:C	1:E:198:LEU:HD12	2.30	0.52
1:D:67:LEU:HD11	1:D:248:PHE:HB2	1.92	0.52
1:C:204:VAL:HG13	1:C:204:VAL:O	2.09	0.52
1:D:34:LEU:CD1	1:D:34:LEU:H	2.22	0.52
1:E:81:TRP:HH2	1:E:232:LEU:HD13	1.75	0.52
1:B:265:LEU:O	1:B:269:LEU:HD23	2.10	0.52
1:C:123:PHE:HB3	1:C:126:ARG:CG	2.40	0.51
1:A:294:GLU:CD	1:A:294:GLU:H	2.14	0.51
1:E:88:LEU:CD2	1:E:232:LEU:HD23	2.41	0.51
1:A:271:ARG:HH12	1:A:306:THR:HG21	1.74	0.51
1:C:249:ILE:HD12	1:C:249:ILE:N	2.26	0.51
1:C:44:GLY:HA2	1:C:57:SER:O	2.11	0.51
1:E:90:TRP:HH2	1:E:131:LEU:CD1	2.23	0.51
1:B:118:LEU:HD11	1:B:128:GLU:HA	1.93	0.51
1:E:172:PRO:O	1:E:203:VAL:HB	2.11	0.51
1:D:286:GLU:HG2	1:D:287:LYS:HG3	1.93	0.50
1:C:36:GLN:O	1:C:40:ILE:HG13	2.11	0.50
1:D:176:ARG:HH11	1:D:176:ARG:HG3	1.75	0.50
1:D:106:VAL:CG1	1:D:108:ILE:HG12	2.41	0.50
1:D:78:ARG:HG2	1:D:303:PRO:HG2	1.92	0.50
1:E:89:LEU:O	1:E:93:LYS:HG3	2.12	0.50
1:E:263:GLU:N	1:E:264:PRO:HD2	2.27	0.50
1:D:74:LEU:HD22	1:D:74:LEU:N	2.25	0.50
1:B:267:ILE:HD12	1:B:267:ILE:C	2.32	0.50
1:B:114:SER:O	1:B:118:LEU:HG	2.12	0.50
1:D:113:GLY:O	1:D:128:GLU:HG3	2.11	0.50
1:C:48:ASP:HB3	1:C:52:GLY:HA2	1.93	0.50
1:B:301:TYR:CE1	1:B:303:PRO:HG3	2.47	0.50
1:B:97:ASN:HD21	1:B:99:LYS:HB2	1.77	0.50
1:C:88:LEU:HD23	1:C:236:MET:HE1	1.92	0.49
1:C:211:GLN:NE2	1:C:251:THR:OG1	2.45	0.49
1:D:115:ARG:CD	1:D:128:GLU:HB2	2.43	0.49
1:E:102:SER:HB3	1:E:110:ASP:OD2	2.13	0.49
1:D:75:THR:HG21	1:D:274:ARG:O	2.12	0.49
1:B:87:GLU:O	1:B:90:TRP:HB3	2.13	0.49
1:D:164:VAL:HG21	1:D:179:MET:HG3	1.95	0.49
1:B:108:ILE:HG13	1:B:109:TRP:HD1	1.78	0.49
1:C:114:SER:O	1:C:118:LEU:HG	2.12	0.49
1:E:259:LEU:HA	1:E:262:ILE:CG1	2.43	0.49
1:D:71:PHE:CE2	1:D:279:LEU:HD22	2.49	0.48
1:D:251:THR:HG21	1:E:251:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:PHE:C	1:D:292:LYS:HD2	2.34	0.48
1:D:96:THR:HG21	1:D:137:PHE:HB2	1.95	0.48
1:D:249:ILE:HD12	1:D:249:ILE:N	2.28	0.48
1:A:187:LEU:HD23	1:A:190:MET:CE	2.44	0.48
1:D:82:LYS:HE3	1:D:105:GLY:HA3	1.94	0.48
1:C:261:HIS:C	1:C:264:PRO:HD2	2.33	0.48
1:A:205:ASN:HD21	1:B:45:VAL:HG11	1.78	0.48
1:C:82:LYS:NZ	1:C:105:GLY:HA3	2.28	0.48
1:D:55:THR:HB	1:D:257:ILE:O	2.14	0.48
1:A:271:ARG:HH22	1:A:306:THR:CB	2.22	0.47
1:D:270:GLN:CA	1:D:270:GLN:HE21	2.26	0.47
1:B:106:VAL:HG12	1:B:108:ILE:HG12	1.96	0.47
1:E:138:GLN:HA	1:E:138:GLN:OE1	2.14	0.47
1:D:51:THR:O	1:D:51:THR:HG22	2.14	0.47
1:D:50:ARG:NH2	1:E:176:ARG:NH1	2.61	0.47
1:C:277:PRO:CG	1:C:301:TYR:HD1	2.26	0.47
1:C:263:GLU:O	1:C:267:ILE:HG13	2.15	0.47
1:A:108:ILE:HG13	1:A:109:TRP:CD1	2.50	0.47
1:A:198:LEU:C	1:A:198:LEU:HD12	2.35	0.47
1:C:294:GLU:N	1:C:294:GLU:CD	2.67	0.47
1:D:149:MET:HG2	1:D:150:GLU:N	2.30	0.47
1:C:40:ILE:HD12	1:C:219:MET:HG3	1.97	0.47
1:C:32:GLN:O	1:C:36:GLN:HG3	2.14	0.47
1:D:106:VAL:HG12	1:D:108:ILE:HG12	1.95	0.47
1:C:198:LEU:C	1:C:198:LEU:HD12	2.34	0.47
1:D:114:SER:O	1:D:118:LEU:HG	2.14	0.47
1:D:187:LEU:HB3	1:D:188:PRO:HD3	1.97	0.47
1:A:164:VAL:O	1:A:168:ILE:HG12	2.15	0.47
1:C:147:ARG:HH12	1:E:302:ASN:ND2	2.12	0.47
1:E:207:GLU:HA	1:E:244:LYS:O	2.15	0.47
1:D:66:SER:C	1:D:67:LEU:HD23	2.36	0.47
1:E:267:ILE:H	1:E:267:ILE:HD12	1.79	0.47
1:C:69:ASP:O	1:C:278:LYS:HE2	2.15	0.47
1:C:109:TRP:CE3	1:C:131:LEU:HD13	2.49	0.46
1:E:190:MET:SD	1:E:194:PRO:HD3	2.55	0.46
1:B:149:MET:HG3	1:B:150:GLU:HG2	1.97	0.46
1:B:50:ARG:CB	1:B:50:ARG:HH11	2.24	0.46
1:C:28:HIS:HD2	1:C:30:GLU:HB3	1.80	0.46
1:D:301:TYR:CZ	1:D:303:PRO:HG3	2.50	0.46
1:A:187:LEU:HD23	1:A:190:MET:HE3	1.98	0.46
1:A:192:LEU:CD1	1:A:192:LEU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ARG:NH1	1:D:303:PRO:O	2.48	0.46
1:C:285:VAL:CG1	1:C:290:ASP:HB2	2.44	0.46
1:D:82:LYS:CE	1:D:105:GLY:HA3	2.46	0.46
1:E:244:LYS:HB2	1:E:244:LYS:NZ	2.30	0.46
1:D:281:ILE:HA	1:D:295:ASP:O	2.16	0.46
1:C:28:HIS:CD2	1:C:30:GLU:H	2.33	0.46
1:D:301:TYR:O	1:D:303:PRO:HD3	2.16	0.46
1:C:259:LEU:O	1:C:262:ILE:HG12	2.15	0.46
1:B:135:TYR:OH	1:B:195:CYS:N	2.48	0.46
1:D:204:VAL:HG21	1:E:45:VAL:CG2	2.42	0.46
1:D:133:PRO:HD2	1:D:189:LEU:O	2.15	0.46
1:C:280:ARG:CB	1:C:280:ARG:HH11	2.13	0.46
1:A:187:LEU:HA	1:A:190:MET:CE	2.45	0.46
1:D:77:LYS:HD2	1:D:78:ARG:O	2.16	0.46
1:B:135:TYR:O	1:B:136:GLY:C	2.55	0.46
1:D:34:LEU:HD12	1:D:34:LEU:N	2.30	0.45
1:D:293:ALA:C	1:D:295:ASP:H	2.19	0.45
1:C:206:SER:HA	1:C:243:LEU:CD2	2.45	0.45
1:E:34:LEU:HD11	1:E:76:THR:HG21	1.98	0.45
1:A:211:GLN:HG3	1:A:249:ILE:HB	1.99	0.45
1:D:123:PHE:CB	1:D:126:ARG:HD2	2.38	0.45
1:E:132:GLY:HA2	1:E:146:TYR:CE2	2.51	0.45
1:A:240:ILE:HD11	1:A:288:ILE:HA	1.98	0.45
1:B:108:ILE:HG13	1:B:109:TRP:CD1	2.52	0.45
1:D:196:HIS:ND1	1:D:214:GLN:HG3	2.32	0.44
1:B:252:LEU:HD13	1:B:255:ALA:CB	2.47	0.44
1:D:168:ILE:HG23	1:D:203:VAL:HG21	1.99	0.44
1:A:187:LEU:HA	1:A:190:MET:HE2	2.00	0.44
1:C:28:HIS:CD2	1:C:30:GLU:HB3	2.52	0.44
1:C:30:GLU:OE1	1:C:76:THR:HG23	2.17	0.44
1:C:184:PRO:HA	1:C:187:LEU:HD12	1.99	0.44
1:B:109:TRP:CE3	1:B:131:LEU:HD13	2.52	0.44
1:D:88:LEU:HD23	1:D:232:LEU:CD2	2.47	0.44
1:D:66:SER:O	1:D:67:LEU:HD23	2.18	0.44
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.99	0.44
1:D:139:TRP:CG	1:D:179:MET:HE1	2.52	0.44
1:A:130:ASP:HB2	1:A:149:MET:CE	2.47	0.44
1:E:133:PRO:O	1:E:190:MET:HE3	2.17	0.44
1:D:102:SER:HA	1:D:106:VAL:O	2.18	0.44
1:E:115:ARG:HH21	1:E:115:ARG:HB2	1.83	0.44
1:C:87:GLU:O	1:C:90:TRP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:MET:HB2	1:B:199:CYS:SG	2.57	0.44
1:B:44:GLY:O	1:B:56:LEU:HD22	2.18	0.44
1:E:88:LEU:HD23	1:E:232:LEU:HD23	1.99	0.44
1:D:96:THR:CG2	1:D:137:PHE:HB2	2.48	0.43
1:D:215:ARG:HH11	1:D:215:ARG:HG3	1.82	0.43
1:D:88:LEU:CD2	1:D:232:LEU:HD23	2.48	0.43
1:D:285:VAL:HG12	1:D:286:GLU:N	2.30	0.43
1:C:37:ILE:CD1	1:C:219:MET:HB3	2.49	0.43
1:D:27:PRO:HB2	1:D:31:LEU:HD12	2.00	0.43
1:E:77:LYS:HB3	1:E:78:ARG:H	1.52	0.43
1:D:164:VAL:O	1:D:168:ILE:HG13	2.18	0.43
1:A:205:ASN:ND2	1:B:45:VAL:HG11	2.33	0.43
1:D:173:ASP:HB2	1:E:47:LYS:HE3	2.00	0.43
1:B:126:ARG:CG	1:B:130:ASP:HB3	2.49	0.43
1:A:32:GLN:O	1:A:36:GLN:HG3	2.19	0.43
1:C:164:VAL:HG13	1:C:177:ILE:HG22	2.01	0.43
1:B:288:ILE:HG23	1:B:289:ASP:OD2	2.19	0.43
1:A:102:SER:C	1:A:104:LYS:H	2.22	0.42
1:D:140:ARG:HH11	1:D:140:ARG:HG3	1.84	0.42
1:D:34:LEU:HD12	1:D:34:LEU:H	1.84	0.42
1:A:126:ARG:HD3	1:A:130:ASP:CG	2.40	0.42
1:D:301:TYR:CE1	1:D:303:PRO:HG3	2.54	0.42
1:C:75:THR:HG21	1:C:274:ARG:O	2.19	0.42
1:B:88:LEU:HD21	1:B:233:LEU:HD13	2.01	0.42
1:E:211:GLN:HA	1:E:249:ILE:O	2.20	0.42
1:A:268:GLN:HA	1:A:271:ARG:HD2	2.02	0.42
1:A:126:ARG:HG2	1:A:130:ASP:CB	2.44	0.42
1:D:83:GLY:HA2	1:D:106:VAL:CG2	2.49	0.42
1:C:147:ARG:HH12	1:E:302:ASN:CG	2.23	0.42
1:D:115:ARG:HD3	1:D:128:GLU:HB2	2.02	0.42
1:B:102:SER:HA	1:B:106:VAL:O	2.19	0.42
1:D:301:TYR:C	1:D:303:PRO:HD3	2.40	0.42
1:D:131:LEU:O	1:D:134:VAL:HG13	2.20	0.42
1:D:34:LEU:CD1	1:D:34:LEU:N	2.83	0.41
1:E:68:ARG:HE	1:E:207:GLU:CD	2.23	0.41
1:A:223:VAL:O	1:A:227:ILE:HG13	2.20	0.41
1:A:214:GLN:OE1	1:A:250:HIS:HE1	2.03	0.41
1:D:213:TYR:OH	1:E:200:GLN:NE2	2.52	0.41
1:E:186:ASP:O	1:E:190:MET:HG3	2.20	0.41
1:B:283:ARG:HG2	1:B:284:LYS:N	2.35	0.41
1:D:86:GLU:HB3	1:D:106:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLN:OE1	1:D:165:ILE:HD12	2.20	0.41
1:D:270:GLN:NE2	1:D:270:GLN:HA	2.29	0.41
1:A:184:PRO:HD2	1:B:142:PHE:CE2	2.55	0.41
1:C:283:ARG:NH1	1:C:285:VAL:HG22	2.36	0.41
1:B:153:TYR:O	1:B:156:GLN:HB2	2.20	0.41
1:A:91:PHE:CD1	1:A:135:TYR:HB2	2.55	0.41
1:D:148:ASP:OD1	1:D:151:SER:HB2	2.20	0.41
1:A:112:ASN:HB3	1:A:191:ALA:HB1	2.03	0.41
1:A:45:VAL:CG2	1:B:204:VAL:HG21	2.50	0.41
1:A:185:ARG:HH21	1:A:185:ARG:HG3	1.86	0.41
1:C:106:VAL:HG12	1:C:108:ILE:HG12	2.03	0.41
1:D:176:ARG:HG3	1:D:176:ARG:NH1	2.35	0.41
1:D:193:PRO:HG3	1:E:176:ARG:HD3	2.02	0.41
1:D:202:TYR:HB2	1:E:59:PHE:CD2	2.55	0.41
1:D:30:GLU:O	1:D:34:LEU:HD13	2.21	0.41
1:D:115:ARG:HH21	1:D:127:GLU:HA	1.81	0.41
1:B:38:GLN:OE1	1:B:269:LEU:HD12	2.21	0.41
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.75	0.41
1:A:215:ARG:HG3	1:A:215:ARG:NH1	2.36	0.41
1:C:104:LYS:HE2	1:C:104:LYS:HB3	1.90	0.41
1:D:280:ARG:CZ	1:D:280:ARG:HB3	2.50	0.41
2:D:565:UFP:H5'2	1:E:175:ARG:NH2	2.34	0.41
1:A:30:GLU:O	1:A:34:LEU:HG	2.21	0.40
1:B:74:LEU:HD12	1:B:224:PRO:HB3	2.03	0.40
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.56	0.40
1:D:124:SER:C	1:D:126:ARG:H	2.25	0.40
1:D:214:GLN:HB3	1:D:252:LEU:CD2	2.44	0.40
1:E:138:GLN:O	1:E:142:PHE:HB2	2.21	0.40
1:D:272:GLU:HA	1:D:273:PRO:HD2	1.91	0.40
1:D:263:GLU:N	1:D:264:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	279/313 (89%)	262 (94%)	15 (5%)	2 (1%)	26 51
1	B	279/313 (89%)	250 (90%)	25 (9%)	4 (1%)	14 31
1	C	279/313 (89%)	247 (88%)	24 (9%)	8 (3%)	6 12
1	D	278/313 (89%)	234 (84%)	32 (12%)	12 (4%)	3 6
1	E	279/313 (89%)	246 (88%)	29 (10%)	4 (1%)	14 31
All	All	1394/1565 (89%)	1239 (89%)	125 (9%)	30 (2%)	8 19

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	53	THR
1	D	68	ARG
1	B	135	TYR
1	B	222	GLY
1	C	46	ARG
1	C	54	GLY
1	D	173	ASP
1	E	45	VAL
1	C	282	LEU
1	D	80	PHE
1	D	125	THR
1	D	172	PRO
1	D	275	PRO
1	D	283	ARG
1	D	294	GLU
1	B	108	ILE
1	C	43	CYS
1	E	42	ARG
1	E	135	TYR
1	A	80	PHE
1	D	135	TYR
1	A	177	ILE
1	C	74	LEU
1	D	303	PRO
1	B	220	GLY
1	C	72	PRO
1	C	303	PRO
1	D	277	PRO

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Mol	Chain	Res	Type
1	E	72	PRO
1	C	277	PRO

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	245/271 (90%)	239 (98%)	6 (2%)	57	82
1	B	245/271 (90%)	234 (96%)	11 (4%)	34	61
1	C	245/271 (90%)	235 (96%)	10 (4%)	37	66
1	D	244/271 (90%)	223 (91%)	21 (9%)	13	26
1	E	245/271 (90%)	229 (94%)	16 (6%)	21	43
All	All	1224/1355 (90%)	1160 (95%)	64 (5%)	29	54

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	A	229	SER
1	A	276	PHE
1	A	288	ILE
1	A	289	ASP
1	A	302	ASN
1	B	46	ARG
1	B	77	LYS
1	B	88	LEU
1	B	101	LEU
1	B	176	ARG
1	B	198	LEU
1	B	221	LEU
1	B	259	LEU
1	B	260	ASN
1	B	263	GLU
1	B	272	GLU

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Mol	Chain	Res	Type
1	C	48	ASP
1	C	125	THR
1	C	138	GLN
1	C	147	ARG
1	C	192	LEU
1	C	229	SER
1	C	263	GLU
1	C	280	ARG
1	C	289	ASP
1	C	306	THR
1	D	68	ARG
1	D	69	ASP
1	D	77	LYS
1	D	100	GLU
1	D	147	ARG
1	D	148	ASP
1	D	149	MET
1	D	179	MET
1	D	216	SER
1	D	219	MET
1	D	229	SER
1	D	240	ILE
1	D	263	GLU
1	D	270	GLN
1	D	275	PRO
1	D	286	GLU
1	D	289	ASP
1	D	291	PHE
1	D	292	LYS
1	D	298	ILE
1	D	304	HIS
1	E	32	GLN
1	E	42	ARG
1	E	48	ASP
1	E	49	ASP
1	E	56	LEU
1	E	69	ASP
1	E	78	ARG
1	E	115	ARG
1	E	150	GLU
1	E	173	ASP
1	E	185	ARG

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Mol	Chain	Res	Type
1	E	187	LEU
1	E	269	LEU
1	E	286	GLU
1	E	299	GLU
1	E	302	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	171	ASN
1	A	196	HIS
1	A	205	ASN
1	A	211	GLN
1	A	250	HIS
1	A	302	ASN
1	B	156	GLN
1	B	211	GLN
1	B	268	GLN
1	B	270	GLN
1	C	28	HIS
1	C	32	GLN
1	C	38	GLN
1	C	156	GLN
1	C	200	GLN
1	C	211	GLN
1	C	302	ASN
1	D	39	HIS
1	D	171	ASN
1	D	200	GLN
1	D	211	GLN
1	D	270	GLN
1	E	32	GLN
1	E	62	GLN
1	E	200	GLN
1	E	268	GLN
1	E	297	GLN
1	E	302	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

7 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	UFP	A	400	-	18,22,22	1.78	4 (22%)	21,33,33	2.16	4 (19%)
3	EDO	A	401	-	3,3,3	0.60	0	2,2,2	0.14	0
2	UFP	B	400	-	18,22,22	1.79	4 (22%)	21,33,33	1.89	4 (19%)
3	EDO	B	401	-	3,3,3	0.55	0	2,2,2	0.03	0
4	PO4	C	365	-	4,4,4	1.11	0	6,6,6	0.27	0
2	UFP	D	565	-	18,22,22	1.76	4 (22%)	21,33,33	2.23	4 (19%)
4	PO4	D	616	-	4,4,4	1.09	0	6,6,6	0.27	0

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	UFP	A	400	-	-	0/6/22/22	0/2/2/2
3	EDO	A	401	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UFP	B	400	-	-	0/6/22/22	0/2/2/2
3	EDO	B	401	-	-	0/1/1/1	0/0/0/0
4	PO4	C	365	-	-	0/0/0/0	0/0/0/0
2	UFP	D	565	-	-	0/6/22/22	0/2/2/2
4	PO4	D	616	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	565	UFP	P-O1P	2.21	1.58	1.51
2	D	565	UFP	C4-N3	2.34	1.37	1.33
2	A	400	UFP	C4-N3	2.40	1.37	1.33
2	B	400	UFP	C4-N3	2.41	1.37	1.33
2	A	400	UFP	P-O1P	2.52	1.59	1.51
2	B	400	UFP	P-O1P	2.91	1.60	1.51
2	D	565	UFP	C6-N1	3.14	1.39	1.35
2	A	400	UFP	C6-N1	3.18	1.39	1.35
2	B	400	UFP	C6-N1	3.55	1.40	1.35
2	B	400	UFP	C4-C5	4.39	1.43	1.38
2	D	565	UFP	C4-C5	4.83	1.44	1.38
2	A	400	UFP	C4-C5	4.93	1.44	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	UFP	C4'-O4'-C1'	-4.01	99.32	109.47
2	D	565	UFP	C4'-O4'-C1'	-3.94	99.52	109.47
2	B	400	UFP	C4'-O4'-C1'	-3.21	101.35	109.47
2	D	565	UFP	C5-C4-N3	-2.70	119.33	122.34
2	A	400	UFP	C5-C4-N3	-2.52	119.53	122.34
2	B	400	UFP	C5-C4-N3	-2.20	119.89	122.34
2	B	400	UFP	O4'-C1'-N1	2.70	112.39	107.72
2	A	400	UFP	O4'-C1'-N1	3.65	114.04	107.72
2	D	565	UFP	O4'-C1'-N1	4.07	114.76	107.72
2	B	400	UFP	C4-N3-C2	6.72	121.06	115.25
2	A	400	UFP	C4-N3-C2	6.99	121.29	115.25
2	D	565	UFP	C4-N3-C2	7.28	121.54	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	UFP	1	0
2	D	565	UFP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	281/313 (89%)	-0.27	1 (0%)	93	94	28, 47, 71, 83	0
1	B	281/313 (89%)	-0.03	7 (2%)	61	59	27, 58, 93, 105	0
1	C	281/313 (89%)	-0.12	1 (0%)	93	94	30, 54, 84, 106	0
1	D	280/313 (89%)	0.29	9 (3%)	51	50	36, 80, 109, 128	0
1	E	281/313 (89%)	-0.05	3 (1%)	82	82	30, 64, 107, 129	0
All	All	1404/1565 (89%)	-0.03	21 (1%)	76	75	27, 58, 101, 129	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	GLU	4.2
1	B	121	LEU	3.1
1	E	50	ARG	3.0
1	B	147	ARG	2.9
1	D	119	ASP	2.6
1	E	266	LYS	2.6
1	B	123	PHE	2.6
1	D	280	ARG	2.5
1	D	272	GLU	2.5
1	A	282	LEU	2.4
1	D	69	ASP	2.4
1	E	263	GLU	2.4
1	B	116	ASP	2.3
1	D	282	LEU	2.3
1	C	52	GLY	2.3
1	D	290	ASP	2.3
1	B	125	THR	2.2
1	B	127	GLU	2.2
1	D	300	GLY	2.2
1	D	286	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	297	GLN	2.1

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	UFP	B	400	21/21	0.90	0.34	11.83	71,86,88,89	17
2	UFP	D	565	21/21	0.92	0.32	6.85	55,90,99,102	17
2	UFP	A	400	21/21	0.94	0.27	3.92	52,90,106,111	0
4	PO4	C	365	5/5	0.95	0.18	-0.21	99,100,101,102	0
4	PO4	D	616	5/5	0.94	0.18	-0.50	97,97,98,99	0
3	EDO	A	401	4/4	0.89	0.25	-	76,80,80,81	0
3	EDO	B	401	4/4	0.83	0.21	-	73,78,80,83	0

6.5 Other polymers (i)

There are no such residues in this entry.