



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 AM GMT

PDB ID : 2VGF
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE: T384M MUTANT
Authors : Valentini, G.; Chiarelli, L.R.; Fortin, R.; Dolzan, M.; Galizzi, A.; Abraham, D.J.; Wang, C.; Bianchi, P.; Zanella, A.; Mattevi, A.
Deposited on : 2007-11-12
Resolution : 2.75 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 ⓘ symbol.

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

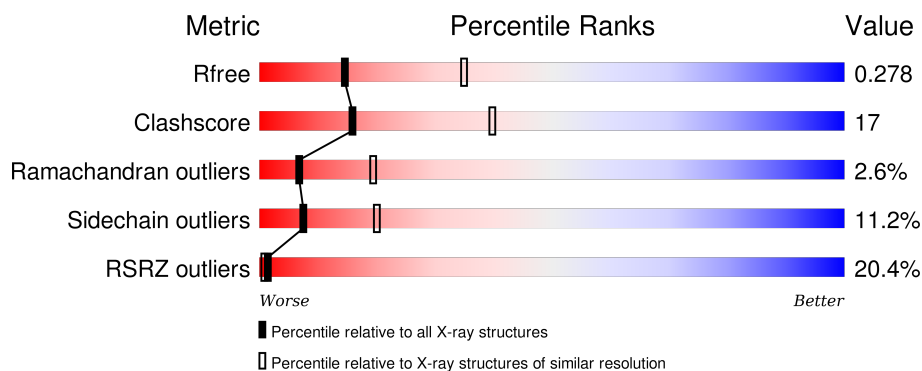
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	<div> <div>27%</div> <div>58%</div> <div>32%</div> <div>7%</div> <div>..</div> </div>
1	B	528	<div> <div>15%</div> <div>56%</div> <div>32%</div> <div>5%</div> <div>7%</div> <div>.</div> </div>
1	C	528	<div> <div>13%</div> <div>63%</div> <div>31%</div> <div>.</div> <div>..</div> </div>
1	D	528	<div> <div>24%</div> <div>58%</div> <div>32%</div> <div>6%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15550 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.

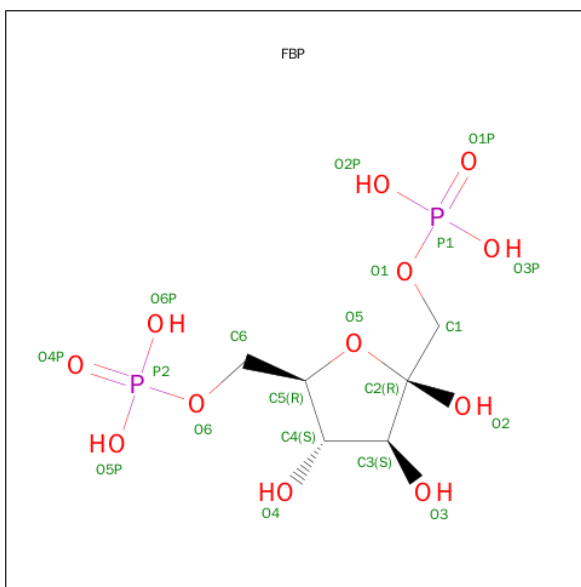
- Molecule 1 is a protein called PYRUVATE KINASE ISOZYMES R/L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3913	2458	709	727	19			
1	B	491	Total	C	N	O	S	0	0	0
			3720	2340	673	688	19			
1	C	517	Total	C	N	O	S	0	0	0
			3913	2458	709	727	19			
1	D	512	Total	C	N	O	S	7	0	0
			3880	2437	703	721	19			

There are 4 discrepancies between the modelled and reference sequences:

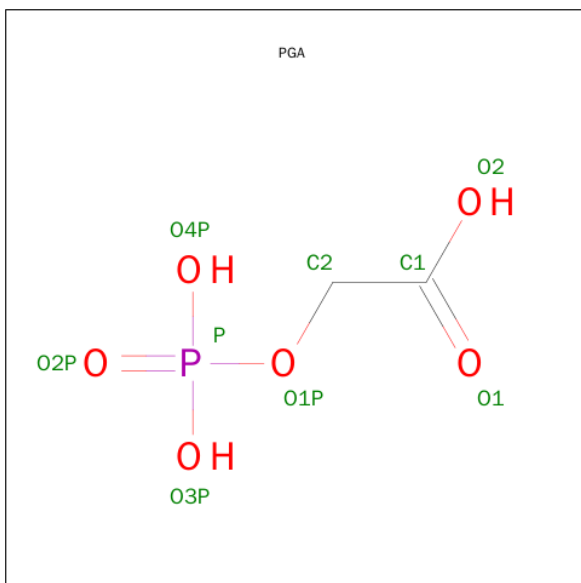
Chain	Residue	Modelled	Actual	Comment	Reference
A	384	MET	THR	ENGINEERED MUTATION	UNP P30613
B	384	MET	THR	ENGINEERED MUTATION	UNP P30613
C	384	MET	THR	ENGINEERED MUTATION	UNP P30613
D	384	MET	THR	ENGINEERED MUTATION	UNP P30613

- Molecule 2 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: C₆H₁₄O₁₂P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is SUGAR (2-PHOSPHOGLYCOLIC ACID) (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			9	2	6	1		
3	B	1	Total	C	O	P	0	0
			9	2	6	1		
3	C	1	Total	C	O	P	0	0
			9	2	6	1		
3	D	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

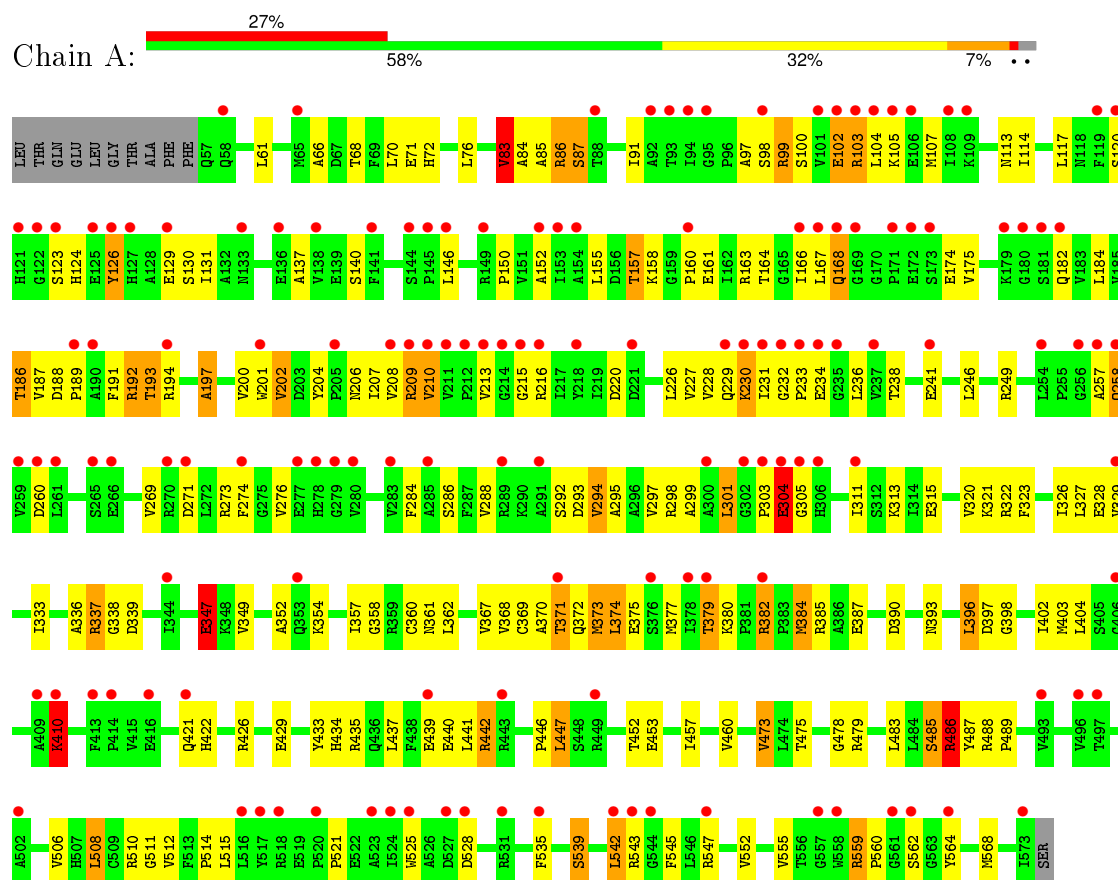
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		

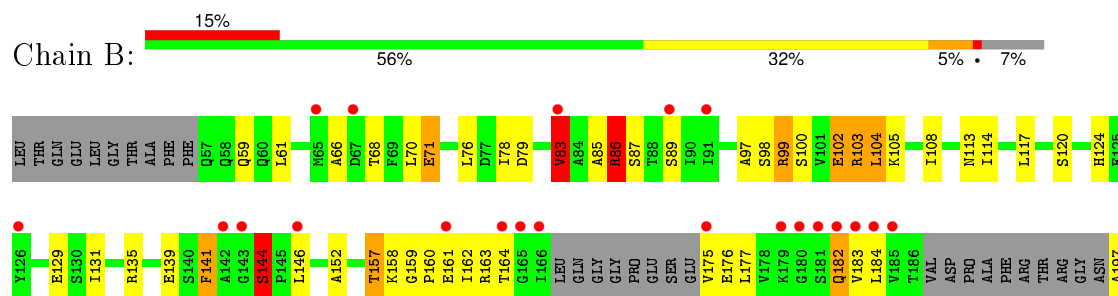
3 Residue-property plots

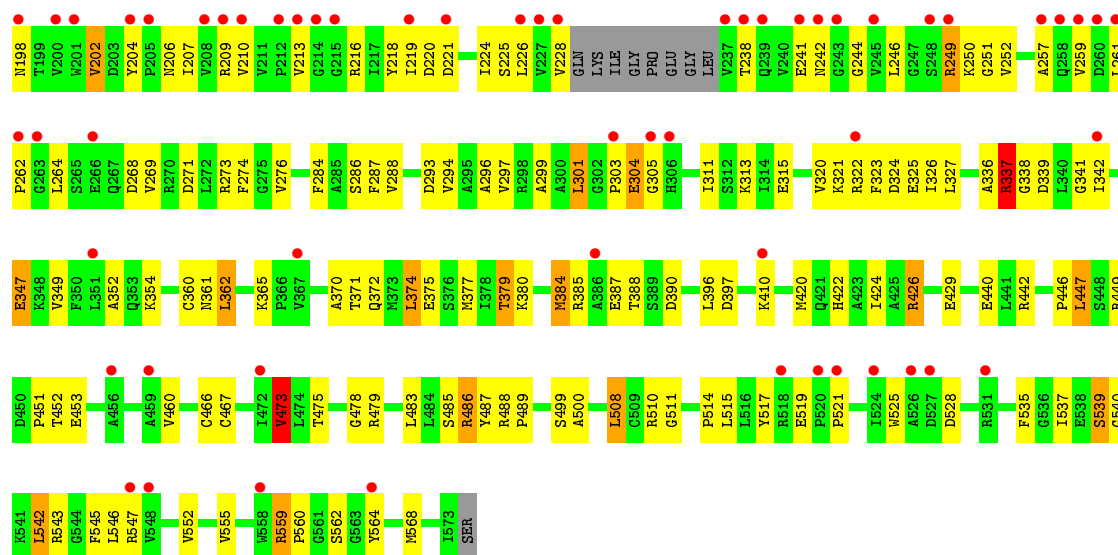
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PYRUVATE KINASE ISOZYMES R/L



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

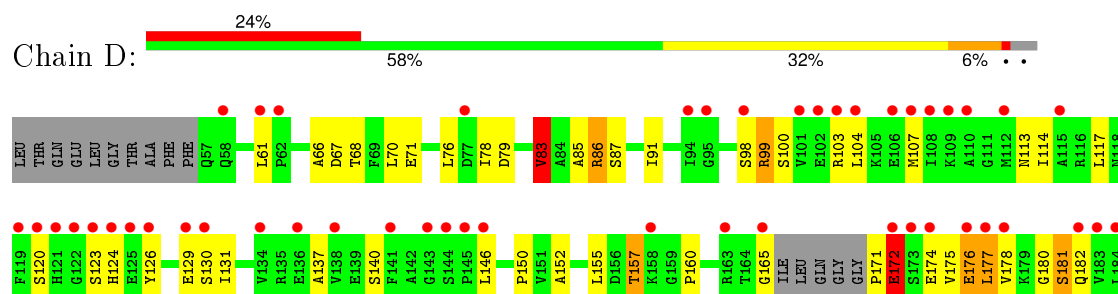


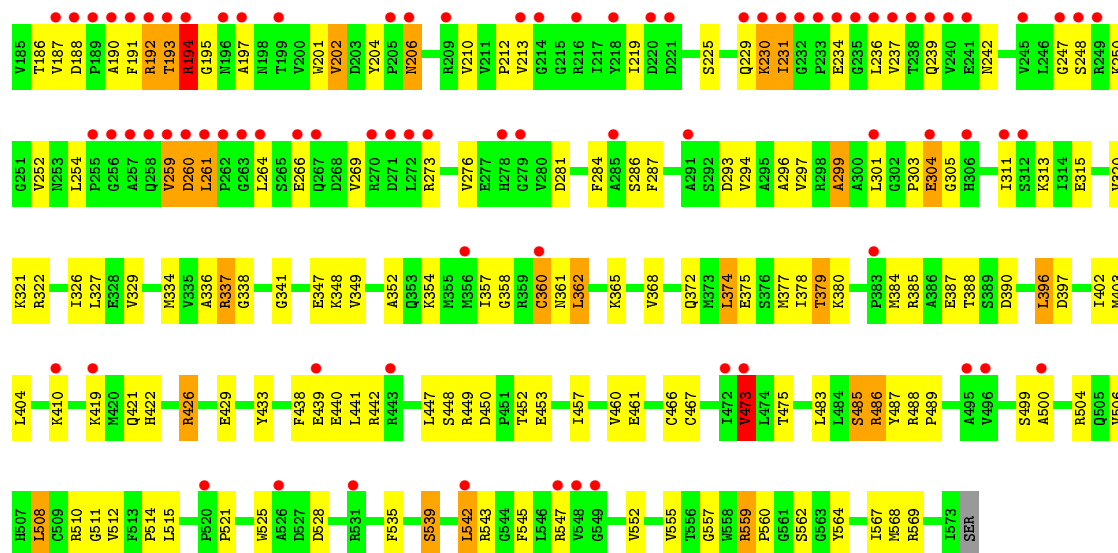


• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.30 Å 172.98 Å 85.78 Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 19.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.75) 93.7 (19.98-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.75 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.303 0.242 , 0.278	Depositor DCC
R_{free} test set	1102 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 53824 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	15550	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: K, FBP, PGA, MN

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	1.00	11/3977 (0.3%)	0.94	13/5390 (0.2%)
1	B	1.04	8/3777 (0.2%)	0.90	11/5115 (0.2%)
1	C	1.02	7/3977 (0.2%)	0.89	9/5390 (0.2%)
1	D	1.94	25/3943 (0.6%)	1.24	17/5342 (0.3%)
All	All	1.31	51/15674 (0.3%)	1.00	50/21237 (0.2%)

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	D	0	3
All	All	0	4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	GLU	CD-OE1	79.59	2.13	1.25
1	D	194	ARG	CZ-NH1	38.64	1.83	1.33
1	D	230	LYS	CE-NZ	32.91	2.31	1.49
1	D	176	GLU	CD-OE1	27.53	1.55	1.25
1	D	171	PRO	C-N	26.51	1.95	1.34
1	A	382	ARG	CZ-NH2	22.43	1.62	1.33
1	B	144	SER	CB-OG	21.73	1.70	1.42
1	C	230	LYS	CE-NZ	21.47	2.02	1.49
1	D	176	GLU	CD-OE2	19.25	1.46	1.25
1	D	172	GLU	CG-CD	18.67	1.79	1.51
1	C	241	GLU	CD-OE2	17.96	1.45	1.25
1	B	176	GLU	CD-OE1	17.53	1.45	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	241	GLU	CD-OE1	16.82	1.44	1.25
1	B	176	GLU	CD-OE2	16.63	1.44	1.25
1	A	410	LYS	CE-NZ	15.88	1.88	1.49
1	D	192	ARG	CZ-NH1	14.32	1.51	1.33
1	A	168	GLN	CD-NE2	12.55	1.64	1.32
1	A	102	GLU	CD-OE2	11.12	1.37	1.25
1	D	260	ASP	CG-OD1	10.41	1.49	1.25
1	B	249	ARG	CZ-NH2	9.51	1.45	1.33
1	D	165	GLY	C-O	8.56	1.37	1.23
1	D	180	GLY	C-O	-8.47	1.10	1.23
1	A	126	TYR	CE2-CZ	-8.35	1.27	1.38
1	A	126	TYR	CE1-CZ	8.35	1.49	1.38
1	D	360	CYS	CB-SG	-8.31	1.68	1.82
1	B	182	GLN	CD-OE1	7.85	1.41	1.24
1	D	230	LYS	CG-CD	7.82	1.79	1.52
1	B	209	ARG	CZ-NH1	7.65	1.43	1.33
1	A	260	ASP	C-O	7.11	1.36	1.23
1	C	230	LYS	CD-CE	6.95	1.68	1.51
1	A	230	LYS	CE-NZ	6.91	1.66	1.49
1	C	209	ARG	CZ-NH1	6.88	1.42	1.33
1	D	194	ARG	NE-CZ	6.87	1.42	1.33
1	D	67	ASP	CG-OD2	6.50	1.40	1.25
1	A	209	ARG	CZ-NH1	6.30	1.41	1.33
1	D	247	GLY	C-O	6.29	1.33	1.23
1	A	241	GLU	CD-OE1	6.08	1.32	1.25
1	D	181	SER	C-O	6.05	1.34	1.23
1	C	401	CYS	CB-SG	-5.95	1.72	1.81
1	D	192	ARG	CD-NE	5.86	1.56	1.46
1	D	181	SER	CB-OG	5.86	1.49	1.42
1	D	195	GLY	C-O	5.70	1.32	1.23
1	D	99	ARG	CZ-NH1	5.69	1.40	1.33
1	D	439	GLU	CG-CD	5.45	1.60	1.51
1	B	102	GLU	CG-CD	5.40	1.60	1.51
1	C	209	ARG	CZ-NH2	5.35	1.40	1.33
1	D	192	ARG	CZ-NH2	5.29	1.40	1.33
1	B	71	GLU	CG-CD	5.27	1.59	1.51
1	A	439	GLU	CG-CD	5.14	1.59	1.51
1	D	174	GLU	CD-OE2	5.13	1.31	1.25
1	D	192	ARG	CG-CD	5.04	1.64	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ARG	NE-CZ-NH1	-43.84	98.38	120.30
1	D	171	PRO	O-C-N	-24.57	83.38	122.70
1	D	260	ASP	CB-CG-OD1	-23.99	96.71	118.30
1	A	382	ARG	NE-CZ-NH2	-18.45	111.08	120.30
1	D	192	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	D	171	PRO	CA-C-N	14.81	149.78	117.20
1	A	410	LYS	CD-CE-NZ	11.67	138.55	111.70
1	A	102	GLU	OE1-CD-OE2	-10.61	110.57	123.30
1	D	194	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	D	171	PRO	C-N-CA	9.30	144.95	121.70
1	D	192	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	D	194	ARG	NH1-CZ-NH2	8.71	128.98	119.40
1	C	230	LYS	CD-CE-NZ	-8.66	91.79	111.70
1	B	426	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	D	172	GLU	OE1-CD-OE2	8.54	133.54	123.30
1	C	508	LEU	CA-CB-CG	8.03	133.77	115.30
1	B	209	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	B	508	LEU	CA-CB-CG	7.53	132.62	115.30
1	D	347	GLU	CB-CA-C	-7.25	95.90	110.40
1	B	249	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	D	172	GLU	CG-CD-OE1	-6.84	104.61	118.30
1	B	337	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	473	VAL	CB-CA-C	-6.80	98.48	111.40
1	D	508	LEU	CA-CB-CG	6.80	130.94	115.30
1	B	184	LEU	O-C-N	6.57	133.22	122.70
1	C	241	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	A	508	LEU	CA-CB-CG	6.29	129.76	115.30
1	C	86	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	176	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	B	473	VAL	CB-CA-C	-6.03	99.94	111.40
1	C	86	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	D	450	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	347	GLU	CB-CA-C	-5.93	98.53	110.40
1	A	368	VAL	CB-CA-C	-5.91	100.17	111.40
1	A	347	GLU	CB-CA-C	-5.82	98.75	110.40
1	B	347	GLU	CB-CA-C	-5.75	98.89	110.40
1	C	77	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	426	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	126	TYR	OH-CZ-CE2	-5.68	104.78	120.10
1	A	373	MET	CG-SD-CE	-5.49	91.41	100.20
1	C	473	VAL	CB-CA-C	-5.49	100.98	111.40
1	D	396	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	A	230	LYS	CD-CE-NZ	-5.42	99.24	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	102	GLU	CG-CD-OE2	5.31	128.92	118.30
1	A	410	LYS	CG-CD-CE	-5.17	96.38	111.90
1	B	86	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	86	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	442	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	382	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ARG	Sidechain
1	D	172	GLU	Sidechain
1	D	194	ARG	Sidechain
1	D	260	ASP	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3913	0	3994	157	0
1	B	3720	0	3804	146	0
1	C	3913	0	3994	130	0
1	D	3880	0	3957	138	0
2	A	20	0	10	1	0
2	B	20	0	10	1	0
2	C	20	0	10	0	0
2	D	20	0	10	2	0
3	A	9	0	2	1	0
3	B	9	0	2	0	0
3	C	9	0	2	0	0
3	D	9	0	2	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	15550	0	15797	530	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 17.

All (530) 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:230:LYS:CG	1:D:230:LYS:CD	1.79	1.55
1:D:172:GLU:CG	1:D:172:GLU:CD	1.80	1.48
1:D:194:ARG:NH1	1:D:194:ARG:CZ	1.83	1.42
1:B:144:SER:OG	1:B:144:SER:CB	1.70	1.39
1:A:410:LYS:NZ	1:A:410:LYS:CE	1.88	1.36
1:C:230:LYS:NZ	1:C:230:LYS:CE	2.02	1.20
1:B:315:GLU:OE2	1:B:339:ASP:OD2	1.78	1.00
1:D:86:ARG:HB3	1:D:426:ARG:HG2	1.44	0.98
1:B:379:THR:HG22	1:B:380:LYS:HG3	1.45	0.97
1:D:379:THR:HG22	1:D:380:LYS:HG3	1.44	0.96
1:A:86:ARG:HB3	1:A:426:ARG:HG2	1.45	0.96
1:A:442:ARG:HH21	1:B:442:ARG:HH21	1.06	0.95
1:A:442:ARG:HH21	1:B:442:ARG:NH2	1.65	0.94
1:C:379:THR:HG22	1:C:380:LYS:HG3	1.48	0.94
1:A:379:THR:HG22	1:A:380:LYS:HG3	1.49	0.94
1:D:230:LYS:NZ	1:D:230:LYS:CE	2.31	0.93
1:B:86:ARG:HB3	1:B:426:ARG:HG2	1.48	0.92
1:B:261:LEU:HD12	1:B:262:PRO:HD2	1.51	0.91
1:C:86:ARG:HB3	1:C:426:ARG:HG2	1.53	0.90
1:B:162:ILE:HB	1:B:252:VAL:HB	1.50	0.90
1:C:452:THR:HG22	1:C:483:LEU:HD12	1.54	0.89
1:B:452:THR:HG22	1:B:483:LEU:HD12	1.56	0.86
1:D:172:GLU:OE1	1:D:172:GLU:CD	2.13	0.86
1:D:114:ILE:HG12	1:D:152:ALA:HB3	1.58	0.85
1:C:208:VAL:HA	1:C:236:LEU:HD11	1.60	0.83
1:A:442:ARG:NH2	1:B:442:ARG:HH21	1.76	0.83
1:C:453:GLU:HG2	1:C:483:LEU:HD13	1.62	0.82
1:B:175:VAL:HG13	1:B:197:ALA:HA	1.62	0.81
1:C:269:VAL:O	1:C:273:ARG:HG2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:THR:HG22	1:D:483:LEU:HD12	1.63	0.81
1:C:535:PHE:O	1:C:539:SER:OG	1.99	0.81
1:C:374:LEU:HD12	1:C:387:GLU:HB3	1.64	0.80
1:C:442:ARG:HH21	1:D:442:ARG:HH21	1.27	0.80
1:A:374:LEU:HD12	1:A:387:GLU:HB3	1.63	0.78
1:A:86:ARG:HD3	1:A:422:HIS:ND1	1.98	0.78
1:C:114:ILE:HG12	1:C:152:ALA:HB3	1.66	0.78
1:D:204:TYR:CE1	1:D:261:LEU:HD13	2.19	0.77
1:A:453:GLU:HG2	1:A:483:LEU:HD13	1.66	0.76
1:B:535:PHE:O	1:B:539:SER:OG	2.04	0.76
1:B:374:LEU:HD12	1:B:387:GLU:HB3	1.68	0.76
1:C:177:LEU:HD12	1:C:183:VAL:HG21	1.68	0.76
1:A:535:PHE:O	1:A:539:SER:OG	2.05	0.75
1:D:453:GLU:HG2	1:D:483:LEU:HD13	1.67	0.75
1:A:191:PHE:C	1:A:193:THR:H	1.90	0.75
1:A:163:ARG:NH1	1:A:249:ARG:O	2.21	0.74
1:A:191:PHE:O	1:A:193:THR:N	2.21	0.74
1:D:374:LEU:HD12	1:D:387:GLU:HB3	1.68	0.74
1:A:321:LYS:HE3	1:C:79:ASP:OD2	1.86	0.74
1:A:452:THR:HG22	1:A:483:LEU:HD12	1.70	0.72
1:C:85:ALA:HB2	1:C:545:PHE:CE2	2.25	0.72
1:D:86:ARG:HD3	1:D:422:HIS:ND1	2.05	0.71
1:B:114:ILE:HG12	1:B:152:ALA:HB3	1.71	0.71
1:B:269:VAL:O	1:B:273:ARG:HG2	1.91	0.71
1:A:83:VAL:O	1:A:83:VAL:CG1	2.39	0.70
1:B:202:VAL:HG13	1:B:204:TYR:H	1.56	0.70
1:D:535:PHE:O	1:D:539:SER:OG	2.10	0.70
1:B:539:SER:O	1:B:543:ARG:HG3	1.91	0.70
1:D:204:TYR:HE1	1:D:261:LEU:HD13	1.57	0.70
1:D:187:VAL:HG12	1:D:202:VAL:HG12	1.74	0.70
1:B:514:PRO:O	1:B:515:LEU:HD23	1.91	0.69
1:B:83:VAL:CG1	1:B:83:VAL:O	2.40	0.69
1:D:488:ARG:NH1	1:D:510:ARG:HB3	2.07	0.69
1:B:453:GLU:HG2	1:B:483:LEU:HD13	1.74	0.69
1:D:204:TYR:CZ	1:D:206:ASN:HB2	2.28	0.69
1:D:269:VAL:O	1:D:273:ARG:HG2	1.91	0.69
1:B:146:LEU:HB2	1:B:542:LEU:HD12	1.73	0.69
1:C:372:GLN:HG2	1:C:375:GLU:HG3	1.73	0.69
1:B:66:ALA:HB1	1:B:71:GLU:HB3	1.75	0.69
1:C:442:ARG:NH2	1:D:442:ARG:HH21	1.91	0.69
1:D:225:SER:HB3	1:D:242:ASN:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HG12	1:A:152:ALA:HB3	1.75	0.68
1:A:315:GLU:HG2	1:A:336:ALA:CB	2.22	0.68
1:D:487:TYR:O	1:D:488:ARG:HB2	1.92	0.68
1:C:354:LYS:NZ	1:C:397:ASP:OD1	2.26	0.68
1:A:87:SER:HB3	1:A:511:GLY:HA2	1.75	0.68
1:B:86:ARG:HD3	1:B:422:HIS:ND1	2.10	0.67
1:C:177:LEU:HD21	1:C:246:LEU:HD22	1.76	0.67
1:A:360:CYS:SG	1:A:367:VAL:HB	2.35	0.67
1:B:559:ARG:HD2	1:B:564:TYR:CD1	2.28	0.67
1:A:85:ALA:HB2	1:A:545:PHE:CE2	2.30	0.66
1:D:146:LEU:HB2	1:D:542:LEU:HD12	1.77	0.66
1:A:166:ILE:HD12	1:A:166:ILE:H	1.60	0.66
1:B:204:TYR:CE1	1:B:261:LEU:HB2	2.30	0.66
1:C:337:ARG:NH2	1:C:390:ASP:OD1	2.28	0.66
1:C:83:VAL:O	1:C:83:VAL:CG1	2.42	0.66
1:D:230:LYS:CG	1:D:230:LYS:CE	2.73	0.65
1:A:384:MET:CE	1:C:375:GLU:HB2	2.27	0.65
1:A:384:MET:HE3	1:C:375:GLU:HB2	1.79	0.65
1:A:216:ARG:HA	1:A:226:LEU:O	1.97	0.65
1:A:322:ARG:O	1:A:326:ILE:HG13	1.97	0.65
1:B:475:THR:HA	2:B:580:FBP:H61	1.78	0.65
1:A:442:ARG:NH2	1:B:442:ARG:NH2	2.40	0.65
1:A:514:PRO:O	1:A:515:LEU:HD23	1.97	0.65
1:A:68:THR:HB	1:C:440:GLU:OE2	1.97	0.64
1:A:372:GLN:HG2	1:A:375:GLU:HG3	1.80	0.64
1:C:86:ARG:HD3	1:C:422:HIS:ND1	2.12	0.64
1:D:542:LEU:O	1:D:542:LEU:HD22	1.96	0.64
1:D:402:ILE:HG13	1:D:421:GLN:NE2	2.12	0.64
1:B:175:VAL:CG1	1:B:197:ALA:HA	2.26	0.64
1:C:442:ARG:HH21	1:D:442:ARG:NH2	1.95	0.64
1:D:83:VAL:CG1	1:D:83:VAL:O	2.45	0.64
1:B:321:LYS:HE3	1:D:79:ASP:OD2	1.98	0.64
1:B:210:VAL:HG12	1:B:257:ALA:HB1	1.78	0.63
1:C:210:VAL:O	1:C:212:PRO:HD3	1.98	0.63
1:A:375:GLU:HB2	1:C:384:MET:CE	2.29	0.63
1:B:146:LEU:CB	1:B:542:LEU:HD12	2.29	0.63
1:A:402:ILE:HG13	1:A:421:GLN:NE2	2.14	0.63
1:A:488:ARG:NH1	1:A:510:ARG:HB3	2.14	0.62
1:C:559:ARG:HD2	1:C:564:TYR:CD1	2.33	0.62
1:C:337:ARG:HH22	1:C:390:ASP:CG	2.02	0.62
1:A:83:VAL:HG12	1:A:83:VAL:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ARG:HD2	1:A:564:TYR:CD1	2.35	0.62
1:D:453:GLU:CG	1:D:483:LEU:HD13	2.30	0.62
1:D:322:ARG:O	1:D:326:ILE:HG13	2.00	0.62
1:B:117:LEU:HD11	1:B:131:ILE:HG13	1.82	0.62
1:A:204:TYR:CZ	1:A:206:ASN:HB2	2.35	0.61
1:C:210:VAL:O	1:C:212:PRO:CD	2.48	0.61
1:A:506:VAL:HG13	1:A:512:VAL:HG11	1.82	0.61
1:B:542:LEU:O	1:B:542:LEU:HD22	2.00	0.61
1:D:315:GLU:HG2	1:D:336:ALA:CB	2.31	0.61
1:C:473:VAL:HG13	1:C:555:VAL:HB	1.82	0.61
1:A:539:SER:O	1:A:543:ARG:HG3	2.01	0.60
1:B:372:GLN:HG2	1:B:375:GLU:HG3	1.83	0.60
1:D:349:VAL:O	1:D:352:ALA:N	2.34	0.60
1:D:230:LYS:CB	1:D:230:LYS:CD	2.75	0.60
1:D:194:ARG:NE	1:D:194:ARG:NH1	2.47	0.60
1:B:177:LEU:HD12	1:B:183:VAL:HG21	1.82	0.60
1:D:86:ARG:HB3	1:D:426:ARG:CG	2.24	0.60
1:D:85:ALA:HB2	1:D:545:PHE:CE2	2.36	0.60
1:D:337:ARG:HH22	1:D:390:ASP:CG	2.04	0.60
1:C:460:VAL:HG22	1:C:489:PRO:HG3	1.82	0.60
1:C:66:ALA:HB1	1:C:71:GLU:HB3	1.83	0.59
1:B:99:ARG:NH2	1:B:129:GLU:OE1	2.33	0.59
1:B:79:ASP:OD2	1:D:321:LYS:HE3	2.02	0.59
1:D:557:GLY:HA3	2:D:580:FBP:O3	2.02	0.59
1:D:315:GLU:HG2	1:D:336:ALA:HB3	1.83	0.59
1:D:514:PRO:O	1:D:515:LEU:HD23	2.02	0.59
1:A:320:VAL:HG11	1:C:78:ILE:HD13	1.84	0.59
1:B:225:SER:HB3	1:B:242:ASN:HB2	1.83	0.59
1:C:225:SER:HB3	1:C:242:ASN:HB2	1.84	0.59
1:D:506:VAL:CG1	1:D:512:VAL:HG11	2.32	0.59
1:A:192:ARG:HG2	1:A:192:ARG:O	2.02	0.59
1:A:117:LEU:HD11	1:A:131:ILE:HG13	1.84	0.58
1:B:420:MET:O	1:B:424:ILE:HG13	2.04	0.58
1:D:460:VAL:HG22	1:D:489:PRO:HG3	1.86	0.58
1:B:183:VAL:O	1:B:238:THR:OG1	2.18	0.58
1:C:177:LEU:CD1	1:C:183:VAL:HG21	2.34	0.58
1:D:506:VAL:CG1	1:D:512:VAL:CG1	2.82	0.58
1:A:215:GLY:O	1:A:227:VAL:HA	2.04	0.58
1:C:230:LYS:CD	1:C:230:LYS:NZ	2.67	0.58
1:D:83:VAL:HG12	1:D:83:VAL:O	2.03	0.58
1:D:506:VAL:HG13	1:D:512:VAL:HG11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:NZ	1:A:397:ASP:OD1	2.33	0.57
1:C:539:SER:O	1:C:543:ARG:HG3	2.05	0.57
1:A:85:ALA:HB2	1:A:545:PHE:HE2	1.70	0.57
1:D:441:LEU:O	1:D:442:ARG:C	2.39	0.57
1:D:559:ARG:HD2	1:D:564:TYR:CD1	2.39	0.57
1:B:86:ARG:HB3	1:B:426:ARG:CG	2.29	0.57
1:B:213:VAL:HA	1:B:228:VAL:HG12	1.87	0.57
1:D:137:ALA:O	1:D:140:SER:OG	2.15	0.57
1:B:85:ALA:HB2	1:B:545:PHE:CE2	2.39	0.56
1:A:204:TYR:CE2	1:A:206:ASN:HB2	2.39	0.56
1:C:167:LEU:O	1:C:170:GLY:N	2.33	0.56
1:C:230:LYS:HB2	1:C:237:VAL:HB	1.88	0.56
1:D:539:SER:O	1:D:543:ARG:HG3	2.05	0.56
1:D:281:ASP:OD2	1:D:504:ARG:NE	2.32	0.56
1:B:219:ILE:HA	1:B:251:GLY:O	2.05	0.56
1:A:375:GLU:HB2	1:C:384:MET:HE3	1.87	0.56
1:D:157:THR:HG22	1:D:286:SER:HB2	1.87	0.56
1:A:440:GLU:OE2	1:C:68:THR:HB	2.05	0.56
1:A:155:LEU:C	1:A:155:LEU:HD23	2.26	0.56
1:A:506:VAL:CG1	1:A:512:VAL:CG1	2.83	0.56
1:C:86:ARG:HG2	1:C:422:HIS:CE1	2.41	0.55
1:C:488:ARG:NH1	1:C:510:ARG:HB3	2.22	0.55
1:A:487:TYR:O	1:A:488:ARG:HB2	2.06	0.55
1:B:286:SER:HA	1:B:313:LYS:HE2	1.89	0.55
1:A:506:VAL:CG1	1:A:512:VAL:HG11	2.36	0.55
1:C:162:ILE:HG22	1:C:252:VAL:HB	1.86	0.55
1:D:175:VAL:HG12	1:D:177:LEU:CD2	2.37	0.55
1:C:117:LEU:HD11	1:C:131:ILE:HG13	1.88	0.55
1:A:228:VAL:HG22	1:A:238:THR:HG22	1.89	0.55
1:B:288:VAL:HG12	1:B:326:ILE:HD13	1.89	0.55
1:B:159:GLY:O	1:B:161:GLU:N	2.36	0.55
1:B:86:ARG:NH2	1:B:113:ASN:OD1	2.40	0.55
1:C:453:GLU:CG	1:C:483:LEU:HD13	2.35	0.55
1:A:337:ARG:HH22	1:A:390:ASP:CG	2.11	0.55
1:D:230:LYS:HB2	1:D:237:VAL:HB	1.89	0.54
1:D:337:ARG:NH2	1:D:390:ASP:OD1	2.39	0.54
1:A:473:VAL:HG13	1:A:555:VAL:HB	1.90	0.54
1:C:86:ARG:NH2	1:C:113:ASN:OD1	2.40	0.54
1:A:191:PHE:C	1:A:193:THR:N	2.55	0.54
1:A:453:GLU:CG	1:A:483:LEU:HD13	2.38	0.54
1:B:87:SER:HB2	1:B:511:GLY:CA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:PRO:HG2	1:D:514:PRO:HG2	1.88	0.54
1:A:228:VAL:HA	1:A:238:THR:HG22	1.89	0.54
1:B:460:VAL:HG22	1:B:489:PRO:HG3	1.90	0.54
1:C:349:VAL:O	1:C:352:ALA:N	2.41	0.54
1:A:475:THR:HA	2:A:580:FBP:H61	1.89	0.54
1:A:158:LYS:HG2	1:A:161:GLU:HG3	1.89	0.54
1:B:322:ARG:O	1:B:326:ILE:HG13	2.07	0.54
1:B:87:SER:CB	1:B:511:GLY:HA2	2.38	0.54
1:C:514:PRO:O	1:C:515:LEU:HD23	2.08	0.54
1:C:446:PRO:O	1:C:447:LEU:O	2.25	0.54
1:D:194:ARG:CD	1:D:194:ARG:NH1	2.70	0.54
1:B:259:VAL:HG12	1:B:261:LEU:HB3	1.90	0.53
1:A:293:ASP:O	1:A:297:VAL:HG23	2.07	0.53
1:C:542:LEU:HD22	1:C:542:LEU:O	2.08	0.53
1:D:86:ARG:NH2	1:D:113:ASN:OD1	2.42	0.53
1:A:288:VAL:HG12	1:A:326:ILE:HD13	1.89	0.53
1:D:372:GLN:HG2	1:D:375:GLU:HG3	1.89	0.53
1:D:473:VAL:HG13	1:D:555:VAL:HB	1.89	0.53
1:B:183:VAL:HG22	1:B:198:ASN:HA	1.90	0.53
1:D:117:LEU:HD11	1:D:131:ILE:HG13	1.91	0.53
1:A:271:ASP:O	1:A:274:PHE:HB3	2.08	0.53
1:B:488:ARG:NH1	1:B:510:ARG:HB3	2.22	0.53
1:C:322:ARG:O	1:C:326:ILE:HG13	2.09	0.53
1:D:181:SER:O	1:D:239:GLN:HG3	2.08	0.53
1:B:85:ALA:HB2	1:B:545:PHE:HE2	1.73	0.53
1:A:369:CYS:SG	1:A:373:MET:CE	2.97	0.53
1:A:184:LEU:HG	1:A:186:THR:HG22	1.91	0.53
1:A:542:LEU:HD22	1:A:542:LEU:O	2.09	0.53
1:C:461:GLU:OE1	1:D:461:GLU:OE1	2.27	0.53
1:A:87:SER:CB	1:A:511:GLY:HA2	2.37	0.52
1:D:438:PHE:CZ	1:D:442:ARG:HD3	2.45	0.52
1:C:395:VAL:O	1:C:510:ARG:NH1	2.33	0.52
1:D:191:PHE:O	1:D:201:TRP:HB2	2.09	0.52
1:A:447:LEU:HD13	1:B:467:CYS:SG	2.49	0.52
1:C:208:VAL:HA	1:C:236:LEU:CD1	2.36	0.52
1:A:303:PRO:C	1:A:305:GLY:H	2.13	0.52
1:D:499:SER:O	1:D:500:ALA:C	2.48	0.52
1:B:163:ARG:HA	1:B:250:LYS:O	2.10	0.52
1:A:66:ALA:HB1	1:A:71:GLU:HB3	1.90	0.52
1:B:83:VAL:HG13	1:B:83:VAL:O	2.10	0.52
1:C:567:ILE:HG12	1:D:569:ARG:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:THR:HG23	1:B:250:LYS:H	1.75	0.52
1:B:202:VAL:HG11	1:B:207:ILE:HD12	1.91	0.51
1:C:288:VAL:HG12	1:C:326:ILE:HD13	1.92	0.51
1:C:315:GLU:HG2	1:C:336:ALA:CB	2.41	0.51
1:C:87:SER:CB	1:C:511:GLY:HA2	2.41	0.51
1:B:78:ILE:HD13	1:D:320:VAL:HG11	1.93	0.51
1:A:506:VAL:HG13	1:A:512:VAL:CG1	2.41	0.51
1:D:87:SER:CB	1:D:511:GLY:HA2	2.41	0.51
1:A:206:ASN:O	1:A:210:VAL:HG23	2.11	0.51
1:D:66:ALA:HB1	1:D:71:GLU:HB3	1.92	0.51
1:A:284:PHE:HD1	1:A:311:ILE:HB	1.75	0.51
1:B:487:TYR:O	1:B:488:ARG:HB2	2.10	0.50
1:D:296:ALA:O	1:D:299:ALA:HB3	2.11	0.50
1:B:68:THR:HB	1:D:440:GLU:OE2	2.11	0.50
1:C:360:CYS:HB3	1:C:365:LYS:O	2.10	0.50
1:C:150:PRO:HG2	1:C:514:PRO:HG2	1.93	0.50
1:C:446:PRO:C	1:C:447:LEU:O	2.48	0.50
1:B:224:ILE:CD1	1:B:244:GLY:HA3	2.41	0.50
1:B:144:SER:OG	1:B:144:SER:CA	2.53	0.50
1:B:453:GLU:CG	1:B:483:LEU:HD13	2.40	0.50
1:B:87:SER:HB2	1:B:511:GLY:N	2.26	0.50
1:B:183:VAL:HG13	1:B:198:ASN:O	2.11	0.50
1:A:349:VAL:O	1:A:352:ALA:N	2.45	0.50
1:D:87:SER:HB3	1:D:511:GLY:HA2	1.93	0.50
1:B:228:VAL:CG2	1:B:238:THR:HG22	2.42	0.50
1:A:286:SER:HA	1:A:313:LYS:HE2	1.93	0.50
1:D:293:ASP:O	1:D:297:VAL:HG23	2.12	0.50
1:A:91:ILE:HB	1:A:403:MET:HG3	1.94	0.49
1:D:213:VAL:HG13	1:D:229:GLN:HA	1.93	0.49
1:B:349:VAL:O	1:B:352:ALA:N	2.45	0.49
1:D:378:ILE:O	1:D:378:ILE:HG22	2.12	0.49
1:D:286:SER:HA	1:D:313:LYS:HE2	1.93	0.49
1:C:204:TYR:O	1:C:205:PRO:C	2.50	0.49
1:B:164:THR:HG21	1:B:246:LEU:HD11	1.94	0.49
1:C:163:ARG:HD2	1:C:249:ARG:HH21	1.77	0.49
1:A:70:LEU:CD2	1:C:362:LEU:HD12	2.43	0.49
1:A:91:ILE:HG23	1:A:114:ILE:HG22	1.95	0.49
1:B:440:GLU:OE2	1:D:68:THR:HB	2.13	0.49
1:D:219:ILE:HG12	1:D:252:VAL:HG22	1.95	0.49
1:D:403:MET:HG2	1:D:404:LEU:N	2.27	0.49
1:B:473:VAL:HG13	1:B:555:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG11	1:A:258:GLN:O	2.13	0.49
1:B:102:GLU:OE1	1:B:105:LYS:HD2	2.13	0.49
1:C:217:ILE:HG12	1:C:254:LEU:CD2	2.42	0.49
1:B:375:GLU:HB2	1:D:384:MET:CE	2.43	0.49
1:A:269:VAL:O	1:A:273:ARG:HG2	2.11	0.49
1:B:446:PRO:O	1:B:447:LEU:O	2.30	0.49
1:C:448:SER:OG	1:C:449:ARG:N	2.46	0.49
1:B:315:GLU:HG2	1:B:336:ALA:CB	2.43	0.49
1:C:438:PHE:CZ	1:C:442:ARG:HD3	2.48	0.49
1:C:87:SER:HB2	1:C:511:GLY:CA	2.43	0.49
1:A:70:LEU:HD21	1:C:362:LEU:HD12	1.95	0.49
1:B:337:ARG:HH22	1:B:390:ASP:CG	2.14	0.48
1:C:264:LEU:HD12	1:C:268:ASP:CB	2.43	0.48
1:B:158:LYS:O	1:B:161:GLU:HG3	2.13	0.48
1:A:71:GLU:O	1:A:72:HIS:C	2.50	0.48
1:D:210:VAL:O	1:D:212:PRO:HD3	2.12	0.48
1:B:537:ILE:O	1:B:540:GLY:N	2.47	0.48
1:D:448:SER:OG	1:D:449:ARG:N	2.45	0.48
1:D:172:GLU:CD	1:D:172:GLU:CB	2.74	0.48
1:A:87:SER:HB2	1:A:511:GLY:N	2.28	0.48
1:D:194:ARG:HH11	1:D:194:ARG:HD2	1.77	0.48
1:B:219:ILE:HG23	1:B:251:GLY:O	2.13	0.48
1:C:325:GLU:HG3	1:C:326:ILE:N	2.29	0.48
1:A:157:THR:HG22	1:A:286:SER:H	1.77	0.48
1:B:221:ASP:HA	1:B:342:ILE:HD11	1.94	0.48
1:B:216:ARG:HD2	1:B:218:TYR:CZ	2.48	0.48
1:D:485:SER:O	1:D:486:ARG:C	2.52	0.48
1:C:293:ASP:O	1:C:297:VAL:HG23	2.14	0.48
1:A:369:CYS:SG	1:A:373:MET:HE1	2.53	0.48
1:C:315:GLU:HG2	1:C:336:ALA:HB3	1.95	0.48
1:B:271:ASP:O	1:B:274:PHE:HB3	2.14	0.48
1:C:202:VAL:HG13	1:C:204:TYR:H	1.78	0.48
1:A:521:PRO:HA	1:A:528:ASP:OD1	2.13	0.48
1:D:360:CYS:HB3	1:D:365:LYS:O	2.13	0.48
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.69	0.48
1:C:499:SER:O	1:C:500:ALA:C	2.52	0.48
1:C:196:ASN:C	1:C:196:ASN:OD1	2.51	0.48
1:B:144:SER:HG	1:B:144:SER:CB	2.13	0.48
1:A:315:GLU:HG2	1:A:336:ALA:HB3	1.94	0.48
1:C:83:VAL:O	1:C:83:VAL:HG12	2.14	0.47
1:D:348:LYS:O	1:D:349:VAL:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:HA	1:B:264:LEU:HD12	1.73	0.47
1:D:188:ASP:OD2	1:D:190:ALA:HB3	2.14	0.47
1:B:83:VAL:HG12	1:B:83:VAL:O	2.14	0.47
1:D:254:LEU:HD12	1:D:259:VAL:HG22	1.96	0.47
1:B:104:LEU:O	1:B:108:ILE:HG13	2.14	0.47
1:A:315:GLU:HB3	1:A:339:ASP:HB2	1.96	0.47
1:A:367:VAL:O	1:A:367:VAL:HG13	2.13	0.47
1:B:159:GLY:C	1:B:161:GLU:H	2.17	0.47
1:A:129:GLU:O	1:A:130:SER:C	2.53	0.47
1:B:362:LEU:HD12	1:D:70:LEU:CD2	2.44	0.47
1:A:208:VAL:HG12	1:A:236:LEU:HG	1.97	0.47
1:C:559:ARG:HD3	1:C:560:PRO:O	2.15	0.47
1:A:347:GLU:OE2	1:A:347:GLU:N	2.27	0.47
1:A:460:VAL:HG22	1:A:489:PRO:HG3	1.96	0.47
1:D:231:ILE:HG12	1:D:236:LEU:HD23	1.96	0.47
1:A:403:MET:HG2	1:A:404:LEU:N	2.30	0.47
1:D:358:GLY:O	1:D:361:ASN:HB2	2.15	0.47
1:B:337:ARG:NH2	1:B:390:ASP:OD1	2.44	0.46
1:A:164:THR:HA	1:A:201:TRP:O	2.14	0.46
1:D:377:MET:C	1:D:379:THR:H	2.18	0.46
1:C:168:GLN:C	1:C:170:GLY:H	2.17	0.46
1:A:357:ILE:O	1:A:358:GLY:C	2.50	0.46
1:B:141:PHE:N	1:B:141:PHE:CD1	2.83	0.46
1:A:375:GLU:HB2	1:C:384:MET:HE1	1.97	0.46
1:A:323:PHE:CE1	1:A:333:ILE:HG13	2.50	0.46
1:D:354:LYS:NZ	1:D:397:ASP:OD1	2.42	0.46
1:B:559:ARG:HD2	1:B:564:TYR:CE1	2.50	0.46
1:B:341:GLY:HA3	1:D:385:ARG:HE	1.80	0.46
1:B:284:PHE:HD1	1:B:311:ILE:HB	1.79	0.46
1:A:146:LEU:HB2	1:A:542:LEU:HD12	1.98	0.46
1:B:483:LEU:O	1:B:486:ARG:HB2	2.16	0.46
1:B:449:ARG:O	1:B:451:PRO:HD3	2.16	0.46
1:A:97:ALA:O	1:A:103:ARG:HD3	2.16	0.46
1:D:172:GLU:OE1	1:D:172:GLU:N	2.49	0.46
1:B:301:LEU:HD12	1:B:301:LEU:HA	1.70	0.46
1:B:86:ARG:HA	1:B:429:GLU:OE1	2.14	0.46
1:C:525:TRP:CE2	1:C:560:PRO:HG3	2.50	0.46
1:B:225:SER:OG	1:B:241:GLU:HB3	2.15	0.46
1:A:393:ASN:O	1:A:397:ASP:N	2.47	0.46
1:C:166:ILE:CG2	1:C:167:LEU:N	2.79	0.46
1:C:370:ALA:O	1:C:371:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:MET:C	1:B:379:THR:H	2.18	0.45
1:A:276:VAL:HG11	1:A:304:GLU:HB2	1.98	0.45
1:B:452:THR:CG2	1:B:483:LEU:HD12	2.37	0.45
1:D:475:THR:HA	2:D:580:FBP:H61	1.98	0.45
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.82	0.45
1:B:320:VAL:HG11	1:D:78:ILE:HD13	1.98	0.45
1:A:191:PHE:CD1	1:A:191:PHE:N	2.84	0.45
1:B:315:GLU:HG2	1:B:336:ALA:HB3	1.97	0.45
1:C:85:ALA:HB2	1:C:545:PHE:HE2	1.79	0.45
1:B:525:TRP:CE2	1:B:560:PRO:HG3	2.51	0.45
1:C:487:TYR:O	1:C:488:ARG:HB2	2.15	0.45
1:D:403:MET:HG2	1:D:404:LEU:H	1.82	0.45
1:B:296:ALA:O	1:B:299:ALA:HB3	2.17	0.45
1:B:360:CYS:HB3	1:B:365:LYS:O	2.16	0.45
1:B:276:VAL:HG11	1:B:304:GLU:HB2	1.99	0.45
1:D:204:TYR:CE1	1:D:206:ASN:HB2	2.51	0.45
1:A:485:SER:O	1:A:486:ARG:C	2.55	0.45
1:A:384:MET:HE1	1:C:375:GLU:HB2	1.98	0.45
1:A:210:VAL:HG12	1:A:257:ALA:HB1	1.98	0.45
1:B:304:GLU:HG2	1:B:304:GLU:H	1.59	0.45
1:C:83:VAL:O	1:C:83:VAL:HG13	2.17	0.45
1:C:87:SER:HB2	1:C:511:GLY:N	2.32	0.45
1:A:385:ARG:HG2	1:C:372:GLN:OE1	2.17	0.45
1:C:323:PHE:O	1:C:324:ASP:C	2.55	0.45
1:A:377:MET:C	1:A:379:THR:H	2.20	0.44
1:A:87:SER:CB	1:A:511:GLY:CA	2.96	0.44
1:A:372:GLN:HB2	1:C:385:ARG:HB2	1.99	0.44
1:D:336:ALA:HB1	3:D:581:PGA:C1	2.47	0.44
1:B:157:THR:HG22	1:B:286:SER:HB2	1.98	0.44
1:B:384:MET:HE3	1:D:375:GLU:HB2	1.99	0.44
1:C:284:PHE:HD1	1:C:311:ILE:HB	1.82	0.44
1:A:369:CYS:SG	1:A:373:MET:HE3	2.56	0.44
1:B:354:LYS:NZ	1:B:397:ASP:OD1	2.45	0.44
1:B:225:SER:O	1:B:226:LEU:HD23	2.18	0.44
1:C:168:GLN:O	1:C:170:GLY:N	2.51	0.44
1:C:420:MET:O	1:C:424:ILE:HG13	2.16	0.44
1:C:168:GLN:C	1:C:170:GLY:N	2.70	0.44
1:B:384:MET:CE	1:D:375:GLU:HB2	2.48	0.44
1:B:293:ASP:O	1:B:297:VAL:HG23	2.18	0.44
1:C:506:VAL:CG1	1:C:512:VAL:CG1	2.95	0.44
1:B:372:GLN:HA	1:B:375:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:SER:O	1:D:239:GLN:CG	2.65	0.44
1:A:294:VAL:O	1:A:295:ALA:C	2.56	0.44
1:C:86:ARG:HB3	1:C:426:ARG:CG	2.37	0.44
1:B:337:ARG:HD3	1:B:370:ALA:O	2.17	0.44
1:C:286:SER:HA	1:C:313:LYS:HE2	1.99	0.44
1:D:264:LEU:HA	1:D:264:LEU:HD12	1.79	0.44
1:A:86:ARG:HG2	1:A:422:HIS:CE1	2.52	0.44
1:A:441:LEU:O	1:A:442:ARG:C	2.53	0.44
1:C:162:ILE:HG12	1:C:204:TYR:HB2	2.00	0.44
1:A:479:ARG:HG3	1:A:479:ARG:HH11	1.83	0.44
1:A:370:ALA:O	1:A:371:THR:HB	2.17	0.44
1:C:340:LEU:O	1:C:344:ILE:HG12	2.17	0.44
1:D:86:ARG:HA	1:D:429:GLU:OE1	2.18	0.43
1:D:187:VAL:CG1	1:D:202:VAL:HG12	2.46	0.43
1:D:276:VAL:HG11	1:D:304:GLU:HB2	1.99	0.43
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.88	0.43
1:D:521:PRO:HA	1:D:528:ASP:OD1	2.18	0.43
1:D:155:LEU:C	1:D:155:LEU:HD23	2.39	0.43
1:A:102:GLU:OE1	1:A:105:LYS:HD2	2.19	0.43
1:C:192:ARG:HA	1:C:201:TRP:CD2	2.54	0.43
1:B:499:SER:O	1:B:500:ALA:C	2.56	0.43
1:A:202:VAL:HG13	1:A:204:TYR:H	1.83	0.43
1:B:228:VAL:HG23	1:B:238:THR:HG22	1.99	0.43
1:C:506:VAL:HG13	1:C:512:VAL:HG11	2.00	0.43
1:D:87:SER:HB2	1:D:511:GLY:N	2.34	0.43
1:B:89:SER:HA	1:B:113:ASN:OD1	2.18	0.43
1:B:162:ILE:CB	1:B:252:VAL:HB	2.35	0.43
1:B:87:SER:HB2	1:B:511:GLY:HA2	1.95	0.43
1:C:162:ILE:O	1:C:162:ILE:HG22	2.18	0.43
1:C:87:SER:CB	1:C:511:GLY:CA	2.96	0.43
1:D:362:LEU:O	1:D:486:ARG:NH2	2.51	0.43
1:A:434:HIS:O	1:A:435:ARG:C	2.57	0.43
1:D:123:SER:O	1:D:126:TYR:HB3	2.18	0.43
1:C:348:LYS:O	1:C:349:VAL:C	2.57	0.43
1:D:204:TYR:CE1	1:D:261:LEU:CD1	2.95	0.43
1:A:258:GLN:H	1:A:258:GLN:HG2	1.70	0.43
1:A:303:PRO:C	1:A:305:GLY:N	2.72	0.43
1:B:97:ALA:O	1:B:103:ARG:HD3	2.18	0.43
1:B:515:LEU:HD11	1:B:539:SER:HB2	2.00	0.43
1:C:177:LEU:HD21	1:C:246:LEU:CD2	2.48	0.43
1:A:559:ARG:HD3	1:A:560:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLU:HG2	1:C:423:ALA:HB1	2.01	0.43
1:B:218:TYR:C	1:B:219:ILE:HG13	2.39	0.42
1:C:177:LEU:HD23	1:C:246:LEU:HB2	2.01	0.42
1:A:167:LEU:O	1:A:168:GLN:C	2.57	0.42
1:C:388:THR:HG22	1:C:389:SER:N	2.34	0.42
1:D:284:PHE:HD1	1:D:311:ILE:HB	1.84	0.42
1:D:525:TRP:CE2	1:D:560:PRO:HG3	2.54	0.42
1:D:146:LEU:CB	1:D:542:LEU:HD12	2.46	0.42
1:A:150:PRO:HG2	1:A:514:PRO:HG2	2.01	0.42
1:A:475:THR:OG1	1:A:478:GLY:N	2.48	0.42
1:D:303:PRO:C	1:D:305:GLY:H	2.23	0.42
1:C:299:ALA:O	1:C:300:ALA:C	2.57	0.42
1:B:323:PHE:O	1:B:324:ASP:C	2.58	0.42
1:C:231:ILE:HD13	1:C:232:GLY:O	2.18	0.42
1:A:123:SER:O	1:A:126:TYR:HB3	2.19	0.42
1:A:478:GLY:O	1:A:479:ARG:C	2.57	0.42
1:B:259:VAL:HG12	1:B:261:LEU:CB	2.50	0.42
1:A:403:MET:HG2	1:A:404:LEU:H	1.84	0.42
1:C:206:ASN:O	1:C:210:VAL:HG23	2.19	0.42
1:A:194:ARG:CB	1:A:194:ARG:HH11	2.33	0.42
1:C:569:ARG:HG2	1:D:567:ILE:HG12	2.01	0.42
1:D:419:LYS:O	1:D:422:HIS:HB3	2.19	0.42
1:B:385:ARG:NE	1:D:341:GLY:HA3	2.35	0.42
1:A:446:PRO:C	1:A:447:LEU:O	2.57	0.42
1:A:200:VAL:HG12	1:A:246:LEU:HD21	2.00	0.42
1:A:137:ALA:O	1:A:140:SER:OG	2.17	0.42
1:D:466:CYS:O	1:D:467:CYS:C	2.56	0.42
1:B:70:LEU:CD2	1:D:362:LEU:HD12	2.50	0.42
1:B:514:PRO:C	1:B:515:LEU:HD23	2.40	0.42
1:B:135:ARG:O	1:B:139:GLU:HG2	2.19	0.42
1:A:286:SER:CA	1:A:313:LYS:HE2	2.50	0.42
1:A:232:GLY:HA2	1:A:233:PRO:HD3	1.84	0.42
1:B:559:ARG:HD3	1:B:560:PRO:O	2.20	0.41
1:B:466:CYS:O	1:B:467:CYS:C	2.56	0.41
1:A:347:GLU:CG	1:C:423:ALA:HB1	2.49	0.41
1:C:506:VAL:HG13	1:C:512:VAL:CG1	2.51	0.41
1:B:303:PRO:C	1:B:305:GLY:H	2.23	0.41
1:B:264:LEU:HD12	1:B:268:ASP:CB	2.50	0.41
1:D:87:SER:H	1:D:429:GLU:CD	2.23	0.41
1:B:206:ASN:O	1:B:210:VAL:HG23	2.20	0.41
1:C:559:ARG:HD2	1:C:564:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ARG:HG2	1:D:372:GLN:OE1	2.19	0.41
1:A:175:VAL:HG11	1:A:197:ALA:N	2.35	0.41
1:D:129:GLU:O	1:D:130:SER:C	2.58	0.41
1:A:207:ILE:C	1:A:209:ARG:H	2.24	0.41
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.74	0.41
1:C:61:LEU:HA	1:C:61:LEU:HD12	1.95	0.41
1:C:230:LYS:CB	1:C:237:VAL:HB	2.51	0.41
1:D:281:ASP:CG	1:D:504:ARG:HE	2.19	0.41
1:D:157:THR:HG22	1:D:286:SER:CB	2.51	0.41
1:D:98:SER:HB2	1:D:107:MET:SD	2.60	0.41
1:D:175:VAL:HG12	1:D:177:LEU:HD22	2.03	0.41
1:C:87:SER:HB3	1:C:511:GLY:HA2	2.02	0.41
1:C:296:ALA:O	1:C:299:ALA:HB3	2.20	0.41
1:B:478:GLY:O	1:B:479:ARG:C	2.58	0.41
1:A:86:ARG:NH2	1:A:113:ASN:OD1	2.54	0.41
1:A:437:LEU:HD21	1:A:488:ARG:HG3	2.03	0.41
1:D:68:THR:OG1	1:D:71:GLU:HB2	2.20	0.41
1:D:357:ILE:O	1:D:358:GLY:C	2.57	0.41
1:A:188:ASP:HA	1:A:189:PRO:HD3	1.89	0.41
1:A:86:ARG:HA	1:A:429:GLU:OE1	2.20	0.41
1:C:372:GLN:HA	1:C:375:GLU:HG2	2.02	0.41
1:B:446:PRO:C	1:B:447:LEU:O	2.58	0.41
1:C:210:VAL:O	1:C:212:PRO:HD2	2.21	0.41
1:A:559:ARG:HD2	1:A:564:TYR:CE1	2.56	0.41
1:A:274:PHE:C	1:A:274:PHE:CD2	2.94	0.41
1:C:274:PHE:C	1:C:274:PHE:CD2	2.94	0.41
1:A:99:ARG:HD3	1:A:99:ARG:HH11	1.72	0.41
1:B:377:MET:C	1:B:379:THR:N	2.74	0.41
1:A:483:LEU:O	1:A:486:ARG:HB2	2.21	0.41
1:A:194:ARG:NH1	1:A:194:ARG:HB3	2.36	0.41
1:A:188:ASP:OD1	1:A:188:ASP:C	2.60	0.41
1:B:521:PRO:HA	1:B:528:ASP:OD1	2.21	0.41
1:C:182:GLN:O	1:C:198:ASN:OD1	2.39	0.41
1:C:187:VAL:O	1:C:189:PRO:HD3	2.20	0.41
1:C:129:GLU:O	1:C:130:SER:C	2.57	0.41
1:A:336:ALA:HB1	3:A:581:PGA:C1	2.52	0.40
1:A:525:TRP:CE2	1:A:560:PRO:HG3	2.56	0.40
1:A:276:VAL:HG21	1:A:301:LEU:O	2.21	0.40
1:D:334:MET:HA	1:D:368:VAL:HB	2.03	0.40
1:A:98:SER:HB2	1:A:107:MET:SD	2.61	0.40
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:O	1:A:230:LYS:HD3	2.21	0.40
1:B:98:SER:HA	1:B:103:ARG:HG2	2.04	0.40
1:B:325:GLU:HG3	1:B:326:ILE:N	2.36	0.40
1:B:517:TYR:CE2	1:B:519:GLU:HB2	2.57	0.40
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.78	0.40
1:A:87:SER:HB3	1:A:511:GLY:CA	2.47	0.40
1:A:506:VAL:CG1	1:A:512:VAL:HG12	2.51	0.40
1:D:91:ILE:HB	1:D:403:MET:HG3	2.04	0.40
1:C:70:LEU:O	1:C:73:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/528 (98%)	454 (88%)	44 (8%)	17 (3%)	5	14
1	B	483/528 (92%)	436 (90%)	38 (8%)	9 (2%)	10	28
1	C	515/528 (98%)	465 (90%)	37 (7%)	13 (2%)	7	21
1	D	508/528 (96%)	452 (89%)	43 (8%)	13 (3%)	7	19
All	All	2021/2112 (96%)	1807 (89%)	162 (8%)	52 (3%)	7	19

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ARG
1	B	447	LEU
1	C	171	PRO
1	C	433	TYR
1	D	172	GLU
1	D	197	ALA

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Mol	Chain	Res	Type
1	D	447	LEU
1	A	83	VAL
1	A	447	LEU
1	B	59	GLN
1	B	287	PHE
1	C	83	VAL
1	C	168	GLN
1	C	169	GLY
1	C	447	LEU
1	D	83	VAL
1	D	259	VAL
1	D	433	TYR
1	A	197	ALA
1	A	328	GLU
1	A	433	TYR
1	B	83	VAL
1	B	220	ASP
1	C	164	THR
1	D	206	ASN
1	A	84	ALA
1	A	160	PRO
1	A	299	ALA
1	A	304	GLU
1	B	160	PRO
1	D	193	THR
1	D	287	PHE
1	A	193	THR
1	A	220	ASP
1	A	371	THR
1	A	486	ARG
1	B	249	ARG
1	C	160	PRO
1	C	206	ASN
1	C	220	ASP
1	C	566	ASN
1	D	160	PRO
1	D	299	ALA
1	B	371	THR
1	A	213	VAL
1	A	338	GLY
1	B	338	GLY
1	C	205	PRO

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Mol	Chain	Res	Type
1	D	178	VAL
1	D	338	GLY
1	C	338	GLY
1	A	398	GLY

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	414/423 (98%)	366 (88%)	48 (12%)	7	18
1	B	394/423 (93%)	354 (90%)	40 (10%)	9	24
1	C	414/423 (98%)	366 (88%)	48 (12%)	7	18
1	D	411/423 (97%)	364 (89%)	47 (11%)	7	19
All	All	1633/1692 (96%)	1450 (89%)	183 (11%)	7	20

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	83	VAL
1	A	86	ARG
1	A	87	SER
1	A	99	ARG
1	A	100	SER
1	A	103	ARG
1	A	104	LEU
1	A	120	SER
1	A	124	HIS
1	A	157	THR
1	A	174	GLU
1	A	182	GLN
1	A	186	THR
1	A	187	VAL
1	A	202	VAL
1	A	210	VAL

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Mol	Chain	Res	Type
1	A	231	ILE
1	A	234	GLU
1	A	258	GLN
1	A	292	SER
1	A	294	VAL
1	A	298	ARG
1	A	301	LEU
1	A	304	GLU
1	A	327	LEU
1	A	329	VAL
1	A	337	ARG
1	A	347	GLU
1	A	361	ASN
1	A	362	LEU
1	A	374	LEU
1	A	379	THR
1	A	384	MET
1	A	396	LEU
1	A	410	LYS
1	A	457	ILE
1	A	473	VAL
1	A	485	SER
1	A	486	ARG
1	A	508	LEU
1	A	539	SER
1	A	542	LEU
1	A	547	ARG
1	A	552	VAL
1	A	559	ARG
1	A	562	SER
1	A	568	MET
1	B	61	LEU
1	B	83	VAL
1	B	86	ARG
1	B	99	ARG
1	B	100	SER
1	B	103	ARG
1	B	104	LEU
1	B	120	SER
1	B	124	HIS
1	B	141	PHE
1	B	144	SER

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Mol	Chain	Res	Type
1	B	157	THR
1	B	182	GLN
1	B	202	VAL
1	B	294	VAL
1	B	301	LEU
1	B	304	GLU
1	B	327	LEU
1	B	337	ARG
1	B	347	GLU
1	B	361	ASN
1	B	362	LEU
1	B	374	LEU
1	B	379	THR
1	B	384	MET
1	B	388	THR
1	B	396	LEU
1	B	410	LYS
1	B	473	VAL
1	B	485	SER
1	B	486	ARG
1	B	508	LEU
1	B	539	SER
1	B	542	LEU
1	B	546	LEU
1	B	547	ARG
1	B	552	VAL
1	B	559	ARG
1	B	562	SER
1	B	568	MET
1	C	61	LEU
1	C	83	VAL
1	C	86	ARG
1	C	99	ARG
1	C	100	SER
1	C	103	ARG
1	C	104	LEU
1	C	120	SER
1	C	124	HIS
1	C	147	SER
1	C	157	THR
1	C	164	THR
1	C	173	SER

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Mol	Chain	Res	Type
1	C	175	VAL
1	C	188	ASP
1	C	193	THR
1	C	202	VAL
1	C	225	SER
1	C	231	ILE
1	C	234	GLU
1	C	248	SER
1	C	250	LYS
1	C	258	GLN
1	C	294	VAL
1	C	301	LEU
1	C	304	GLU
1	C	327	LEU
1	C	337	ARG
1	C	347	GLU
1	C	362	LEU
1	C	374	LEU
1	C	379	THR
1	C	388	THR
1	C	396	LEU
1	C	410	LYS
1	C	453	GLU
1	C	473	VAL
1	C	485	SER
1	C	486	ARG
1	C	508	LEU
1	C	539	SER
1	C	542	LEU
1	C	546	LEU
1	C	547	ARG
1	C	552	VAL
1	C	559	ARG
1	C	562	SER
1	C	568	MET
1	D	61	LEU
1	D	83	VAL
1	D	86	ARG
1	D	99	ARG
1	D	100	SER
1	D	103	ARG
1	D	104	LEU

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Mol	Chain	Res	Type
1	D	120	SER
1	D	124	HIS
1	D	157	THR
1	D	176	GLU
1	D	177	LEU
1	D	182	GLN
1	D	186	THR
1	D	192	ARG
1	D	193	THR
1	D	202	VAL
1	D	231	ILE
1	D	234	GLU
1	D	248	SER
1	D	250	LYS
1	D	261	LEU
1	D	266	GLU
1	D	294	VAL
1	D	301	LEU
1	D	304	GLU
1	D	327	LEU
1	D	329	VAL
1	D	337	ARG
1	D	362	LEU
1	D	374	LEU
1	D	379	THR
1	D	388	THR
1	D	396	LEU
1	D	410	LYS
1	D	457	ILE
1	D	473	VAL
1	D	485	SER
1	D	486	ARG
1	D	508	LEU
1	D	539	SER
1	D	542	LEU
1	D	547	ARG
1	D	552	VAL
1	D	559	ARG
1	D	562	SER
1	D	568	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	124	HIS
1	A	133	ASN
1	A	182	GLN
1	A	361	ASN
1	A	421	GLN
1	A	434	HIS
1	A	534	GLN
1	B	124	HIS
1	B	133	ASN
1	B	361	ASN
1	B	421	GLN
1	C	124	HIS
1	C	133	ASN
1	C	198	ASN
1	C	421	GLN
1	C	534	GLN
1	D	124	HIS
1	D	133	ASN
1	D	242	ASN
1	D	421	GLN
1	D	434	HIS
1	D	534	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
2	FBP	A	580	-	18,20,20	0.88	0	21,32,32	0.74	0
3	PGA	A	581	5,4	5,8,8	0.79	0	6,11,11	0.86	0
2	FBP	B	580	-	18,20,20	1.05	0	21,32,32	0.79	1 (4%)
3	PGA	B	581	5,4	5,8,8	0.83	0	6,11,11	1.00	1 (16%)
2	FBP	C	580	-	18,20,20	1.06	1 (5%)	21,32,32	0.83	1 (4%)
3	PGA	C	581	5,4	5,8,8	0.95	0	6,11,11	0.89	0
2	FBP	D	580	-	18,20,20	1.06	0	21,32,32	0.83	0
3	PGA	D	581	5,4	5,8,8	0.70	0	6,11,11	0.78	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	FBP	A	580	-	-	0/13/32/32	0/1/1/1
3	PGA	A	581	5,4	-	0/4/6/6	0/0/0/0
2	FBP	B	580	-	-	0/13/32/32	0/1/1/1
3	PGA	B	581	5,4	-	0/4/6/6	0/0/0/0
2	FBP	C	580	-	-	0/13/32/32	0/1/1/1
3	PGA	C	581	5,4	-	0/4/6/6	0/0/0/0
2	FBP	D	580	-	-	0/13/32/32	0/1/1/1
3	PGA	D	581	5,4	-	0/4/6/6	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	580	FBP	O2-C2	2.19	1.44	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	581	PGA	O3P-P-O1P	2.10	112.60	106.56
2	C	580	FBP	O2P-P1-O1	2.16	112.80	106.56
2	B	580	FBP	O2P-P1-O1	2.17	112.81	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	580	FBP	1	0
3	A	581	PGA	1	0
2	B	580	FBP	1	0
2	D	580	FBP	2	0
3	D	581	PGA	1	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, 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	517/528 (97%)	1.50	143 (27%) 1 0	9, 12, 23, 32	0
1	B	491/528 (92%)	1.13	78 (15%) 3 2	10, 12, 22, 32	0
1	C	517/528 (97%)	0.93	66 (12%) 5 3	10, 12, 23, 32	0
1	D	511/528 (96%)	1.41	129 (25%) 1 0	10, 12, 22, 32	0
All	All	2036/2112 (96%)	1.24	416 (20%) 1 1	9, 12, 22, 32	0

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	232	GLY	12.9
1	A	122	GLY	12.2
1	B	165	GLY	10.4
1	D	231	ILE	8.6
1	D	173	SER	8.1
1	B	208	VAL	8.0
1	A	123	SER	7.4
1	D	129	GLU	7.4
1	D	122	GLY	7.3
1	A	523	ALA	7.2
1	A	542	LEU	6.7
1	D	238	THR	6.5
1	A	121	HIS	6.2
1	D	123	SER	6.2
1	D	194	ARG	6.1
1	A	230	LYS	6.1
1	A	256	GLY	6.1
1	D	182	GLN	6.0
1	A	547	ARG	5.9
1	B	213	VAL	5.9
1	D	259	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	103	ARG	5.8
1	A	209	ARG	5.7
1	B	249	ARG	5.7
1	D	256	GLY	5.7
1	C	182	GLN	5.6
1	D	98	SER	5.4
1	D	190	ALA	5.4
1	D	248	SER	5.4
1	B	214	GLY	5.3
1	A	231	ILE	5.2
1	A	259	VAL	5.1
1	D	165	GLY	5.0
1	B	209	ARG	5.0
1	B	180	GLY	4.9
1	D	245	VAL	4.9
1	A	279	GLY	4.9
1	A	235	GLY	4.9
1	D	209	ARG	4.9
1	D	258	GLN	4.8
1	A	95	GLY	4.7
1	B	248	SER	4.7
1	B	237	VAL	4.7
1	A	266	GLU	4.7
1	C	168	GLN	4.7
1	D	187	VAL	4.7
1	B	166	ILE	4.6
1	A	234	GLU	4.6
1	B	303	PRO	4.6
1	B	210	VAL	4.6
1	B	258	GLN	4.6
1	B	142	ALA	4.5
1	A	216	ARG	4.5
1	D	257	ALA	4.5
1	D	233	PRO	4.5
1	B	65	MET	4.5
1	D	184	LEU	4.4
1	B	201	TRP	4.4
1	C	167	LEU	4.4
1	B	527	ASP	4.4
1	A	215	GLY	4.3
1	A	119	PHE	4.2
1	B	239	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	212	PRO	4.2
1	D	189	PRO	4.2
1	B	547	ARG	4.2
1	B	228	VAL	4.2
1	D	262	PRO	4.2
1	D	121	HIS	4.1
1	A	443	ARG	4.1
1	D	126	TYR	4.1
1	B	242	ASN	4.1
1	D	94	ILE	4.1
1	D	62	PRO	4.1
1	A	65	MET	4.1
1	A	120	SER	4.1
1	A	214	GLY	4.1
1	A	125	GLU	4.1
1	D	230	LYS	4.0
1	A	531	ARG	4.0
1	A	171	PRO	4.0
1	B	259	VAL	4.0
1	A	409	ALA	4.0
1	A	378	ILE	4.0
1	B	238	THR	4.0
1	A	306	HIS	4.0
1	A	205	PRO	4.0
1	A	172	GLU	4.0
1	D	176	GLU	3.9
1	A	144	SER	3.9
1	A	211	VAL	3.9
1	B	181	SER	3.9
1	D	239	GLN	3.9
1	C	306	HIS	3.9
1	D	120	SER	3.9
1	B	146	LEU	3.8
1	A	141	PHE	3.8
1	B	520	PRO	3.8
1	C	227	VAL	3.8
1	C	199	THR	3.8
1	A	229	GLN	3.8
1	B	558	TRP	3.8
1	D	193	THR	3.7
1	B	198	ASN	3.7
1	D	304	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	520	PRO	3.7
1	A	257	ALA	3.7
1	A	497	THR	3.7
1	A	258	GLN	3.6
1	D	237	VAL	3.6
1	A	265	SER	3.6
1	A	379	THR	3.5
1	A	213	VAL	3.5
1	D	188	ASP	3.5
1	C	231	ILE	3.5
1	A	92	ALA	3.5
1	A	169	GLY	3.5
1	A	524	ILE	3.5
1	D	235	GLY	3.5
1	A	525	TRP	3.5
1	D	249	ARG	3.5
1	A	233	PRO	3.5
1	C	171	PRO	3.5
1	D	263	GLY	3.5
1	A	414	PRO	3.4
1	A	102	GLU	3.4
1	B	221	ASP	3.4
1	B	524	ILE	3.4
1	C	558	TRP	3.4
1	D	107	MET	3.4
1	D	213	VAL	3.4
1	A	518	ARG	3.4
1	D	234	GLU	3.4
1	B	182	GLN	3.4
1	B	260	ASP	3.4
1	D	270	ARG	3.3
1	B	518	ARG	3.3
1	A	129	GLU	3.3
1	B	266	GLU	3.3
1	A	261	LEU	3.3
1	D	306	HIS	3.3
1	C	208	VAL	3.3
1	C	216	ARG	3.3
1	C	547	ARG	3.2
1	A	167	LEU	3.2
1	B	227	VAL	3.2
1	D	178	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	382	ARG	3.2
1	B	526	ALA	3.2
1	B	342	ILE	3.2
1	D	146	LEU	3.2
1	A	160	PRO	3.2
1	A	562	SER	3.2
1	A	573	ILE	3.2
1	C	233	PRO	3.2
1	A	280	VAL	3.2
1	D	547	ARG	3.2
1	C	242	ASN	3.2
1	B	143	GLY	3.2
1	C	122	GLY	3.2
1	B	261	LEU	3.1
1	A	277	GLU	3.1
1	B	175	VAL	3.1
1	B	185	VAL	3.1
1	A	557	GLY	3.1
1	A	561	GLY	3.1
1	C	247	GLY	3.1
1	D	278	HIS	3.1
1	D	172	GLU	3.1
1	D	191	PHE	3.1
1	B	200	VAL	3.1
1	D	143	GLY	3.1
1	D	177	LEU	3.1
1	A	413	PHE	3.1
1	A	544	GLY	3.1
1	B	548	VAL	3.1
1	C	209	ARG	3.1
1	C	260	ASP	3.1
1	C	194	ARG	3.1
1	D	266	GLU	3.1
1	C	230	LYS	3.0
1	A	502	ALA	3.0
1	A	241	GLU	3.0
1	B	126	TYR	3.0
1	B	564	TYR	3.0
1	A	154	ALA	3.0
1	A	254	LEU	3.0
1	B	243	GLY	3.0
1	D	542	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	300	ALA	3.0
1	A	516	LEU	3.0
1	A	303	PRO	3.0
1	C	94	ILE	3.0
1	C	523	ALA	3.0
1	D	548	VAL	3.0
1	D	214	GLY	3.0
1	B	164	THR	3.0
1	A	105	LYS	3.0
1	A	126	TYR	3.0
1	D	236	LEU	3.0
1	A	304	GLU	3.0
1	A	101	VAL	3.0
1	D	77	ASP	2.9
1	C	367	VAL	2.9
1	D	125	GLU	2.9
1	D	301	LEU	2.9
1	C	191	PHE	2.9
1	D	106	GLU	2.9
1	B	306	HIS	2.9
1	D	61	LEU	2.9
1	B	257	ALA	2.9
1	C	213	VAL	2.9
1	D	260	ASP	2.9
1	D	163	ARG	2.9
1	B	263	GLY	2.9
1	A	210	VAL	2.8
1	A	305	GLY	2.8
1	D	221	ASP	2.8
1	B	305	GLY	2.8
1	D	520	PRO	2.8
1	C	333	ILE	2.8
1	C	263	GLY	2.8
1	D	549	GLY	2.8
1	D	197	ALA	2.8
1	A	136	GLU	2.8
1	A	182	GLN	2.8
1	B	241	GLU	2.8
1	A	181	SER	2.8
1	A	270	ARG	2.8
1	C	170	GLY	2.8
1	B	322	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	221	ASP	2.8
1	C	183	VAL	2.8
1	C	121	HIS	2.7
1	C	342	ILE	2.7
1	A	278	HIS	2.7
1	A	564	TYR	2.7
1	B	262	PRO	2.7
1	D	174	GLU	2.7
1	D	247	GLY	2.7
1	A	166	ILE	2.7
1	A	527	ASP	2.7
1	C	178	VAL	2.7
1	C	237	VAL	2.7
1	D	95	GLY	2.7
1	D	229	GLN	2.7
1	B	351	LEU	2.7
1	D	443	ARG	2.6
1	C	232	GLY	2.6
1	C	175	VAL	2.6
1	D	58	GLN	2.6
1	D	240	VAL	2.6
1	D	103	ARG	2.6
1	C	304	GLU	2.6
1	D	271	ASP	2.6
1	D	101	VAL	2.6
1	C	241	GLU	2.6
1	D	205	PRO	2.6
1	D	255	PRO	2.6
1	D	158	LYS	2.6
1	A	152	ALA	2.6
1	A	173	SER	2.6
1	A	376	SER	2.6
1	D	410	LYS	2.6
1	D	144	SER	2.6
1	A	535	PHE	2.6
1	B	521	PRO	2.6
1	D	145	PRO	2.6
1	C	229	GLN	2.5
1	A	108	ILE	2.5
1	A	180	GLY	2.5
1	D	472	ILE	2.5
1	B	226	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	410	LYS	2.5
1	B	83	VAL	2.5
1	D	312	SER	2.5
1	C	179	LYS	2.5
1	D	291	ALA	2.5
1	A	218	TYR	2.5
1	A	285	ALA	2.5
1	D	192	ARG	2.5
1	A	106	GLU	2.5
1	B	456	ALA	2.5
1	D	110	ALA	2.5
1	D	138	VAL	2.5
1	A	127	HIS	2.5
1	B	204	TYR	2.5
1	A	168	GLN	2.5
1	A	302	GLY	2.5
1	C	530	ASP	2.5
1	D	104	LEU	2.5
1	B	179	LYS	2.5
1	A	260	ASP	2.5
1	D	419	LYS	2.4
1	A	94	ILE	2.4
1	D	183	VAL	2.4
1	D	130	SER	2.4
1	A	146	LEU	2.4
1	A	208	VAL	2.4
1	A	179	LYS	2.4
1	C	65	MET	2.4
1	A	371	THR	2.4
1	A	190	ALA	2.4
1	C	336	ALA	2.4
1	D	109	LYS	2.4
1	D	134	VAL	2.4
1	D	141	PHE	2.4
1	C	115	ALA	2.4
1	C	314	ILE	2.4
1	A	133	ASN	2.4
1	C	184	LEU	2.4
1	D	261	LEU	2.4
1	A	291	ALA	2.4
1	D	285	ALA	2.4
1	A	88	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	416	GLU	2.4
1	A	528	ASP	2.4
1	D	216	ARG	2.4
1	C	169	GLY	2.4
1	C	399	ALA	2.4
1	A	543	ARG	2.4
1	C	239	GLN	2.4
1	C	214	GLY	2.3
1	C	161	GLU	2.3
1	A	311	ILE	2.3
1	A	212	PRO	2.3
1	C	117	LEU	2.3
1	D	119	PHE	2.3
1	C	173	SER	2.3
1	A	58	GLN	2.3
1	B	67	ASP	2.3
1	B	89	SER	2.3
1	C	120	SER	2.3
1	D	267	GLN	2.3
1	D	136	GLU	2.3
1	A	93	THR	2.3
1	C	522	GLU	2.3
1	D	272	LEU	2.3
1	A	189	PRO	2.3
1	B	459	ALA	2.3
1	A	496	VAL	2.3
1	B	245	VAL	2.3
1	D	102	GLU	2.3
1	C	303	PRO	2.3
1	D	500	ALA	2.3
1	A	194	ARG	2.3
1	D	124	HIS	2.3
1	D	473	VAL	2.3
1	B	386	ALA	2.2
1	C	92	ALA	2.2
1	A	517	TYR	2.2
1	C	379	THR	2.2
1	D	199	THR	2.2
1	A	145	PRO	2.2
1	D	526	ALA	2.2
1	C	172	GLU	2.2
1	C	521	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	2.2
1	B	219	ILE	2.2
1	D	311	ILE	2.2
1	D	264	LEU	2.2
1	D	273	ARG	2.2
1	D	383	PRO	2.2
1	D	439	GLU	2.2
1	C	200	VAL	2.2
1	A	98	SER	2.2
1	A	406	GLY	2.2
1	B	531	ARG	2.2
1	C	559	ARG	2.2
1	D	356	MET	2.2
1	D	220	ASP	2.2
1	D	206	ASN	2.2
1	D	115	ALA	2.2
1	A	271	ASP	2.2
1	A	329	VAL	2.2
1	B	183	VAL	2.2
1	A	344	ILE	2.2
1	B	472	ILE	2.2
1	D	531	ARG	2.2
1	D	495	ALA	2.2
1	A	493	VAL	2.2
1	C	186	THR	2.2
1	D	496	VAL	2.2
1	D	279	GLY	2.1
1	D	218	TYR	2.1
1	A	289	ARG	2.1
1	B	161	GLU	2.1
1	A	353	GLN	2.1
1	C	238	THR	2.1
1	A	558	TRP	2.1
1	B	215	GLY	2.1
1	C	458	GLY	2.1
1	B	205	PRO	2.1
1	A	439	GLU	2.1
1	A	109	LYS	2.1
1	A	421	GLN	2.1
1	A	104	LEU	2.1
1	B	91	ILE	2.1
1	B	184	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	449	ARG	2.1
1	D	108	ILE	2.1
1	C	234	GLU	2.1
1	A	274	PHE	2.1
1	A	232	GLY	2.1
1	A	153	ILE	2.1
1	D	241	GLU	2.1
1	A	237	VAL	2.1
1	B	367	VAL	2.1
1	A	201	TRP	2.1
1	C	221	ASP	2.1
1	D	196	ASN	2.0
1	D	112	MET	2.0
1	A	138	VAL	2.0
1	A	149	ARG	2.0
1	A	410	LYS	2.0
1	D	360	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FBP	D	580	20/20	0.92	0.29	1.81	56,61,63,63	0
2	FBP	B	580	20/20	0.93	0.32	1.26	56,61,63,63	0
4	K	D	594	1/1	0.73	0.36	0.61	77,77,77,77	0
2	FBP	C	580	20/20	0.92	0.25	0.29	56,61,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FBP	A	580	20/20	0.87	0.29	0.11	56,61,63,63	0
3	PGA	B	581	9/9	0.91	0.23	0.05	85,86,86,86	0
3	PGA	A	581	9/9	0.89	0.26	0.05	85,86,86,86	0
3	PGA	C	581	9/9	0.93	0.22	-0.18	85,86,86,86	0
4	K	A	582	1/1	0.74	0.25	-0.69	52,52,52,52	0
3	PGA	D	581	9/9	0.92	0.18	-0.83	85,86,86,86	0
4	K	B	586	1/1	0.80	0.19	-1.01	33,33,33,33	0
4	K	C	590	1/1	0.94	0.15	-1.69	41,41,41,41	0
5	MN	B	587	1/1	0.95	0.11	-2.34	35,35,35,35	0
5	MN	D	595	1/1	0.95	0.03	-	38,38,38,38	0
5	MN	C	591	1/1	0.97	0.07	-	37,37,37,37	0
5	MN	A	583	1/1	0.84	0.09	-	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.