



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:09 am GMT

PDB ID : 2VGB  
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE  
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Deposited on : 2007-11-12  
Resolution : 2.73 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

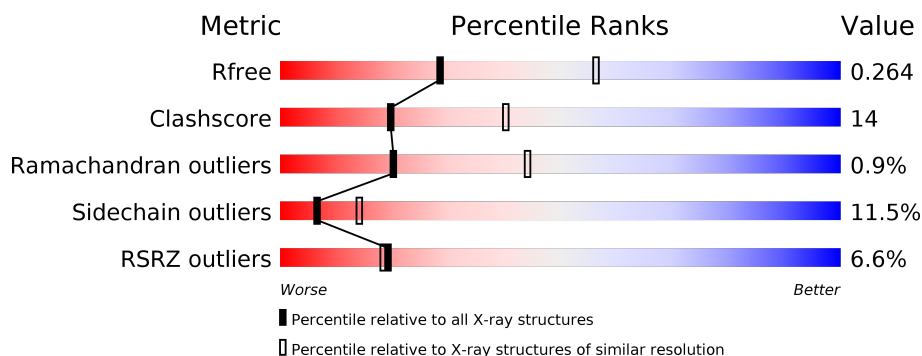
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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))
$R_{free}$	100719	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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  $\geq 3$ , 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>10%</div> <div>64%</div> <div>29%</div> <div>• • •</div> </div>
1	B	528	<div> <div>9%</div> <div>63%</div> <div>26%</div> <div>• • 7%</div> </div>
1	C	528	<div> <div>2%</div> <div>68%</div> <div>26%</div> <div>• • •</div> </div>
1	D	528	<div> <div>5%</div> <div>67%</div> <div>26%</div> <div>• • •</div> </div>

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
3	PGA	D	581	-	-	-	X

## 2 Entry composition [i](#)

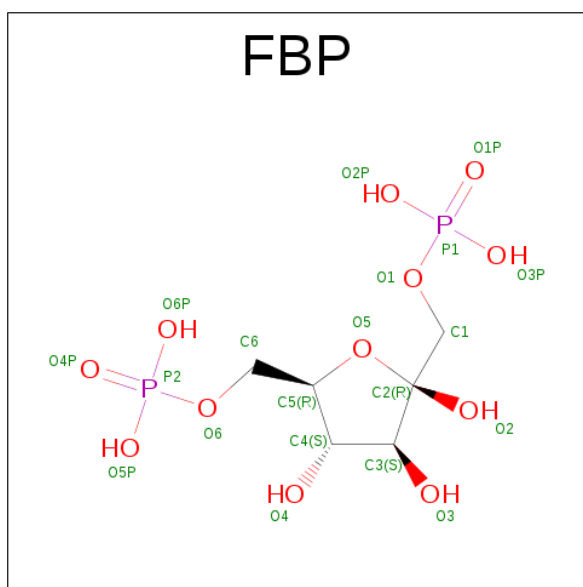
There are 6 unique types of molecules in this entry. The entry contains 15612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			3912	2457	709	728	18			
1	B	491	Total	C	N	O	S	0	0	0
			3719	2339	673	689	18			
1	C	517	Total	C	N	O	S	0	0	0
			3912	2457	709	728	18			
1	D	512	Total	C	N	O	S	0	0	0
			3880	2437	703	722	18			

- Molecule 2 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).



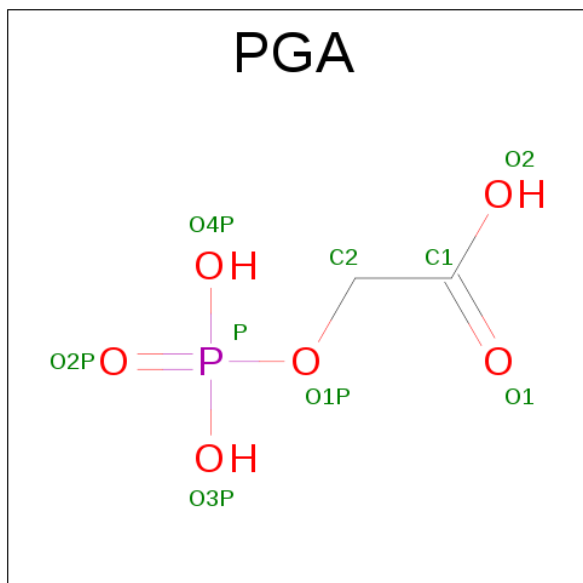
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

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

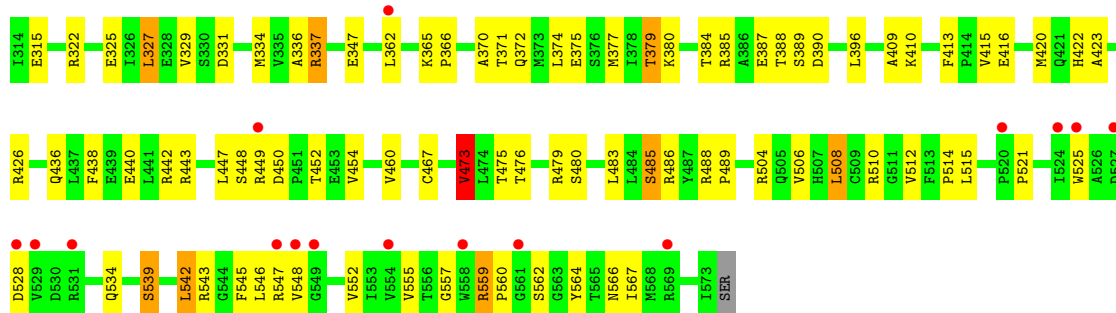
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

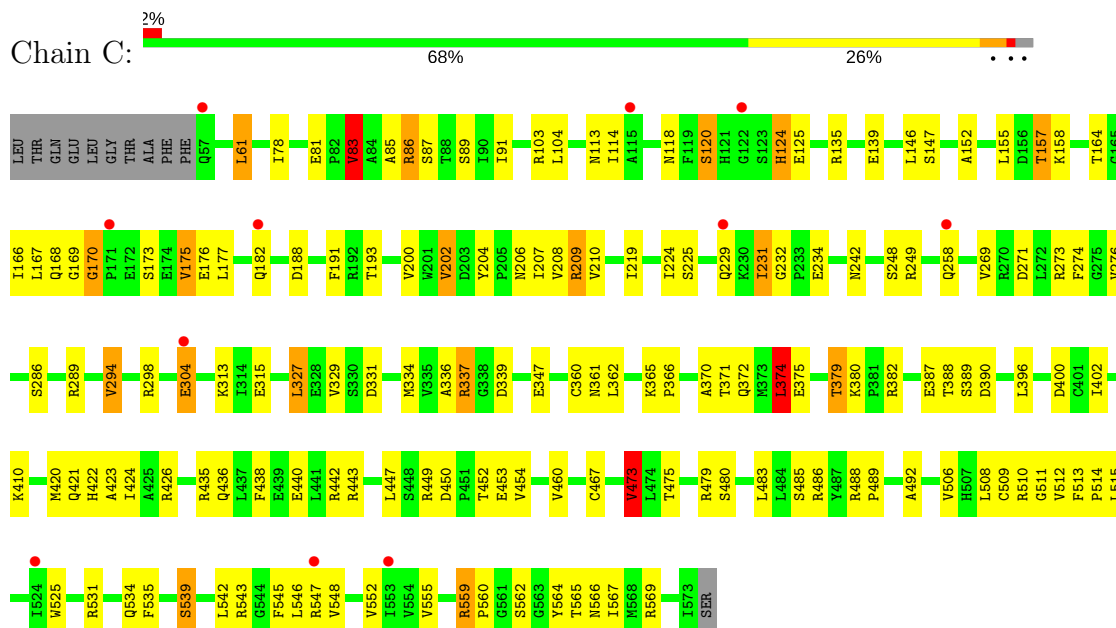
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	16	Total O 16 16	0	0
6	C	20	Total O 20 20	0	0
6	D	17	Total O 17 17	0	0

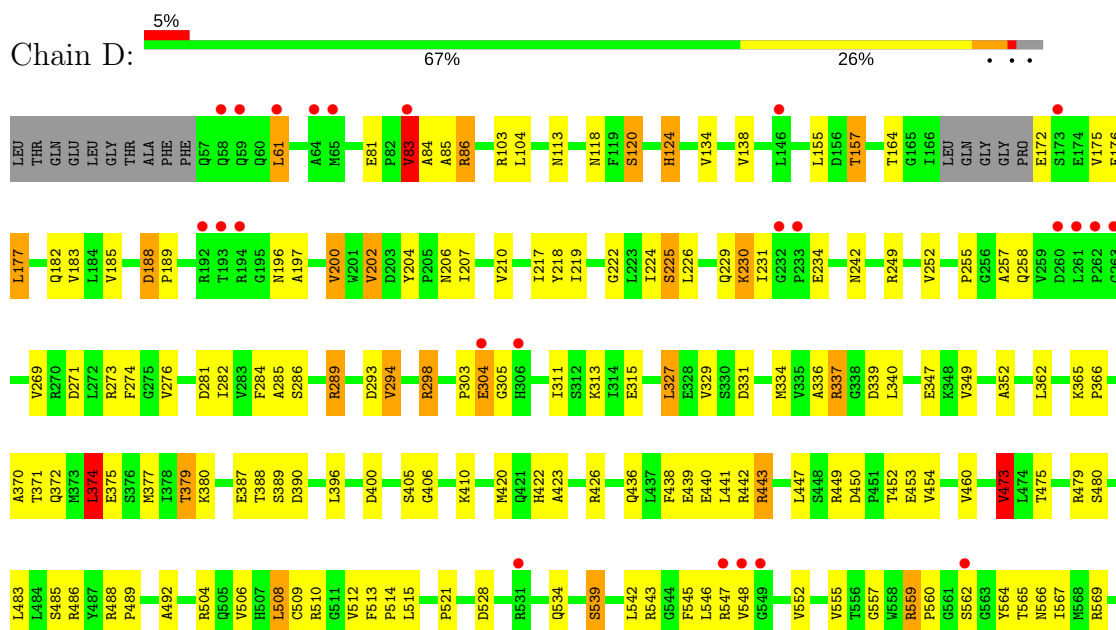




• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L





1573  
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.41Å 172.06Å 85.51Å 90.00° 92.46° 90.00°	Depositor
Resolution (Å)	20.00 – 2.73 25.25 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.73) 96.3 (25.25-2.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.227 , 0.271 0.221 , 0.264	Depositor DCC
$R_{free}$ test set	2782 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MN, PGA, FBP

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	0.69	3/3976 (0.1%)	0.74	2/5390 (0.0%)
1	B	0.78	2/3776 (0.1%)	0.73	2/5115 (0.0%)
1	C	0.66	0/3976	0.77	2/5390 (0.0%)
1	D	0.66	0/3942	0.77	2/5342 (0.0%)
All	All	0.70	5/15670 (0.0%)	0.75	8/21237 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	SER	CB-OG	27.69	1.78	1.42
1	A	410	LYS	CE-NZ	13.54	1.82	1.49
1	A	410	LYS	CD-CE	-6.44	1.35	1.51
1	A	234	GLU	CD-OE1	5.55	1.31	1.25
1	B	260	ASP	CG-OD1	5.32	1.37	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	VAL	CB-CA-C	-7.38	97.37	111.40
1	A	473	VAL	CB-CA-C	-6.69	98.69	111.40
1	D	473	VAL	CB-CA-C	-6.35	99.33	111.40
1	B	473	VAL	CB-CA-C	-6.27	99.48	111.40
1	D	374	LEU	CA-CB-CG	6.04	129.18	115.30
1	B	144	SER	CA-CB-OG	-5.93	95.19	111.20
1	C	374	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	508	LEU	CA-CB-CG	5.26	127.41	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3912	0	3992	130	6
1	B	3719	0	3802	116	6
1	C	3912	0	3992	110	1
1	D	3880	0	3959	120	1
2	A	20	0	10	1	0
2	B	20	0	10	3	0
2	C	20	0	10	2	0
2	D	20	0	10	2	0
3	A	9	0	2	0	0
3	B	9	0	2	0	0
3	C	9	0	2	0	0
3	D	9	0	2	0	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
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
6	A	12	0	0	3	0
6	B	16	0	0	2	0
6	C	20	0	0	3	0
6	D	17	0	0	0	0
All	All	15612	0	15793	446	7

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 (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LYS:NZ	1:A:410:LYS:CE	1.82	1.41
1:B:144:SER:OG	1:B:144:SER:CB	1.78	1.32
1:A:488:ARG:NH1	1:A:510:ARG:HB3	1.56	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ARG:NH1	1:B:510:ARG:HB3	1.56	1.18
1:D:488:ARG:NH1	1:D:510:ARG:HB3	1.58	1.17
1:C:488:ARG:NH1	1:C:510:ARG:HB3	1.64	1.11
1:C:86:ARG:HB3	1:C:426:ARG:HG2	1.41	0.99
1:A:86:ARG:HB3	1:A:426:ARG:HG2	1.42	0.99
1:B:86:ARG:HB3	1:B:426:ARG:HG2	1.45	0.97
1:D:86:ARG:HB3	1:D:426:ARG:HG2	1.46	0.97
1:A:488:ARG:HH12	1:A:510:ARG:HB3	1.30	0.96
1:A:347:GLU:HG2	1:C:423:ALA:HB1	1.49	0.95
1:D:488:ARG:HH12	1:D:510:ARG:HB3	1.29	0.94
1:A:442:ARG:HH21	1:B:442:ARG:NH2	1.67	0.93
1:A:442:ARG:HH21	1:B:442:ARG:HH21	0.92	0.91
1:A:442:ARG:NH2	1:B:442:ARG:HH21	1.69	0.91
1:B:488:ARG:HH12	1:B:510:ARG:HB3	1.35	0.90
1:C:225:SER:HB3	1:C:242:ASN:HB2	1.53	0.90
1:B:488:ARG:NH1	1:B:510:ARG:CB	2.36	0.88
1:C:170:GLY:HA3	1:C:173:SER:OG	1.74	0.86
1:C:479:ARG:HG3	1:C:479:ARG:HH11	1.40	0.86
1:C:442:ARG:HH21	1:D:442:ARG:HH21	1.24	0.86
1:C:488:ARG:NH1	1:C:510:ARG:CB	2.39	0.85
1:D:488:ARG:NH1	1:D:510:ARG:CB	2.40	0.85
1:B:423:ALA:HB1	1:D:347:GLU:HG2	1.58	0.85
1:B:488:ARG:HH11	1:B:510:ARG:HB3	1.42	0.84
1:C:85:ALA:HB2	1:C:545:PHE:CE2	2.13	0.84
1:C:531:ARG:HD2	6:C:2018:HOH:O	1.78	0.83
1:A:488:ARG:HH11	1:A:510:ARG:HB3	1.43	0.83
1:D:506:VAL:CG1	1:D:512:VAL:HG11	2.08	0.83
1:B:347:GLU:HG2	1:D:423:ALA:HB1	1.60	0.83
1:B:506:VAL:CG1	1:B:512:VAL:HG11	2.11	0.80
1:D:488:ARG:HH12	1:D:510:ARG:CB	1.95	0.80
1:C:372:GLN:HG2	1:C:375:GLU:CG	2.11	0.79
1:D:488:ARG:HH11	1:D:510:ARG:HB3	1.48	0.79
1:A:488:ARG:NH1	1:A:510:ARG:CB	2.41	0.79
1:A:479:ARG:HG3	1:A:479:ARG:HH11	1.49	0.78
1:C:488:ARG:HH12	1:C:510:ARG:HB3	1.46	0.78
1:B:488:ARG:HH12	1:B:510:ARG:CB	1.95	0.78
1:D:315:GLU:HG2	1:D:336:ALA:CB	2.14	0.77
1:C:315:GLU:HG2	1:C:336:ALA:CB	2.16	0.76
1:D:86:ARG:HB3	1:D:426:ARG:CG	2.15	0.76
1:A:223:LEU:HD22	1:C:380:LYS:HE2	1.69	0.74
1:A:216:ARG:HD2	1:A:218:TYR:CE1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:GLN:HG2	1:C:375:GLU:HG3	1.66	0.74
1:C:488:ARG:HH11	1:C:510:ARG:HB3	1.45	0.74
1:D:506:VAL:HG11	1:D:512:VAL:HG11	1.68	0.74
1:B:89:SER:OG	6:B:2001:HOH:O	2.06	0.73
1:A:423:ALA:HB1	1:C:347:GLU:HG2	1.71	0.73
1:C:506:VAL:CG1	1:C:512:VAL:HG11	2.19	0.73
1:C:488:ARG:HH12	1:C:510:ARG:CB	2.01	0.72
1:A:86:ARG:HB3	1:A:426:ARG:CG	2.20	0.72
1:C:315:GLU:HG2	1:C:336:ALA:HB3	1.70	0.72
1:A:86:ARG:HD3	1:A:422:HIS:ND1	2.04	0.71
1:B:86:ARG:HD3	1:B:422:HIS:ND1	2.04	0.71
1:C:86:ARG:HD3	1:C:422:HIS:ND1	2.05	0.71
1:A:506:VAL:CG1	1:A:512:VAL:HG11	2.20	0.71
1:B:506:VAL:CG1	1:B:512:VAL:CG1	2.69	0.71
1:A:315:GLU:HG2	1:A:336:ALA:CB	2.20	0.71
1:B:479:ARG:HG3	1:B:479:ARG:HH11	1.55	0.70
1:D:86:ARG:HD3	1:D:422:HIS:ND1	2.07	0.70
1:D:315:GLU:HG2	1:D:336:ALA:HB3	1.71	0.70
1:A:379:THR:HG22	1:A:380:LYS:HG3	1.73	0.70
1:D:506:VAL:CG1	1:D:512:VAL:CG1	2.69	0.70
1:A:488:ARG:HH12	1:A:510:ARG:CB	2.01	0.69
1:A:157:THR:HG22	1:A:286:SER:H	1.58	0.69
1:B:506:VAL:HG11	1:B:512:VAL:HG11	1.74	0.69
1:B:86:ARG:HB3	1:B:426:ARG:CG	2.21	0.69
1:C:379:THR:HG22	1:C:380:LYS:HG3	1.74	0.69
1:B:514:PRO:O	1:B:515:LEU:HD23	1.94	0.68
1:A:506:VAL:HG11	1:A:512:VAL:HG11	1.76	0.68
1:D:372:GLN:HG2	1:D:375:GLU:CG	2.24	0.67
1:A:225:SER:HB3	1:A:242:ASN:H	1.60	0.67
1:B:506:VAL:HG13	1:B:512:VAL:HG11	1.77	0.67
1:C:225:SER:CB	1:C:242:ASN:HB2	2.24	0.67
1:C:514:PRO:O	1:C:515:LEU:HD23	1.95	0.67
1:B:379:THR:HG22	1:B:380:LYS:HG3	1.77	0.66
1:D:485:SER:HB2	1:D:510:ARG:O	1.96	0.66
1:A:315:GLU:HG2	1:A:336:ALA:HB3	1.76	0.66
1:D:157:THR:HG22	1:D:286:SER:H	1.60	0.66
1:B:315:GLU:HG2	1:B:336:ALA:CB	2.25	0.66
1:B:177:LEU:HD13	1:B:183:VAL:HG21	1.77	0.66
1:C:442:ARG:NH2	1:D:442:ARG:HH21	1.95	0.66
1:D:514:PRO:O	1:D:515:LEU:HD23	1.96	0.66
1:A:347:GLU:CG	1:C:423:ALA:HB1	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:SER:HB2	1:A:510:ARG:O	1.96	0.65
1:B:144:SER:O	6:B:2004:HOH:O	2.14	0.65
1:C:86:ARG:HB3	1:C:426:ARG:CG	2.20	0.65
1:C:460:VAL:HG22	1:C:489:PRO:HG3	1.79	0.65
1:C:331:ASP:O	1:C:366:PRO:HD2	1.96	0.64
1:B:539:SER:O	1:B:543:ARG:HG3	1.97	0.64
1:A:223:LEU:CD2	1:C:380:LYS:HE2	2.27	0.64
1:B:144:SER:OG	1:B:144:SER:CA	2.46	0.64
1:B:269:VAL:O	1:B:273:ARG:HG2	1.99	0.63
1:C:166:ILE:HA	1:C:248:SER:HB3	1.80	0.63
1:D:372:GLN:HG2	1:D:375:GLU:HG3	1.80	0.63
1:A:506:VAL:CG1	1:A:512:VAL:CG1	2.76	0.63
1:B:315:GLU:HG2	1:B:336:ALA:HB3	1.81	0.63
1:B:164:THR:O	1:B:249:ARG:HA	1.98	0.63
1:D:506:VAL:HG13	1:D:512:VAL:HG11	1.79	0.62
1:D:315:GLU:OE2	1:D:339:ASP:OD2	2.17	0.62
1:B:485:SER:HB2	1:B:510:ARG:O	1.99	0.62
1:C:567:ILE:HG12	1:D:569:ARG:HG2	1.80	0.62
1:A:269:VAL:O	1:A:273:ARG:HG2	2.00	0.62
1:C:506:VAL:HG11	1:C:512:VAL:HG11	1.81	0.62
1:A:479:ARG:HG3	1:A:479:ARG:NH1	2.13	0.62
1:B:281:ASP:OD2	1:B:504:ARG:NE	2.32	0.62
1:B:331:ASP:O	1:B:366:PRO:HD2	2.00	0.62
1:C:269:VAL:O	1:C:273:ARG:HG2	2.00	0.61
1:D:177:LEU:HD12	1:D:183:VAL:HG21	1.82	0.61
1:C:479:ARG:NH1	1:C:479:ARG:HG3	2.09	0.61
1:D:379:THR:HG22	1:D:380:LYS:HG3	1.82	0.61
1:A:331:ASP:O	1:A:366:PRO:HD2	2.01	0.61
1:D:188:ASP:C	1:D:188:ASP:OD1	2.38	0.61
1:B:337:ARG:HD3	1:B:370:ALA:O	2.01	0.60
1:D:506:VAL:HG11	1:D:512:VAL:CG1	2.31	0.60
1:A:170:GLY:HA3	1:A:173:SER:OG	2.01	0.60
1:B:290:LYS:HB3	1:B:322:ARG:NH1	2.16	0.60
1:C:315:GLU:OE2	1:C:339:ASP:OD2	2.20	0.60
1:C:506:VAL:CG1	1:C:512:VAL:CG1	2.80	0.60
1:A:337:ARG:HD3	1:A:370:ALA:O	2.01	0.60
1:A:460:VAL:HG22	1:A:489:PRO:HG3	1.83	0.59
1:A:447:LEU:HD13	1:B:467:CYS:SG	2.41	0.59
1:C:313:LYS:HD2	1:C:334:MET:SD	2.42	0.59
1:B:372:GLN:HG2	1:B:375:GLU:CG	2.31	0.59
1:D:175:VAL:HG21	1:D:196:ASN:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:VAL:CG1	1:D:197:ALA:HA	2.33	0.59
1:B:313:LYS:HD2	1:B:334:MET:SD	2.43	0.58
1:D:539:SER:O	1:D:543:ARG:HG3	2.02	0.58
1:B:479:ARG:NH1	1:B:479:ARG:HG3	2.17	0.58
1:C:219:ILE:HB	1:C:224:ILE:HB	1.85	0.58
1:D:204:TYR:CE1	1:D:206:ASN:HB2	2.39	0.58
1:C:157:THR:HG22	1:C:286:SER:H	1.69	0.58
1:A:450:ASP:O	1:A:454:VAL:HG23	2.03	0.58
1:B:327:LEU:HD22	1:B:365:LYS:HD2	1.86	0.58
1:A:506:VAL:HG11	1:A:512:VAL:CG1	2.34	0.58
1:B:372:GLN:HA	1:B:375:GLU:HG2	1.84	0.58
1:D:269:VAL:O	1:D:273:ARG:HG2	2.04	0.58
1:A:539:SER:O	1:A:543:ARG:HG3	2.03	0.58
1:C:146:LEU:HD23	1:C:535:PHE:CE1	2.38	0.58
1:C:485:SER:HB2	1:C:510:ARG:O	2.04	0.58
1:A:514:PRO:O	1:A:515:LEU:HD23	2.04	0.58
1:D:436:GLN:O	1:D:440:GLU:HG3	2.03	0.57
1:A:442:ARG:NH2	1:B:442:ARG:NH2	2.38	0.57
1:D:83:VAL:HG12	1:D:83:VAL:O	2.03	0.57
1:A:372:GLN:HA	1:A:375:GLU:HG2	1.87	0.57
1:B:557:GLY:HA3	2:B:580:FBP:O3	2.04	0.57
1:D:327:LEU:HD22	1:D:365:LYS:HD2	1.86	0.57
1:A:194:ARG:HB3	1:A:194:ARG:HH11	1.70	0.57
1:C:506:VAL:HG13	1:C:512:VAL:HG11	1.85	0.57
1:B:473:VAL:HG13	1:B:555:VAL:HB	1.87	0.57
1:B:506:VAL:HG11	1:B:512:VAL:CG1	2.32	0.56
1:D:177:LEU:CD1	1:D:183:VAL:HG21	2.34	0.56
1:A:83:VAL:HG12	1:A:83:VAL:O	2.04	0.56
1:D:83:VAL:CG1	1:D:83:VAL:O	2.54	0.56
1:D:172:GLU:N	1:D:172:GLU:CD	2.59	0.56
1:A:210:VAL:HG12	1:A:257:ALA:HB1	1.88	0.56
1:A:157:THR:CG2	1:A:286:SER:H	2.18	0.56
1:D:460:VAL:HG22	1:D:489:PRO:HG3	1.88	0.55
1:D:134:VAL:O	1:D:138:VAL:HG23	2.06	0.55
1:A:83:VAL:O	1:A:83:VAL:CG1	2.53	0.55
1:B:157:THR:HG22	1:B:286:SER:H	1.72	0.55
1:B:134:VAL:O	1:B:138:VAL:HG23	2.06	0.55
1:D:479:ARG:HH11	1:D:479:ARG:HG3	1.72	0.55
1:D:331:ASP:O	1:D:366:PRO:HD2	2.06	0.55
1:A:276:VAL:HG11	1:A:304:GLU:HB2	1.89	0.55
1:B:157:THR:HG22	1:B:286:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:TYR:CE1	1:B:206:ASN:HB2	2.42	0.55
1:B:337:ARG:HH22	1:B:390:ASP:CG	2.09	0.55
1:C:276:VAL:HG11	1:C:304:GLU:HB2	1.89	0.55
1:C:372:GLN:HA	1:C:375:GLU:HG2	1.89	0.55
1:C:442:ARG:HH21	1:D:442:ARG:NH2	2.01	0.55
1:C:539:SER:O	1:C:543:ARG:HG3	2.07	0.55
1:A:162:ILE:HG22	1:A:252:VAL:HB	1.88	0.55
1:D:559:ARG:HD2	1:D:564:TYR:CD1	2.42	0.54
1:D:118:ASN:OD1	1:D:120:SER:HB2	2.06	0.54
1:B:385:ARG:HG2	1:B:385:ARG:HH11	1.72	0.54
1:D:337:ARG:HH22	1:D:390:ASP:CG	2.11	0.54
1:A:347:GLU:HG2	1:C:423:ALA:CB	2.31	0.54
1:A:208:VAL:HA	1:A:236:LEU:HD21	1.90	0.54
1:C:327:LEU:HD22	1:C:365:LYS:HD2	1.88	0.54
1:C:164:THR:O	1:C:249:ARG:HA	2.08	0.54
1:A:506:VAL:HG13	1:A:512:VAL:HG11	1.91	0.53
1:C:231:ILE:HD13	1:C:232:GLY:H	1.73	0.53
1:A:118:ASN:OD1	1:A:120:SER:HB2	2.08	0.53
1:A:465:LYS:HE3	1:B:448:SER:HB3	1.90	0.53
1:A:155:LEU:HD23	1:A:155:LEU:C	2.28	0.53
1:C:81:GLU:HA	1:C:81:GLU:OE1	2.08	0.53
1:D:164:THR:O	1:D:249:ARG:HA	2.09	0.53
1:B:436:GLN:O	1:B:440:GLU:HG3	2.08	0.53
1:C:209:ARG:HG2	1:C:209:ARG:O	2.09	0.53
1:D:219:ILE:HG12	1:D:252:VAL:HG22	1.90	0.53
1:B:460:VAL:HG22	1:B:489:PRO:HG3	1.91	0.52
1:B:118:ASN:OD1	1:B:120:SER:HB2	2.09	0.52
1:B:327:LEU:CD2	1:B:365:LYS:HD2	2.39	0.52
1:B:86:ARG:NH2	1:B:113:ASN:OD1	2.41	0.52
1:C:188:ASP:HB3	1:C:191:PHE:HD1	1.74	0.52
1:B:124:HIS:HE1	1:B:271:ASP:OD1	1.93	0.52
1:C:86:ARG:NH2	1:C:113:ASN:OD1	2.42	0.52
1:D:438:PHE:O	1:D:442:ARG:HG3	2.09	0.52
1:A:85:ALA:HB2	1:A:545:PHE:CE2	2.44	0.52
1:C:124:HIS:HE1	1:C:271:ASP:OD1	1.93	0.52
1:C:475:THR:HA	2:C:580:FBP:H61	1.92	0.51
1:A:337:ARG:HH22	1:A:390:ASP:CG	2.13	0.51
1:D:479:ARG:HG3	1:D:479:ARG:NH1	2.26	0.51
1:C:114:ILE:HG12	1:C:152:ALA:HB3	1.93	0.51
1:D:185:VAL:HG22	1:D:200:VAL:HG22	1.93	0.51
1:A:436:GLN:O	1:A:440:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:HIS:HE1	1:D:271:ASP:OD1	1.93	0.51
1:A:559:ARG:HD2	1:A:564:TYR:CD1	2.46	0.51
1:A:337:ARG:CD	1:A:370:ALA:O	2.58	0.51
1:B:559:ARG:HD2	1:B:564:TYR:CD1	2.46	0.51
1:D:366:PRO:HB3	1:D:508:LEU:O	2.10	0.51
1:D:366:PRO:HA	1:D:400:ASP:OD2	2.11	0.51
1:A:124:HIS:HE1	1:A:271:ASP:OD1	1.94	0.50
1:C:89:SER:OG	6:C:2001:HOH:O	2.19	0.50
1:A:185:VAL:HA	1:A:200:VAL:O	2.12	0.50
1:D:219:ILE:HB	1:D:224:ILE:HB	1.94	0.50
1:D:315:GLU:HG2	1:D:336:ALA:HB1	1.91	0.50
1:A:134:VAL:O	1:A:138:VAL:HG23	2.12	0.50
1:A:327:LEU:HD22	1:A:365:LYS:HD2	1.93	0.50
1:D:557:GLY:HA3	2:D:580:FBP:O3	2.12	0.50
1:D:175:VAL:HG13	1:D:197:ALA:HA	1.94	0.50
1:D:289:ARG:HG3	1:D:293:ASP:OD2	2.12	0.50
1:D:327:LEU:CD2	1:D:365:LYS:HD2	2.42	0.50
1:D:81:GLU:HA	1:D:81:GLU:OE1	2.11	0.50
1:C:135:ARG:O	1:C:139:GLU:HG2	2.12	0.49
1:B:275:GLY:O	1:B:280:VAL:HG22	2.11	0.49
1:A:372:GLN:HG2	1:A:375:GLU:CG	2.43	0.49
1:B:276:VAL:HG11	1:B:304:GLU:HB2	1.94	0.49
1:B:372:GLN:HG2	1:B:375:GLU:HG3	1.94	0.49
1:B:281:ASP:C	1:B:282:ILE:HG13	2.33	0.49
1:C:87:SER:CB	1:C:511:GLY:HA2	2.42	0.49
1:A:286:SER:HA	1:A:313:LYS:HE2	1.93	0.49
1:B:85:ALA:HB2	1:B:545:PHE:CE2	2.48	0.49
1:A:168:GLN:HB2	1:A:195:GLY:O	2.12	0.49
1:C:402:ILE:HG13	1:C:421:GLN:NE2	2.28	0.49
1:D:372:GLN:HA	1:D:375:GLU:HG2	1.93	0.49
1:D:86:ARG:NH2	1:D:113:ASN:OD1	2.45	0.49
1:C:168:GLN:O	1:C:169:GLY:C	2.51	0.49
1:C:436:GLN:O	1:C:440:GLU:HG3	2.13	0.49
1:C:453:GLU:HG2	1:C:483:LEU:HD13	1.95	0.49
1:B:420:MET:CE	1:D:347:GLU:HG3	2.43	0.48
1:A:313:LYS:HD2	1:A:334:MET:SD	2.53	0.48
1:B:366:PRO:HB3	1:B:508:LEU:O	2.13	0.48
1:A:186:THR:HB	1:A:188:ASP:H	1.78	0.48
1:A:206:ASN:O	1:A:210:VAL:HG23	2.14	0.48
1:A:229:GLN:NE2	1:A:239:GLN:HB2	2.29	0.48
1:C:438:PHE:O	1:C:442:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:H	1:A:125:GLU:CD	2.16	0.48
1:C:569:ARG:HG2	1:D:567:ILE:HG12	1.95	0.48
1:B:384:THR:OG1	1:B:387:GLU:HG3	2.13	0.48
1:C:337:ARG:CD	1:C:370:ALA:O	2.62	0.48
1:A:209:ARG:HG2	1:A:209:ARG:O	2.12	0.48
1:C:452:THR:HG23	1:C:565:THR:HB	1.95	0.47
1:A:87:SER:CB	1:A:511:GLY:HA2	2.44	0.47
1:C:337:ARG:HH22	1:C:390:ASP:CG	2.18	0.47
1:D:475:THR:HA	2:D:580:FBP:H61	1.96	0.47
1:B:476:THR:HB	2:B:580:FBP:O4P	2.13	0.47
1:B:83:VAL:O	1:B:84:ALA:HB2	2.15	0.47
1:A:225:SER:HB3	1:A:242:ASN:N	2.27	0.47
1:A:438:PHE:O	1:A:442:ARG:HG3	2.14	0.47
1:A:521:PRO:HA	1:A:528:ASP:OD1	2.13	0.47
1:A:230:LYS:HB2	1:A:237:VAL:HB	1.95	0.47
1:D:225:SER:HB3	1:D:242:ASN:HD22	1.79	0.47
1:A:315:GLU:HG2	1:A:336:ALA:HB1	1.96	0.47
1:B:207:ILE:HD11	1:B:254:LEU:HD21	1.96	0.47
1:B:347:GLU:HG3	1:D:420:MET:CE	2.44	0.47
1:B:506:VAL:HG13	1:B:512:VAL:CG1	2.40	0.47
1:C:157:THR:HG22	1:C:286:SER:HB2	1.97	0.47
1:D:271:ASP:O	1:D:274:PHE:HB3	2.15	0.47
1:A:226:LEU:HD23	1:A:240:VAL:HA	1.96	0.47
1:B:297:VAL:CG1	1:B:310:ILE:HD13	2.45	0.47
1:B:452:THR:HG22	1:B:483:LEU:HD12	1.96	0.47
1:D:452:THR:HG23	1:D:565:THR:HB	1.96	0.47
1:C:177:LEU:HD23	1:C:177:LEU:N	2.30	0.47
1:D:521:PRO:HA	1:D:528:ASP:OD1	2.15	0.47
1:C:366:PRO:HA	1:C:400:ASP:OD2	2.14	0.46
1:A:222:GLY:O	1:C:382:ARG:HG3	2.14	0.46
1:A:452:THR:HG22	1:A:483:LEU:HD12	1.96	0.46
1:C:506:VAL:HG11	1:C:512:VAL:CG1	2.44	0.46
1:B:146:LEU:CB	1:B:542:LEU:HD12	2.45	0.46
1:A:384:THR:OG1	1:A:387:GLU:HG3	2.16	0.46
1:C:467:CYS:SG	1:D:447:LEU:HD13	2.56	0.46
1:D:313:LYS:HD2	1:D:334:MET:SD	2.55	0.46
1:A:297:VAL:CG1	1:A:310:ILE:HD13	2.45	0.46
1:D:294:VAL:HG11	1:D:329:VAL:HG12	1.98	0.46
1:B:413:PHE:HB3	1:B:416:GLU:HB2	1.97	0.46
1:B:488:ARG:HH11	1:B:510:ARG:CB	2.19	0.46
1:C:231:ILE:HD13	1:C:232:GLY:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ARG:HD3	1:C:370:ALA:O	2.16	0.46
1:A:473:VAL:HG13	1:A:555:VAL:HB	1.98	0.46
1:C:450:ASP:O	1:C:454:VAL:HG23	2.15	0.46
1:B:450:ASP:O	1:B:454:VAL:HG23	2.15	0.46
1:A:177:LEU:HD13	1:A:183:VAL:HG21	1.98	0.45
1:A:340:LEU:O	1:A:344:ILE:HG12	2.16	0.45
1:A:374:LEU:HD12	1:A:387:GLU:HB3	1.97	0.45
1:B:294:VAL:HG11	1:B:329:VAL:HG12	1.99	0.45
1:C:225:SER:HB3	1:C:242:ASN:H	1.81	0.45
1:B:83:VAL:HG12	1:B:83:VAL:O	2.16	0.45
1:C:206:ASN:O	1:C:210:VAL:HG23	2.16	0.45
1:C:488:ARG:HH12	1:C:510:ARG:HB2	1.80	0.45
1:B:521:PRO:HA	1:B:528:ASP:OD1	2.16	0.45
1:C:87:SER:HB3	1:C:511:GLY:HA2	1.99	0.45
1:A:188:ASP:HA	1:A:189:PRO:HD2	1.67	0.45
1:B:515:LEU:HD13	1:B:539:SER:CB	2.46	0.45
1:B:69:PHE:O	1:B:72:HIS:HB3	2.16	0.45
1:A:515:LEU:HD13	1:A:539:SER:CB	2.47	0.45
1:C:118:ASN:OD1	1:C:120:SER:HB2	2.17	0.45
1:C:327:LEU:CD2	1:C:365:LYS:HD2	2.46	0.45
1:C:202:VAL:HG13	1:C:204:TYR:H	1.81	0.45
1:C:515:LEU:HD13	1:C:539:SER:CB	2.47	0.45
1:A:86:ARG:NH2	1:A:113:ASN:OD1	2.49	0.45
1:A:192:ARG:HG2	1:A:192:ARG:O	2.15	0.45
1:A:184:LEU:HD11	1:A:235:GLY:HA3	1.98	0.45
1:D:473:VAL:HG13	1:D:555:VAL:HB	1.99	0.45
1:A:177:LEU:CD1	1:A:183:VAL:HG21	2.47	0.45
1:B:337:ARG:CD	1:B:370:ALA:O	2.64	0.45
1:D:286:SER:HA	1:D:313:LYS:HE2	1.99	0.45
1:A:216:ARG:O	1:A:217:ILE:HG13	2.17	0.45
1:C:559:ARG:HD2	1:C:564:TYR:CD1	2.51	0.45
1:D:276:VAL:HG11	1:D:304:GLU:HB2	1.98	0.45
1:D:303:PRO:C	1:D:305:GLY:H	2.19	0.45
1:D:85:ALA:HB2	1:D:545:PHE:CE2	2.51	0.45
1:D:229:GLN:O	1:D:230:LYS:HG2	2.17	0.45
1:A:164:THR:O	1:A:249:ARG:HA	2.16	0.44
1:B:255:PRO:C	1:B:257:ALA:H	2.19	0.44
1:B:438:PHE:O	1:B:442:ARG:HG3	2.17	0.44
1:C:559:ARG:HD3	1:C:560:PRO:O	2.18	0.44
1:D:450:ASP:O	1:D:454:VAL:HG23	2.18	0.44
1:A:68:THR:HB	1:C:440:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:VAL:HG13	1:C:555:VAL:HB	1.98	0.44
1:A:249:ARG:NH1	6:A:2005:HOH:O	2.25	0.44
1:A:441:LEU:O	1:A:442:ARG:C	2.57	0.44
1:C:294:VAL:HG11	1:C:329:VAL:HG12	2.00	0.43
1:B:135:ARG:O	1:B:139:GLU:HG2	2.19	0.43
1:D:506:VAL:HG13	1:D:512:VAL:CG1	2.45	0.43
1:A:175:VAL:CG1	1:A:197:ALA:HA	2.48	0.43
1:B:228:VAL:HA	1:B:238:THR:HA	2.01	0.43
1:D:337:ARG:CD	1:D:370:ALA:O	2.67	0.43
1:A:480:SER:OG	2:A:580:FBP:O6P	2.33	0.43
1:D:206:ASN:O	1:D:207:ILE:C	2.55	0.43
1:D:285:ALA:O	1:D:313:LYS:HG3	2.18	0.43
1:A:276:VAL:CG1	1:A:304:GLU:HB2	2.49	0.43
1:D:202:VAL:HG13	1:D:204:TYR:H	1.83	0.43
1:D:441:LEU:O	1:D:442:ARG:C	2.56	0.43
1:A:275:GLY:O	1:A:280:VAL:HG22	2.18	0.43
1:C:125:GLU:H	1:C:125:GLU:CD	2.21	0.43
1:C:374:LEU:HD12	1:C:387:GLU:HB3	2.00	0.43
1:B:559:ARG:HD3	1:B:560:PRO:O	2.19	0.43
1:D:439:GLU:O	1:D:443:ARG:HB2	2.17	0.43
1:A:166:ILE:HD12	1:A:166:ILE:N	2.34	0.43
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.92	0.43
1:B:83:VAL:CG1	1:B:83:VAL:O	2.65	0.43
1:C:83:VAL:O	1:C:83:VAL:CG1	2.67	0.43
1:D:374:LEU:HD12	1:D:387:GLU:HB3	2.00	0.43
1:A:253:ASN:O	1:A:254:LEU:HD23	2.19	0.43
1:A:372:GLN:HG2	1:A:375:GLU:HG3	2.00	0.43
1:C:207:ILE:CG2	1:C:208:VAL:N	2.81	0.43
1:D:339:ASP:O	1:D:340:LEU:C	2.57	0.43
1:B:102:GLU:HA	1:B:102:GLU:OE1	2.18	0.43
1:B:125:GLU:H	1:B:125:GLU:CD	2.22	0.43
1:B:475:THR:HA	2:B:580:FBP:H61	2.00	0.43
1:A:281:ASP:C	1:A:282:ILE:HG13	2.39	0.42
1:D:281:ASP:OD2	1:D:504:ARG:NE	2.48	0.42
1:B:303:PRO:C	1:B:305:GLY:H	2.23	0.42
1:D:453:GLU:HG2	1:D:483:LEU:HD13	2.02	0.42
1:A:135:ARG:O	1:A:139:GLU:HG2	2.19	0.42
1:C:271:ASP:O	1:C:274:PHE:HB3	2.19	0.42
1:A:434:HIS:O	1:A:435:ARG:C	2.57	0.42
1:B:385:ARG:NH1	1:B:385:ARG:HG2	2.33	0.42
1:A:184:LEU:CD1	1:A:235:GLY:HA3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:NH2	1:B:390:ASP:OD1	2.52	0.42
1:C:175:VAL:HG22	6:C:2008:HOH:O	2.19	0.42
1:D:284:PHE:HD1	1:D:311:ILE:HB	1.84	0.42
1:B:156:ASP:OD1	1:B:156:ASP:C	2.58	0.42
1:B:81:GLU:OE1	1:B:81:GLU:HA	2.20	0.42
1:C:562:SER:HB2	2:C:580:FBP:O4P	2.18	0.42
1:D:157:THR:CG2	1:D:286:SER:H	2.31	0.42
1:D:349:VAL:O	1:D:352:ALA:N	2.53	0.42
1:A:175:VAL:HG11	1:A:197:ALA:HA	2.02	0.42
1:A:230:LYS:HD3	1:A:230:LYS:HA	1.82	0.42
1:B:107:MET:HG3	1:B:415:VAL:HG22	2.02	0.42
1:C:509:CYS:O	1:C:510:ARG:C	2.56	0.42
1:A:157:THR:HG22	1:A:286:SER:CB	2.50	0.42
1:B:315:GLU:HG2	1:B:336:ALA:HB1	1.99	0.42
1:D:175:VAL:HG11	1:D:197:ALA:HA	2.01	0.42
1:D:337:ARG:HD3	1:D:370:ALA:O	2.20	0.42
1:C:435:ARG:NH1	1:D:443:ARG:HE	2.18	0.42
1:A:219:ILE:HB	1:A:224:ILE:HB	2.01	0.42
1:C:61:LEU:HA	1:C:61:LEU:HD12	1.95	0.42
1:A:104:LEU:O	1:A:108:ILE:HG13	2.19	0.41
1:B:61:LEU:HA	1:B:61:LEU:HD12	1.98	0.41
1:D:377:MET:HA	1:D:380:LYS:O	2.20	0.41
1:D:83:VAL:O	1:D:84:ALA:HB2	2.20	0.41
1:A:207:ILE:HD11	1:A:254:LEU:HD21	2.02	0.41
1:A:348:LYS:HD3	1:C:78:ILE:O	2.21	0.41
1:C:155:LEU:HD23	1:C:155:LEU:C	2.41	0.41
1:C:492:ALA:HB1	1:C:513:PHE:CE1	2.55	0.41
1:C:157:THR:HG22	1:C:286:SER:CB	2.49	0.41
1:D:255:PRO:C	1:D:257:ALA:H	2.23	0.41
1:D:281:ASP:C	1:D:282:ILE:HG13	2.41	0.41
1:B:420:MET:HE1	1:D:347:GLU:HG3	2.02	0.41
1:D:452:THR:HG22	1:D:483:LEU:HD12	2.03	0.41
1:B:146:LEU:HB3	1:B:542:LEU:HD12	2.01	0.41
1:C:525:TRP:CE2	1:C:560:PRO:HG3	2.56	0.41
1:D:492:ALA:HB1	1:D:513:PHE:CE1	2.56	0.41
1:D:515:LEU:HD13	1:D:539:SER:CB	2.51	0.41
1:D:61:LEU:HA	1:D:61:LEU:HD12	1.88	0.41
1:B:204:TYR:CE1	1:B:261:LEU:HD13	2.55	0.41
1:B:322:ARG:O	1:B:325:GLU:HG2	2.20	0.41
1:A:377:MET:HA	1:A:380:LYS:O	2.20	0.41
1:A:559:ARG:HD3	1:A:560:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:HG12	1:C:114:ILE:HB	2.02	0.41
1:B:347:GLU:HG3	1:D:420:MET:HE1	2.01	0.41
1:B:114:ILE:HG12	1:B:152:ALA:HB3	2.03	0.41
1:B:313:LYS:HD2	1:B:334:MET:CE	2.51	0.41
1:C:360:CYS:O	1:C:361:ASN:C	2.57	0.41
1:D:230:LYS:HD3	1:D:230:LYS:HA	1.80	0.41
1:D:509:CYS:O	1:D:510:ARG:C	2.59	0.41
1:A:144:SER:HB3	6:A:2003:HOH:O	2.21	0.41
1:B:157:THR:HG22	1:B:286:SER:CB	2.50	0.41
1:B:219:ILE:HB	1:B:224:ILE:HB	2.02	0.41
1:B:96:PRO:HD2	1:B:409:ALA:O	2.21	0.41
1:B:525:TRP:CE2	1:B:560:PRO:HG3	2.56	0.41
1:D:559:ARG:HD3	1:D:560:PRO:O	2.20	0.41
1:A:327:LEU:CD2	1:A:365:LYS:HD2	2.51	0.41
1:B:102:GLU:OE1	1:B:105:LYS:HD2	2.21	0.41
1:D:218:TYR:HB3	1:D:222:GLY:HA2	2.02	0.41
1:A:133:ASN:ND2	6:A:2002:HOH:O	2.54	0.41
1:B:377:MET:C	1:B:379:THR:N	2.74	0.41
1:A:271:ASP:O	1:A:274:PHE:HB3	2.21	0.40
1:A:569:ARG:HG2	1:B:567:ILE:HG12	2.03	0.40
1:A:69:PHE:O	1:A:72:HIS:HB3	2.21	0.40
1:D:155:LEU:C	1:D:155:LEU:HD23	2.41	0.40
1:A:488:ARG:HH11	1:A:510:ARG:CB	2.23	0.40
1:A:61:LEU:O	1:A:62:PRO:C	2.59	0.40
1:C:420:MET:HE3	1:C:424:ILE:HG13	2.03	0.40
1:D:315:GLU:CG	1:D:336:ALA:HB3	2.48	0.40
1:D:337:ARG:NH2	1:D:390:ASP:OD1	2.54	0.40
1:D:405:SER:O	1:D:406:GLY:C	2.60	0.40
1:A:297:VAL:HG12	1:A:310:ILE:HD13	2.04	0.40
1:A:360:CYS:O	1:A:361:ASN:C	2.59	0.40
1:A:465:LYS:HE3	1:B:448:SER:CB	2.51	0.40
1:D:188:ASP:HA	1:D:189:PRO:HD3	1.83	0.40
1:D:217:ILE:HB	1:D:226:LEU:HB2	2.02	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:HIS:CE1	1:B:322:ARG:NH1[1_655]	1.57	0.63
1:A:306:HIS:CE1	1:B:322:ARG:NH2[1_655]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:HIS:NE2	1:B:322:ARG:NH1[1_655]	1.65	0.55
1:A:306:HIS:CE1	1:B:322:ARG:CZ[1_655]	1.67	0.53
1:A:306:HIS:NE2	1:B:322:ARG:CZ[1_655]	2.09	0.11
1:C:258:GLN:NE2	1:D:298:ARG:O[1_556]	2.17	0.03
1:A:306:HIS:ND1	1:B:322:ARG:NH2[1_655]	2.19	0.01

## 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%)	476 (92%)	35 (7%)	4 (1%)	22	47
1	B	483/528 (92%)	452 (94%)	25 (5%)	6 (1%)	15	34
1	C	515/528 (98%)	482 (94%)	28 (5%)	5 (1%)	18	40
1	D	508/528 (96%)	479 (94%)	26 (5%)	3 (1%)	28	54
All	All	2021/2112 (96%)	1889 (94%)	114 (6%)	18 (1%)	20	44

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	B	83	VAL
1	C	83	VAL
1	D	83	VAL
1	A	566	ASN
1	C	447	LEU
1	C	566	ASN
1	A	371	THR
1	B	447	LEU
1	B	566	ASN
1	D	371	THR
1	D	566	ASN

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Mol	Chain	Res	Type
1	B	84	ALA
1	B	371	THR
1	C	371	THR
1	A	486	ARG
1	C	170	GLY
1	B	213	VAL

### 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%)	367 (89%)	47 (11%)	7	14
1	B	394/423 (93%)	350 (89%)	44 (11%)	7	15
1	C	414/423 (98%)	366 (88%)	48 (12%)	6	14
1	D	411/423 (97%)	363 (88%)	48 (12%)	6	13
All	All	1633/1692 (96%)	1446 (88%)	187 (12%)	6	14

All (187) 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	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	177	LEU
1	A	182	GLN
1	A	194	ARG
1	A	200	VAL
1	A	202	VAL

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Mol	Chain	Res	Type
1	A	209	ARG
1	A	221	ASP
1	A	231	ILE
1	A	234	GLU
1	A	258	GLN
1	A	289	ARG
1	A	294	VAL
1	A	298	ARG
1	A	304	GLU
1	A	327	LEU
1	A	337	ARG
1	A	362	LEU
1	A	374	LEU
1	A	379	THR
1	A	389	SER
1	A	396	LEU
1	A	410	LYS
1	A	443	ARG
1	A	449	ARG
1	A	473	VAL
1	A	480	SER
1	A	486	ARG
1	A	508	LEU
1	A	534	GLN
1	A	539	SER
1	A	542	LEU
1	A	546	LEU
1	A	547	ARG
1	A	548	VAL
1	A	552	VAL
1	A	559	ARG
1	A	562	SER
1	B	61	LEU
1	B	83	VAL
1	B	86	ARG
1	B	103	ARG
1	B	104	LEU
1	B	120	SER
1	B	124	HIS
1	B	144	SER
1	B	157	THR
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	182	GLN
1	B	202	VAL
1	B	210	VAL
1	B	258	GLN
1	B	260	ASP
1	B	289	ARG
1	B	294	VAL
1	B	298	ARG
1	B	304	GLU
1	B	327	LEU
1	B	337	ARG
1	B	362	LEU
1	B	374	LEU
1	B	379	THR
1	B	388	THR
1	B	389	SER
1	B	396	LEU
1	B	410	LYS
1	B	443	ARG
1	B	449	ARG
1	B	473	VAL
1	B	480	SER
1	B	485	SER
1	B	486	ARG
1	B	508	LEU
1	B	534	GLN
1	B	539	SER
1	B	542	LEU
1	B	546	LEU
1	B	547	ARG
1	B	548	VAL
1	B	552	VAL
1	B	559	ARG
1	B	562	SER
1	C	61	LEU
1	C	83	VAL
1	C	86	ARG
1	C	103	ARG
1	C	104	LEU
1	C	120	SER
1	C	124	HIS
1	C	147	SER

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Mol	Chain	Res	Type
1	C	157	THR
1	C	158	LYS
1	C	167	LEU
1	C	175	VAL
1	C	176	GLU
1	C	182	GLN
1	C	193	THR
1	C	200	VAL
1	C	202	VAL
1	C	209	ARG
1	C	229	GLN
1	C	231	ILE
1	C	234	GLU
1	C	289	ARG
1	C	294	VAL
1	C	298	ARG
1	C	304	GLU
1	C	327	LEU
1	C	337	ARG
1	C	362	LEU
1	C	374	LEU
1	C	379	THR
1	C	388	THR
1	C	389	SER
1	C	396	LEU
1	C	410	LYS
1	C	443	ARG
1	C	449	ARG
1	C	473	VAL
1	C	480	SER
1	C	486	ARG
1	C	508	LEU
1	C	534	GLN
1	C	539	SER
1	C	542	LEU
1	C	546	LEU
1	C	547	ARG
1	C	548	VAL
1	C	552	VAL
1	C	559	ARG
1	D	61	LEU
1	D	83	VAL

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Mol	Chain	Res	Type
1	D	86	ARG
1	D	103	ARG
1	D	104	LEU
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	188	ASP
1	D	200	VAL
1	D	202	VAL
1	D	210	VAL
1	D	225	SER
1	D	230	LYS
1	D	231	ILE
1	D	234	GLU
1	D	258	GLN
1	D	289	ARG
1	D	294	VAL
1	D	298	ARG
1	D	304	GLU
1	D	327	LEU
1	D	337	ARG
1	D	362	LEU
1	D	374	LEU
1	D	379	THR
1	D	388	THR
1	D	389	SER
1	D	396	LEU
1	D	410	LYS
1	D	443	ARG
1	D	449	ARG
1	D	473	VAL
1	D	480	SER
1	D	486	ARG
1	D	508	LEU
1	D	534	GLN
1	D	539	SER
1	D	542	LEU
1	D	546	LEU
1	D	547	ARG

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Mol	Chain	Res	Type
1	D	548	VAL
1	D	552	VAL
1	D	559	ARG
1	D	562	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	133	ASN
1	A	168	GLN
1	A	229	GLN
1	A	421	GLN
1	A	534	GLN
1	B	124	HIS
1	B	133	ASN
1	B	242	ASN
1	B	258	GLN
1	B	421	GLN
1	B	534	GLN
1	C	124	HIS
1	C	133	ASN
1	C	229	GLN
1	C	253	ASN
1	C	421	GLN
1	C	534	GLN
1	D	124	HIS
1	D	133	ASN
1	D	182	GLN
1	D	242	ASN
1	D	258	GLN
1	D	421	GLN

### 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 [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	1.02	1 (5%)	23,32,32	1.03	1 (4%)
3	PGA	A	581	5,4	5,8,8	0.83	0	6,11,11	0.81	0
2	FBP	B	580	-	18,20,20	0.96	1 (5%)	23,32,32	0.86	0
3	PGA	B	581	5,4	5,8,8	0.65	0	6,11,11	0.86	0
2	FBP	C	580	-	18,20,20	1.12	1 (5%)	23,32,32	0.87	0
3	PGA	C	581	5,4	5,8,8	0.75	0	6,11,11	0.89	0
2	FBP	D	580	-	18,20,20	1.02	1 (5%)	23,32,32	1.00	1 (4%)
3	PGA	D	581	5,4	5,8,8	0.61	0	6,11,11	0.77	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	580	FBP	O2-C2	2.01	1.44	1.40
2	B	580	FBP	O2-C2	2.25	1.44	1.40
2	D	580	FBP	O2-C2	2.38	1.44	1.40
2	A	580	FBP	O2-C2	2.60	1.45	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	580	FBP	P1-O1-C1	2.02	123.85	118.30
2	A	580	FBP	P2-O6-C6	2.31	124.64	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	580	FBP	1	0
2	B	580	FBP	3	0
2	C	580	FBP	2	0
2	D	580	FBP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	517/528 (97%)	0.32	51 (9%) 8 7	33, 40, 47, 57	0
1	B	491/528 (92%)	0.42	48 (9%) 8 7	33, 39, 47, 57	0
1	C	517/528 (97%)	-0.00	11 (2%) 64 67	33, 40, 47, 57	0
1	D	512/528 (96%)	0.07	24 (4%) 32 32	33, 40, 47, 57	0
All	All	2037/2112 (96%)	0.20	134 (6%) 19 18	33, 40, 47, 57	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	GLY	6.4
1	B	143	GLY	5.7
1	D	194	ARG	5.4
1	B	142	ALA	5.3
1	B	531	ARG	5.2
1	B	213	VAL	5.2
1	A	168	GLN	4.8
1	A	171	PRO	4.7
1	C	304	GLU	4.7
1	B	239	GLN	4.6
1	A	169	GLY	4.6
1	B	212	PRO	4.3
1	D	548	VAL	4.2
1	A	215	GLY	4.1
1	B	256	GLY	4.0
1	B	527	ASP	4.0
1	A	230	LYS	3.9
1	B	561	GLY	3.9
1	D	59	GLN	3.9
1	A	561	GLY	3.8
1	A	303	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	524	ILE	3.8
1	A	520	PRO	3.8
1	A	173	SER	3.8
1	B	83	VAL	3.8
1	D	549	GLY	3.7
1	C	122	GLY	3.7
1	A	231	ILE	3.7
1	A	167	LEU	3.7
1	B	528	ASP	3.7
1	A	229	GLN	3.7
1	D	173	SER	3.6
1	B	547	ARG	3.6
1	B	145	PRO	3.6
1	B	524	ILE	3.5
1	B	66	ALA	3.5
1	A	261	LEU	3.4
1	A	209	ARG	3.3
1	B	548	VAL	3.3
1	A	302	GLY	3.3
1	D	58	GLN	3.3
1	A	123	SER	3.2
1	A	528	ASP	3.2
1	D	263	GLY	3.2
1	B	207	ILE	3.2
1	B	146	LEU	3.2
1	B	180	GLY	3.2
1	C	57	GLN	3.2
1	B	211	VAL	3.2
1	D	65	MET	3.2
1	D	306	HIS	3.1
1	B	549	GLY	3.1
1	D	547	ARG	3.0
1	A	522	GLU	3.0
1	B	181	SER	2.9
1	A	525	TRP	2.9
1	B	247	GLY	2.9
1	B	306	HIS	2.9
1	B	241	GLU	2.8
1	D	531	ARG	2.8
1	A	239	GLN	2.8
1	B	182	GLN	2.8
1	A	65	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	2.7
1	A	472	ILE	2.7
1	A	542	LEU	2.7
1	B	65	MET	2.7
1	A	307	GLY	2.7
1	B	210	VAL	2.7
1	B	558	TRP	2.7
1	B	249	ARG	2.7
1	B	240	VAL	2.7
1	B	259	VAL	2.7
1	A	260	ASP	2.6
1	D	233	PRO	2.6
1	B	291	ALA	2.6
1	B	362	LEU	2.6
1	D	61	LEU	2.6
1	B	529	VAL	2.6
1	A	523	ALA	2.5
1	A	170	GLY	2.5
1	A	180	GLY	2.5
1	A	554	VAL	2.5
1	A	531	ARG	2.5
1	A	259	VAL	2.5
1	A	57	GLN	2.5
1	D	304	GLU	2.5
1	A	75	LEU	2.5
1	A	306	HIS	2.4
1	A	59	GLN	2.4
1	C	553	ILE	2.4
1	A	521	PRO	2.4
1	C	115	ALA	2.4
1	D	261	LEU	2.4
1	B	520	PRO	2.4
1	C	258	GLN	2.4
1	B	121	HIS	2.4
1	D	146	LEU	2.4
1	B	166	ILE	2.4
1	D	262	PRO	2.3
1	D	83	VAL	2.3
1	A	161	GLU	2.3
1	A	284	PHE	2.3
1	C	171	PRO	2.3
1	A	122	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	562	SER	2.2
1	A	125	GLU	2.2
1	B	64	ALA	2.2
1	A	166	ILE	2.2
1	D	260	ASP	2.2
1	A	527	ASP	2.2
1	B	569	ARG	2.2
1	B	81	GLU	2.2
1	A	245	VAL	2.2
1	A	172	GLU	2.1
1	B	449	ARG	2.1
1	B	144	SER	2.1
1	C	524	ILE	2.1
1	D	232	GLY	2.1
1	A	92	ALA	2.1
1	A	194	ARG	2.1
1	B	262	PRO	2.1
1	C	182	GLN	2.1
1	B	554	VAL	2.1
1	D	64	ALA	2.1
1	C	547	ARG	2.1
1	D	192	ARG	2.1
1	A	568	MET	2.1
1	A	121	HIS	2.0
1	B	525	TRP	2.0
1	C	229	GLN	2.0
1	B	227	VAL	2.0
1	D	193	THR	2.0
1	A	549	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PGA	D	581	9/9	0.96	0.23	2.41	103,106,107,108	0
3	PGA	C	581	9/9	0.94	0.27	1.96	103,105,107,108	0
3	PGA	B	581	9/9	0.95	0.23	1.22	104,106,108,108	0
3	PGA	A	581	9/9	0.94	0.22	0.60	104,106,107,108	0
2	FBP	D	580	20/20	0.95	0.18	-0.07	69,73,76,77	0
2	FBP	A	580	20/20	0.94	0.17	-0.71	70,75,77,78	0
4	K	A	582	1/1	0.93	0.14	-0.86	78,78,78,78	0
2	FBP	C	580	20/20	0.96	0.15	-0.89	68,73,76,77	0
2	FBP	B	580	20/20	0.93	0.16	-0.91	71,75,77,78	0
4	K	D	594	1/1	0.98	0.10	-2.29	60,60,60,60	0
4	K	C	590	1/1	0.98	0.06	-2.58	67,67,67,67	0
4	K	B	586	1/1	0.90	0.15	-2.80	81,81,81,81	0
5	MN	D	595	1/1	0.98	0.10	-	59,59,59,59	0
5	MN	C	591	1/1	0.99	0.08	-	58,58,58,58	0
5	MN	B	587	1/1	0.97	0.06	-	64,64,64,64	0
5	MN	A	583	1/1	0.98	0.06	-	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.