



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 30, 2017 – 07:12 AM EDT

PDB ID : 5NAQ
Title : Crystal structure of native 6-phospho-glucosidase LpBgl from *Lactobacillus plantarum*
Authors : Acebron, I.; Mancheno, J.M.
Deposited on : unknown
Resolution : 2.48 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
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) : rb-20029824

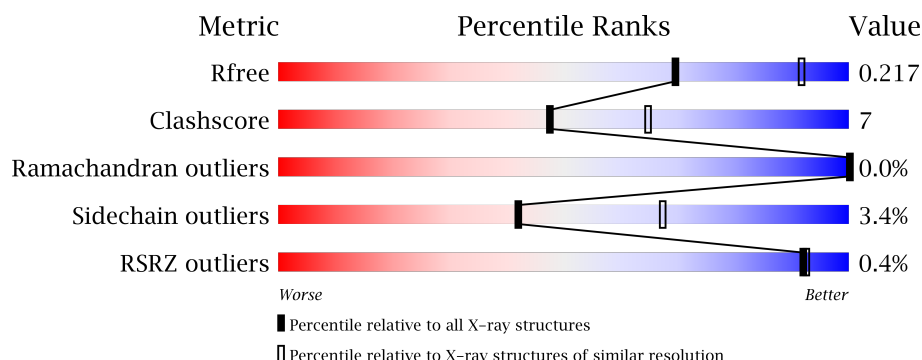
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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	477	
1	B	477	
1	C	477	
1	D	477	
1	E	477	

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Mol	Chain	Length	Quality of chain
1	F	477	 <div>79% 16% . .</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	501	-	-	-	X
2	PO4	E	502	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24057 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	As	C	N	O	S	0	0	0
			3732	1	2403	628	682	18			
1	B	461	Total	As	C	N	O	S	0	0	0
			3732	1	2403	628	682	18			
1	C	461	Total	As	C	N	O	S	0	0	0
			3732	1	2403	628	682	18			
1	D	461	Total	As	C	N	O	S	0	0	0
			3732	1	2403	628	682	18			
1	E	461	Total	As	C	N	O	S	0	0	0
			3732	1	2403	628	682	18			
1	F	461	Total	As	C	N	O	S	0	0	0
			3732	1	2403	628	682	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP F9ULH8
A	-14	GLY	-	expression tag	UNP F9ULH8
A	-13	GLY	-	expression tag	UNP F9ULH8
A	-12	SER	-	expression tag	UNP F9ULH8
A	-11	HIS	-	expression tag	UNP F9ULH8
A	-10	HIS	-	expression tag	UNP F9ULH8
A	-9	HIS	-	expression tag	UNP F9ULH8
A	-8	HIS	-	expression tag	UNP F9ULH8
A	-7	HIS	-	expression tag	UNP F9ULH8
A	-6	HIS	-	expression tag	UNP F9ULH8
A	-5	GLY	-	expression tag	UNP F9ULH8
A	-4	ASP	-	expression tag	UNP F9ULH8
A	-3	ASP	-	expression tag	UNP F9ULH8
A	-2	ASP	-	expression tag	UNP F9ULH8
A	-1	ASP	-	expression tag	UNP F9ULH8
A	0	LYS	-	expression tag	UNP F9ULH8
B	-15	MET	-	initiating methionine	UNP F9ULH8

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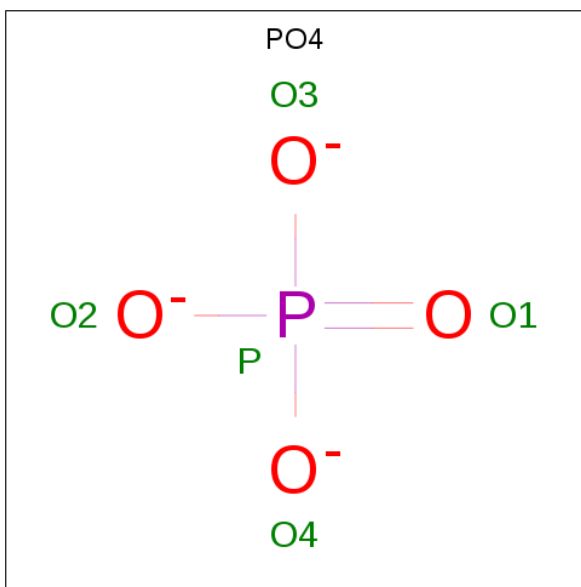
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP F9ULH8
B	-13	GLY	-	expression tag	UNP F9ULH8
B	-12	SER	-	expression tag	UNP F9ULH8
B	-11	HIS	-	expression tag	UNP F9ULH8
B	-10	HIS	-	expression tag	UNP F9ULH8
B	-9	HIS	-	expression tag	UNP F9ULH8
B	-8	HIS	-	expression tag	UNP F9ULH8
B	-7	HIS	-	expression tag	UNP F9ULH8
B	-6	HIS	-	expression tag	UNP F9ULH8
B	-5	GLY	-	expression tag	UNP F9ULH8
B	-4	ASP	-	expression tag	UNP F9ULH8
B	-3	ASP	-	expression tag	UNP F9ULH8
B	-2	ASP	-	expression tag	UNP F9ULH8
B	-1	ASP	-	expression tag	UNP F9ULH8
B	0	LYS	-	expression tag	UNP F9ULH8
C	-15	MET	-	initiating methionine	UNP F9ULH8
C	-14	GLY	-	expression tag	UNP F9ULH8
C	-13	GLY	-	expression tag	UNP F9ULH8
C	-12	SER	-	expression tag	UNP F9ULH8
C	-11	HIS	-	expression tag	UNP F9ULH8
C	-10	HIS	-	expression tag	UNP F9ULH8
C	-9	HIS	-	expression tag	UNP F9ULH8
C	-8	HIS	-	expression tag	UNP F9ULH8
C	-7	HIS	-	expression tag	UNP F9ULH8
C	-6	HIS	-	expression tag	UNP F9ULH8
C	-5	GLY	-	expression tag	UNP F9ULH8
C	-4	ASP	-	expression tag	UNP F9ULH8
C	-3	ASP	-	expression tag	UNP F9ULH8
C	-2	ASP	-	expression tag	UNP F9ULH8
C	-1	ASP	-	expression tag	UNP F9ULH8
C	0	LYS	-	expression tag	UNP F9ULH8
D	-15	MET	-	initiating methionine	UNP F9ULH8
D	-14	GLY	-	expression tag	UNP F9ULH8
D	-13	GLY	-	expression tag	UNP F9ULH8
D	-12	SER	-	expression tag	UNP F9ULH8
D	-11	HIS	-	expression tag	UNP F9ULH8
D	-10	HIS	-	expression tag	UNP F9ULH8
D	-9	HIS	-	expression tag	UNP F9ULH8
D	-8	HIS	-	expression tag	UNP F9ULH8
D	-7	HIS	-	expression tag	UNP F9ULH8
D	-6	HIS	-	expression tag	UNP F9ULH8
D	-5	GLY	-	expression tag	UNP F9ULH8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ASP	-	expression tag	UNP F9ULH8
D	-3	ASP	-	expression tag	UNP F9ULH8
D	-2	ASP	-	expression tag	UNP F9ULH8
D	-1	ASP	-	expression tag	UNP F9ULH8
D	0	LYS	-	expression tag	UNP F9ULH8
E	-15	MET	-	initiating methionine	UNP F9ULH8
E	-14	GLY	-	expression tag	UNP F9ULH8
E	-13	GLY	-	expression tag	UNP F9ULH8
E	-12	SER	-	expression tag	UNP F9ULH8
E	-11	HIS	-	expression tag	UNP F9ULH8
E	-10	HIS	-	expression tag	UNP F9ULH8
E	-9	HIS	-	expression tag	UNP F9ULH8
E	-8	HIS	-	expression tag	UNP F9ULH8
E	-7	HIS	-	expression tag	UNP F9ULH8
E	-6	HIS	-	expression tag	UNP F9ULH8
E	-5	GLY	-	expression tag	UNP F9ULH8
E	-4	ASP	-	expression tag	UNP F9ULH8
E	-3	ASP	-	expression tag	UNP F9ULH8
E	-2	ASP	-	expression tag	UNP F9ULH8
E	-1	ASP	-	expression tag	UNP F9ULH8
E	0	LYS	-	expression tag	UNP F9ULH8
F	-15	MET	-	initiating methionine	UNP F9ULH8
F	-14	GLY	-	expression tag	UNP F9ULH8
F	-13	GLY	-	expression tag	UNP F9ULH8
F	-12	SER	-	expression tag	UNP F9ULH8
F	-11	HIS	-	expression tag	UNP F9ULH8
F	-10	HIS	-	expression tag	UNP F9ULH8
F	-9	HIS	-	expression tag	UNP F9ULH8
F	-8	HIS	-	expression tag	UNP F9ULH8
F	-7	HIS	-	expression tag	UNP F9ULH8
F	-6	HIS	-	expression tag	UNP F9ULH8
F	-5	GLY	-	expression tag	UNP F9ULH8
F	-4	ASP	-	expression tag	UNP F9ULH8
F	-3	ASP	-	expression tag	UNP F9ULH8
F	-2	ASP	-	expression tag	UNP F9ULH8
F	-1	ASP	-	expression tag	UNP F9ULH8
F	0	LYS	-	expression tag	UNP F9ULH8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

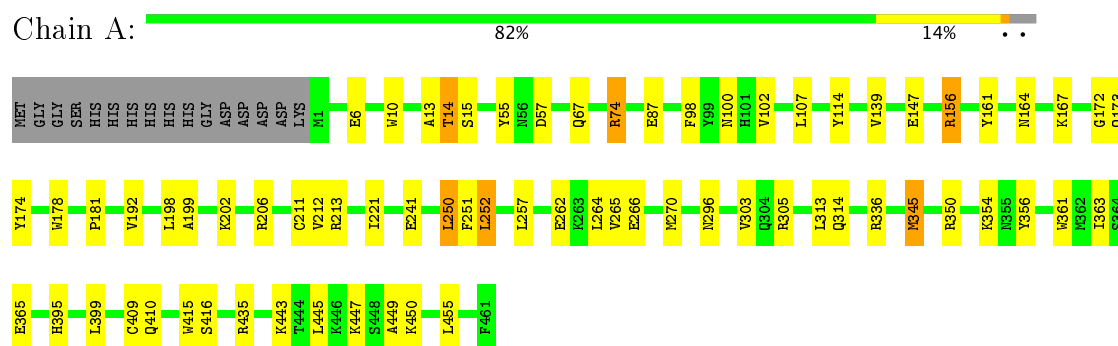
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	333	Total 333	O 333	0	0
3	B	324	Total 324	O 324	0	0
3	C	271	Total 271	O 271	0	0
3	D	271	Total 271	O 271	0	0
3	E	231	Total 231	O 231	0	0
3	F	175	Total 175	O 175	0	0

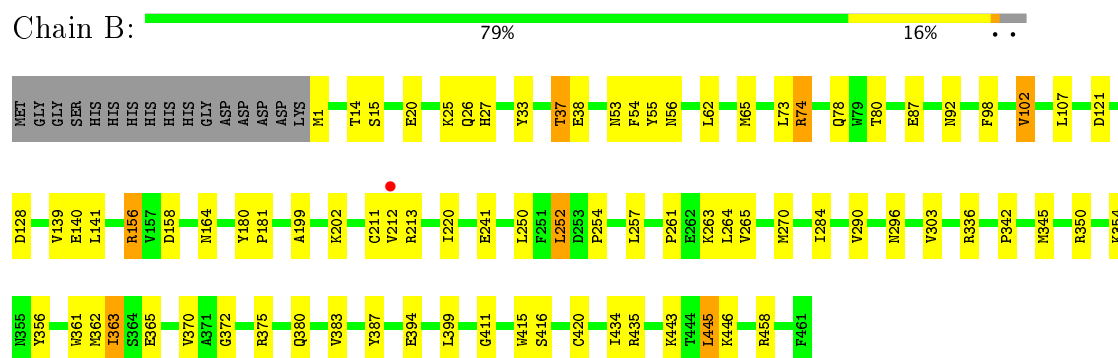
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

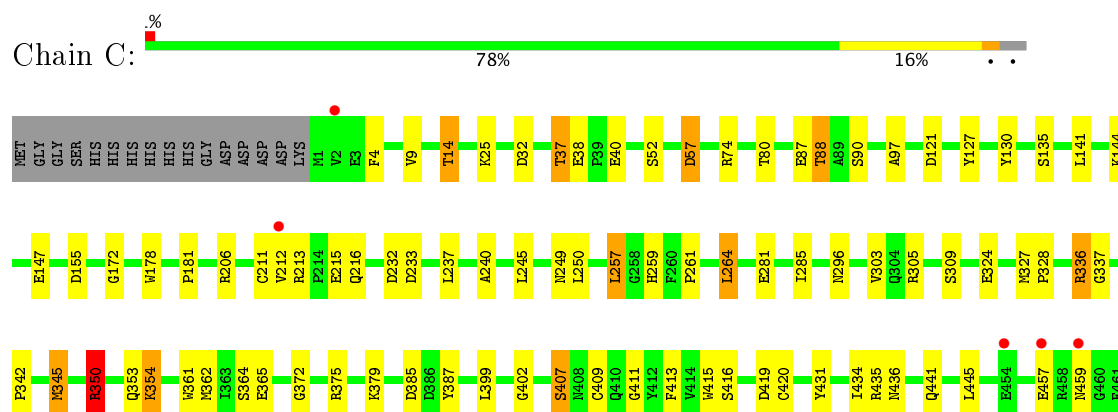
• Molecule 1: Beta-galactosidase

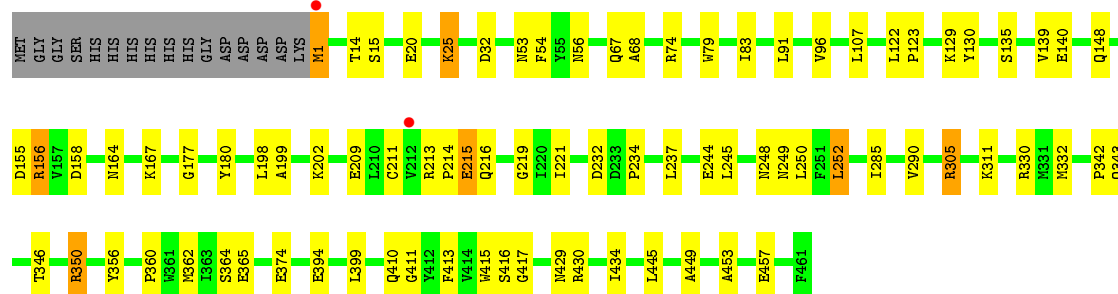


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.69Å 191.68Å 105.93Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	61.23 – 2.48 61.23 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.9 (61.23-2.48) 93.9 (61.23-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.159 , 0.217 0.158 , 0.217	Depositor DCC
R_{free} test set	6364 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24057	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, PO4

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	0.44	0/3843	0.61	0/5236
1	B	0.43	0/3843	0.61	1/5236 (0.0%)
1	C	0.48	3/3843 (0.1%)	0.61	2/5236 (0.0%)
1	D	0.42	0/3843	0.59	2/5236 (0.0%)
1	E	0.50	3/3843 (0.1%)	0.57	0/5236
1	F	0.43	1/3843 (0.0%)	0.56	0/5236
All	All	0.45	7/23058 (0.0%)	0.59	5/31416 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	374	GLU	CD-OE1	-11.86	1.12	1.25
1	E	374	GLU	CD-OE2	-11.16	1.13	1.25
1	C	350	ARG	CZ-NH1	-9.79	1.20	1.33
1	C	350	ARG	NE-CZ	-7.90	1.22	1.33
1	F	215	GLU	CD-OE1	-6.41	1.18	1.25
1	E	374	GLU	CG-CD	-5.21	1.44	1.51
1	C	457	GLU	CD-OE1	-5.03	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	C	350	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	D	379	LYS	CD-CE-NZ	5.43	124.20	111.70
1	B	445	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	445	LEU	CA-CB-CG	5.12	127.08	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	3732	0	3509	46	0
1	B	3732	0	3509	52	0
1	C	3732	0	3509	57	0
1	D	3732	0	3509	39	0
1	E	3732	0	3508	50	0
1	F	3732	0	3509	58	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	2	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	10	0	0	0	0
3	A	333	0	0	11	0
3	B	324	0	0	5	0
3	C	271	0	0	8	0
3	D	271	0	0	7	0
3	E	231	0	0	10	0
3	F	175	0	0	16	0
All	All	24057	0	21053	304	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 7.

All (304) 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:E:104:ASP:OD1	1:E:156:ARG:NH1	1.56	1.37
1:F:53:ASN:HD21	1:F:56:ASN:HD22	1.17	0.89
1:B:241:GLU:OE1	3:B:601:HOH:O	1.88	0.88
1:C:37:THR:HG22	1:C:38:GLU:HG3	1.56	0.88
1:E:158:ASP:OD2	1:E:213:ARG:NH1	2.08	0.87
1:B:53:ASN:HD21	1:B:56:ASN:HD22	1.21	0.87
1:E:182:GLN:NE2	3:E:601:HOH:O	1.84	0.86
1:E:101:HIS:ND1	3:E:603:HOH:O	2.07	0.86
1:C:350:ARG:HH12	1:C:407:SER:HB2	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LYS:NZ	1:B:78:GLN:OE1	2.09	0.85
1:D:452:PHE:O	3:D:601:HOH:O	1.96	0.83
1:B:140:GLU:OE1	3:B:602:HOH:O	1.96	0.82
1:D:57:ASP:OD2	3:D:602:HOH:O	1.99	0.81
1:A:241:GLU:OE2	3:A:601:HOH:O	2.00	0.78
1:F:249:ASN:OD1	3:F:603:HOH:O	2.00	0.78
1:A:67:GLN:O	3:A:602:HOH:O	2.01	0.77
1:F:245:LEU:HD23	1:F:249:ASN:HD22	1.50	0.77
1:D:65:MET:HE1	1:D:73:LEU:HD13	1.68	0.76
1:A:74:ARG:HD2	3:A:716:HOH:O	1.84	0.75
1:E:383:VAL:HB	1:E:446:LYS:HG2	1.66	0.75
1:E:154:GLY:O	1:E:213:ARG:NH2	2.20	0.75
1:E:354:LYS:NZ	3:E:607:HOH:O	2.19	0.74
1:A:345:MET:HE1	1:A:395:HIS:HB3	1.68	0.74
2:E:502:PO4:O4	3:E:602:HOH:O	2.06	0.73
1:B:1:MET:N	3:B:606:HOH:O	2.22	0.72
1:F:155:ASP:OD2	1:F:156:ARG:NE	2.23	0.71
1:F:1:MET:N	3:F:606:HOH:O	2.18	0.71
1:E:233:ASP:OD2	3:E:604:HOH:O	2.09	0.70
1:D:140:GLU:OE1	3:D:603:HOH:O	2.10	0.69
1:E:26:GLN:HE21	1:E:92:ASN:HD22	1.39	0.69
1:A:74:ARG:NH2	1:A:164:ASN:OD1	2.25	0.68
1:F:53:ASN:ND2	1:F:56:ASN:HD22	1.91	0.68
1:F:429:ASN:O	3:F:605:HOH:O	2.10	0.68
1:C:337:GLY:O	3:C:601:HOH:O	2.12	0.68
1:A:13:ALA:HB1	1:A:74:ARG:HH11	1.57	0.67
1:B:128:ASP:OD1	3:B:604:HOH:O	2.13	0.67
1:D:380:GLN:HB3	1:D:382:VAL:HG23	1.75	0.67
1:A:167:LYS:HG3	3:A:619:HOH:O	1.95	0.66
1:C:324:GLU:OE2	3:C:603:HOH:O	2.14	0.66
1:A:206:ARG:NH2	3:A:609:HOH:O	2.27	0.66
1:E:434:ILE:HG12	1:E:445:LEU:HD22	1.79	0.65
1:C:57:ASP:OD2	3:C:602:HOH:O	2.14	0.65
1:B:26:GLN:HE21	1:B:92:ASN:HD22	1.42	0.65
1:F:434:ILE:HG12	1:F:445:LEU:HD22	1.77	0.65
1:E:26:GLN:NE2	1:E:92:ASN:HD22	1.96	0.64
1:A:447:LYS:HA	1:A:450:LYS:HE3	1.80	0.64
1:C:233:ASP:OD1	1:C:305:ARG:NH2	2.31	0.63
1:E:1:MET:N	3:E:608:HOH:O	2.24	0.61
1:B:350:ARG:HH21	1:B:354:LYS:HE3	1.66	0.61
1:D:374:GLU:OE2	3:D:604:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLN:OE1	1:B:380:GLN:N	2.34	0.61
1:F:213:ARG:HG3	1:F:215:GLU:OE1	2.01	0.60
1:C:97:ALA:HA	3:C:814:HOH:O	2.00	0.60
1:C:372:GLY:O	1:C:375:ARG:HD3	2.02	0.60
1:F:158:ASP:OD2	1:F:213:ARG:NH1	2.35	0.59
1:B:361:TRP:CZ3	1:B:363:ILE:HD12	2.37	0.59
1:F:180:TYR:OH	3:F:601:HOH:O	1.86	0.59
1:A:212:VAL:HG23	1:A:213:ARG:HG3	1.85	0.59
1:B:252:LEU:HD13	1:B:356:TYR:CZ	2.39	0.58
1:C:212:VAL:HG23	1:C:213:ARG:HG3	1.86	0.58
1:B:25:LYS:HZ1	1:B:78:GLN:CD	2.01	0.58
1:C:155:ASP:OD1	3:C:604:HOH:O	2.17	0.58
1:A:212:VAL:HG23	1:A:213:ARG:H	1.68	0.58
1:B:361:TRP:HZ3	1:B:363:ILE:HD12	1.69	0.58
1:E:211:CYS:O	3:E:605:HOH:O	2.16	0.57
1:A:345:MET:HE3	1:A:363:ILE:HD13	1.86	0.57
1:F:311:LYS:NZ	3:F:621:HOH:O	2.31	0.57
1:E:273:VAL:O	3:E:606:HOH:O	2.17	0.57
1:D:361:TRP:CZ2	1:D:409:CYS:HB2	2.40	0.56
1:A:147:GLU:OE1	1:A:206:ARG:NH1	2.35	0.56
1:D:295:VAL:HG11	1:D:348:ILE:HG21	1.89	0.55
1:A:173:GLN:HG2	1:A:181:PRO:HD2	1.88	0.55
1:B:254:PRO:O	3:B:605:HOH:O	2.18	0.55
1:B:372:GLY:O	1:B:375:ARG:HD3	2.06	0.55
1:C:436:ASN:HD21	1:C:441:GLN:NE2	2.04	0.55
1:A:100:ASN:OD1	1:A:156:ARG:NH2	2.22	0.55
1:C:240:ALA:HA	1:C:303:VAL:HG21	1.87	0.55
1:F:14:THR:HG21	3:F:635:HOH:O	2.06	0.55
1:C:350:ARG:HH21	1:C:353:GLN:CG	2.19	0.54
1:C:4:PHE:O	1:C:459:ASN:ND2	2.40	0.54
1:F:139:VAL:HG13	1:F:199:ALA:HB2	1.89	0.54
1:C:350:ARG:HH21	1:C:353:GLN:CD	2.10	0.54
1:C:361:TRP:CZ2	1:C:409:CYS:HB2	2.42	0.54
1:E:436:ASN:HD21	1:E:441:GLN:HA	1.72	0.54
2:C:502:PO4:O4	3:C:605:HOH:O	2.18	0.53
1:F:252:LEU:HD13	1:F:356:TYR:CZ	2.43	0.53
1:D:74:ARG:NH2	1:D:365:GLU:HG3	2.24	0.53
1:D:1:MET:N	1:D:458:ARG:HH22	2.05	0.53
1:C:232:ASP:HA	1:C:237:LEU:HD11	1.89	0.53
1:F:148:GLN:NE2	3:F:631:HOH:O	2.42	0.53
1:F:91:LEU:HD13	1:F:96:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:SER:HA	1:C:441:GLN:HE22	1.74	0.53
1:B:212:VAL:HG23	1:B:213:ARG:HG3	1.90	0.52
1:D:303:VAL:HG13	1:D:322:PHE:HB2	1.91	0.52
1:F:232:ASP:O	1:F:237:LEU:HD11	2.09	0.52
1:C:336:ARG:NH2	3:C:624:HOH:O	2.43	0.52
1:F:213:ARG:HG2	1:F:216:GLN:HG3	1.91	0.52
1:C:296:ASN:ND2	1:C:365:GLU:HB2	2.25	0.52
1:A:13:ALA:HB1	1:A:74:ARG:NH1	2.23	0.52
1:B:107:LEU:HD21	1:B:156:ARG:HB2	1.92	0.52
1:B:158:ASP:OD2	1:B:213:ARG:NH2	2.26	0.52
1:B:296:ASN:OD1	1:B:365:GLU:HB2	2.09	0.51
1:B:26:GLN:NE2	1:B:92:ASN:HD22	2.07	0.51
1:C:211:CYS:SG	3:C:627:HOH:O	2.60	0.51
1:E:212:VAL:HG23	1:E:213:ARG:H	1.75	0.51
1:A:252:LEU:HD13	1:A:356:TYR:CZ	2.45	0.51
1:C:362:MET:HG2	1:C:411:GLY:N	2.24	0.51
1:E:252:LEU:HD13	1:E:356:TYR:CZ	2.46	0.51
1:F:374:GLU:CD	1:F:374:GLU:H	2.14	0.51
1:C:213:ARG:HB3	1:C:215:GLU:OE2	2.11	0.51
1:F:244:GLU:OE1	3:F:607:HOH:O	2.18	0.51
1:B:53:ASN:ND2	1:B:56:ASN:HD22	1.99	0.51
1:D:235:ALA:O	3:D:605:HOH:O	2.20	0.51
1:D:30:VAL:HG13	1:D:180:TYR:HB3	1.94	0.50
1:F:140:GLU:OE1	1:F:202:LYS:HE2	2.11	0.50
1:E:25:LYS:HE3	1:E:27:HIS:O	2.11	0.50
1:A:55:TYR:HA	1:A:98:PHE:CE1	2.46	0.50
1:D:213:ARG:HB3	1:D:215:GLU:OE1	2.11	0.50
1:A:445:LEU:HD13	1:A:449:ALA:HB1	1.93	0.50
1:C:25:LYS:HE3	1:C:80:THR:OG1	2.11	0.50
1:F:107:LEU:HD11	1:F:156:ARG:HB2	1.93	0.50
1:E:232:ASP:OD1	1:E:232:ASP:N	2.39	0.50
1:F:122:LEU:HD12	1:F:123:PRO:HD2	1.93	0.50
1:F:364:SER:HA	1:F:413:PHE:HB2	1.94	0.50
1:C:88:THR:HG22	1:C:90:SER:H	1.76	0.50
1:C:172:GLY:HA2	1:C:178:TRP:HB2	1.94	0.50
1:A:74:ARG:HA	1:A:114:TYR:O	2.11	0.50
1:B:65:MET:CE	1:B:73:LEU:HD22	2.42	0.50
1:D:296:ASN:ND2	1:D:365:GLU:HB2	2.27	0.50
1:F:209:GLU:OE1	3:F:609:HOH:O	2.20	0.50
1:F:167:LYS:HG3	3:F:612:HOH:O	2.11	0.49
1:E:305:ARG:HD2	1:E:305:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ASN:HD21	1:C:441:GLN:HE22	1.60	0.49
1:E:20:GLU:HA	1:E:54:PHE:HB3	1.95	0.49
1:F:248:ASN:OD1	3:F:608:HOH:O	2.20	0.49
1:A:350:ARG:CZ	1:A:354:LYS:HG3	2.41	0.49
1:A:74:ARG:HB2	1:A:114:TYR:HB2	1.94	0.49
1:E:370:VAL:HG21	1:E:387:TYR:CE1	2.48	0.49
1:A:57:ASP:CB	3:A:614:HOH:O	2.61	0.48
1:E:74:ARG:CZ	1:E:221:ILE:HD13	2.43	0.48
1:F:234:PRO:HA	1:F:237:LEU:HD12	1.96	0.48
1:D:185:ASN:OD1	1:D:187:PRO:HD2	2.14	0.48
1:E:415:TRP:HA	1:E:416:SER:HA	1.63	0.48
1:A:336:ARG:NH1	1:A:336:ARG:O	2.45	0.48
1:A:67:GLN:OE1	3:A:603:HOH:O	2.20	0.48
1:B:27:HIS:HB2	1:B:80:THR:HB	1.95	0.48
1:D:383:VAL:HB	1:D:446:LYS:HG2	1.96	0.48
1:D:55:TYR:HA	1:D:98:PHE:CE1	2.48	0.47
1:C:87:GLU:OE1	1:C:130:TYR:OH	2.24	0.47
1:D:383:VAL:HG12	1:D:385:ASP:HB3	1.96	0.47
1:F:129:LYS:HG2	1:F:130:TYR:CE2	2.49	0.47
1:E:217:GLN:HB2	1:E:292:CAS:CE1	2.45	0.47
1:B:434:ILE:HG12	1:B:445:LEU:HD22	1.95	0.47
1:A:198:LEU:HG	1:A:202:LYS:HD2	1.95	0.47
1:A:361:TRP:CZ2	1:A:409:CYS:HB2	2.50	0.47
1:E:362:MET:HE2	3:E:678:HOH:O	2.14	0.47
1:E:416:SER:O	1:E:432:GLY:HA2	2.14	0.47
1:B:20:GLU:HA	1:B:54:PHE:HB3	1.96	0.47
1:D:415:TRP:HA	1:D:416:SER:HA	1.70	0.47
1:F:25:LYS:NZ	1:F:32:ASP:OD2	2.47	0.47
1:F:362:MET:HG2	1:F:411:GLY:N	2.30	0.47
1:B:33:TYR:O	1:B:37:THR:HB	2.14	0.47
1:F:342:PRO:HG3	1:F:394:GLU:HB3	1.97	0.47
1:B:458:ARG:HH11	1:B:458:ARG:HG3	1.80	0.47
1:E:180:TYR:CG	1:E:181:PRO:HA	2.50	0.47
1:B:212:VAL:HG23	1:B:213:ARG:H	1.79	0.46
1:B:435:ARG:O	1:B:443:LYS:HA	2.15	0.46
1:C:245:LEU:HA	1:C:249:ASN:HB2	1.96	0.46
1:F:330:ARG:HG3	1:F:332:MET:HG2	1.98	0.46
1:C:385:ASP:HA	1:C:387:TYR:CE2	2.50	0.46
1:E:305:ARG:HD2	1:E:305:ARG:C	2.35	0.46
1:F:198:LEU:HA	1:F:285:ILE:HD11	1.96	0.46
1:C:362:MET:HE2	1:C:411:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG22	1:B:290:VAL:HG11	1.97	0.46
1:A:447:LYS:O	1:A:450:LYS:HG2	2.16	0.46
1:E:106:MET:CE	1:E:113:PRO:HB3	2.45	0.46
1:D:372:GLY:O	1:D:375:ARG:HD3	2.16	0.46
1:A:139:VAL:HG13	1:A:199:ALA:HB2	1.98	0.46
1:B:74:ARG:NH2	1:B:164:ASN:OD1	2.47	0.45
1:B:362:MET:HG2	1:B:411:GLY:N	2.31	0.45
1:F:20:GLU:HA	1:F:54:PHE:HB3	1.99	0.45
1:F:453:ALA:O	1:F:457:GLU:HG2	2.16	0.45
1:B:370:VAL:HG21	1:B:387:TYR:CE1	2.51	0.45
1:D:219:GLY:HA2	1:D:290:VAL:HB	1.98	0.45
1:F:14:THR:HB	1:F:15:SER:H	1.61	0.45
1:F:343:GLN:HB2	3:F:674:HOH:O	2.17	0.45
1:F:219:GLY:HA2	1:F:290:VAL:HB	1.97	0.45
1:B:415:TRP:HA	1:B:416:SER:HA	1.81	0.45
1:A:14:THR:HB	1:A:15:SER:H	1.48	0.45
1:D:129:LYS:HD3	1:D:130:TYR:CE2	2.52	0.45
1:A:10:TRP:CZ3	1:A:455:LEU:HD21	2.52	0.44
1:A:266:GLU:O	1:A:270:MET:HG3	2.16	0.44
1:B:62:LEU:HD23	1:B:65:MET:HE2	1.99	0.44
1:C:353:GLN:HG3	1:C:354:LYS:N	2.32	0.44
1:D:14:THR:HG23	1:D:416:SER:OG	2.16	0.44
1:F:415:TRP:HA	1:F:416:SER:HA	1.67	0.44
1:B:458:ARG:HG3	1:B:458:ARG:NH1	2.33	0.44
1:D:45:GLY:HA3	3:D:696:HOH:O	2.18	0.44
1:C:25:LYS:NZ	1:C:32:ASP:OD2	2.47	0.44
1:E:127:TYR:CZ	1:E:181:PRO:HG3	2.52	0.44
1:F:79:TRP:CD1	1:F:83:ILE:HG13	2.53	0.44
1:B:296:ASN:CG	1:B:365:GLU:HB2	2.37	0.44
1:C:415:TRP:HA	1:C:416:SER:HA	1.76	0.44
1:E:252:LEU:HD23	1:E:252:LEU:HA	1.83	0.44
1:E:371:ALA:O	1:E:375:ARG:NH2	2.47	0.44
1:D:74:ARG:HA	1:D:114:TYR:O	2.18	0.44
1:E:55:TYR:HA	1:E:98:PHE:CE2	2.53	0.44
1:F:177:GLY:N	3:F:626:HOH:O	2.36	0.44
1:F:346:THR:O	1:F:350:ARG:HD3	2.18	0.44
1:F:445:LEU:HB3	1:F:449:ALA:HB3	2.00	0.43
1:C:434:ILE:HG12	1:C:445:LEU:HD22	1.99	0.43
1:C:431:TYR:OH	2:C:501:PO4:O1	2.21	0.43
1:B:139:VAL:HG13	1:B:199:ALA:HB2	2.01	0.43
1:A:435:ARG:O	1:A:443:LYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:VAL:O	1:D:196:MET:HG3	2.19	0.43
1:D:362:MET:HE2	1:D:413:PHE:HE1	1.84	0.43
1:F:213:ARG:HA	1:F:214:PRO:HD3	1.83	0.43
1:F:360:PRO:HB3	1:F:410:GLN:NE2	2.33	0.43
1:F:67:GLN:HG2	3:F:617:HOH:O	2.17	0.43
1:A:14:THR:HG21	3:A:622:HOH:O	2.18	0.43
1:F:215:GLU:H	1:F:215:GLU:CD	2.21	0.43
1:B:252:LEU:HD13	1:B:356:TYR:CE1	2.54	0.43
1:C:14:THR:HG22	1:C:420:CYS:SG	2.58	0.43
1:C:350:ARG:NH1	1:C:402:GLY:O	2.52	0.43
1:D:245:LEU:HA	1:D:249:ASN:HB2	2.00	0.43
1:E:14:THR:HG21	3:E:667:HOH:O	2.19	0.43
1:E:303:VAL:HG13	1:E:322:PHE:HB2	2.01	0.43
1:B:14:THR:HB	1:B:15:SER:H	1.57	0.43
1:D:129:LYS:HD3	1:D:130:TYR:CZ	2.53	0.43
1:F:416:SER:OG	1:F:417:GLY:N	2.52	0.43
1:B:98:PHE:O	1:B:102:VAL:HG13	2.19	0.43
1:A:161:TYR:CD1	1:A:221:ILE:HD11	2.54	0.43
1:A:74:ARG:HB2	1:A:114:TYR:CB	2.49	0.43
1:C:365:GLU:HG2	1:C:415:TRP:HB2	1.99	0.43
1:F:430:ARG:HD3	3:F:605:HOH:O	2.19	0.43
1:D:20:GLU:HA	1:D:54:PHE:HB3	2.01	0.42
1:F:445:LEU:HD13	1:F:449:ALA:HB1	2.01	0.42
1:A:296:ASN:CG	1:A:365:GLU:HB2	2.39	0.42
1:E:212:VAL:HG23	1:E:213:ARG:HG3	2.01	0.42
1:D:121:ASP:OD1	1:D:121:ASP:N	2.52	0.42
1:E:361:TRP:CZ2	1:E:409:CYS:HB2	2.54	0.42
1:A:172:GLY:HA2	1:A:178:TRP:HB2	2.00	0.42
1:B:202:LYS:HG3	1:B:284:ILE:HG21	2.02	0.42
1:B:14:THR:HG22	1:B:420:CYS:SG	2.59	0.42
1:E:103:ILE:HA	1:E:106:MET:HE3	2.01	0.42
1:A:6:GLU:HA	3:A:647:HOH:O	2.19	0.42
1:B:263:LYS:HA	1:B:263:LYS:HD3	1.80	0.42
1:C:141:LEU:HD23	1:C:144:LYS:HZ1	1.84	0.42
1:C:419:ASP:OD2	1:C:435:ARG:HA	2.19	0.42
1:C:257:LEU:HB3	1:C:259:HIS:CE1	2.55	0.42
1:C:147:GLU:OE1	1:C:206:ARG:NH1	2.48	0.42
1:D:206:ARG:NH2	3:D:609:HOH:O	2.27	0.42
1:F:213:ARG:NE	1:F:215:GLU:OE1	2.53	0.42
1:D:30:VAL:HG11	1:D:180:TYR:O	2.19	0.42
1:F:198:LEU:O	1:F:202:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:PRO:HG2	1:B:264:LEU:HB3	2.02	0.42
1:C:141:LEU:HD23	1:C:144:LYS:NZ	2.35	0.42
1:C:261:PRO:HG2	1:C:264:LEU:HB2	2.01	0.42
1:C:342:PRO:O	1:C:345:MET:HB2	2.20	0.42
1:C:350:ARG:HA	1:C:350:ARG:NE	2.34	0.42
1:D:165:GLU:OE1	1:D:223:ASN:HB2	2.19	0.42
1:B:37:THR:HG23	1:B:38:GLU:HG3	2.01	0.41
1:F:365:GLU:HG2	1:F:415:TRP:HE3	1.85	0.41
1:D:74:ARG:HH12	1:D:164:ASN:ND2	2.18	0.41
1:E:84:ASP:HB3	1:E:90:SER:OG	2.20	0.41
1:A:410:GLN:NE2	3:A:642:HOH:O	2.53	0.41
1:C:215:GLU:H	1:C:215:GLU:CD	2.23	0.41
1:A:87:GLU:O	3:A:604:HOH:O	2.22	0.41
1:C:121:ASP:OD1	1:C:121:ASP:N	2.53	0.41
1:B:342:PRO:HG3	1:B:394:GLU:HB3	2.02	0.41
1:C:350:ARG:HD2	1:C:350:ARG:HH11	1.59	0.41
1:B:87:GLU:HA	1:B:141:LEU:HD22	2.02	0.41
1:C:127:TYR:CE1	1:C:181:PRO:HG3	2.55	0.41
1:E:435:ARG:O	1:E:443:LYS:HA	2.20	0.41
1:A:313:LEU:HD22	1:A:314:GLN:H	1.86	0.41
1:A:415:TRP:HA	1:A:416:SER:HA	1.84	0.41
1:B:55:TYR:HA	1:B:98:PHE:CE1	2.55	0.41
1:E:117:LEU:HD23	1:E:117:LEU:HA	1.86	0.41
1:C:364:SER:HA	1:C:413:PHE:HB2	2.03	0.41
1:E:10:TRP:CZ3	1:E:455:LEU:HD21	2.55	0.41
1:E:180:TYR:CD1	1:E:181:PRO:HA	2.56	0.41
1:F:164:ASN:HA	1:F:221:ILE:HB	2.02	0.41
1:E:295:VAL:HG11	1:E:348:ILE:HG21	2.03	0.41
1:E:74:ARG:HA	1:E:114:TYR:O	2.20	0.41
1:B:383:VAL:HB	1:B:446:LYS:HG2	2.02	0.41
1:C:281:GLU:O	1:C:285:ILE:HG12	2.20	0.41
1:A:174:TYR:CE1	1:A:192:VAL:HG21	2.56	0.41
1:A:250:LEU:HD13	1:A:251:PHE:CE2	2.56	0.41
1:E:245:LEU:HA	1:E:249:ASN:HB2	2.02	0.41
1:D:9:VAL:HB	1:D:362:MET:CE	2.51	0.40
1:D:433:LEU:O	1:D:449:ALA:HB2	2.21	0.40
1:E:257:LEU:HD12	1:E:257:LEU:HA	1.93	0.40
1:F:68:ALA:HB2	1:F:445:LEU:HD13	2.03	0.40
1:B:121:ASP:OD1	1:B:121:ASP:N	2.54	0.40
1:C:379:LYS:N	1:C:379:LYS:HD2	2.35	0.40
1:E:174:TYR:CE1	1:E:192:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLU:HA	1:A:265:VAL:HG12	2.03	0.40
1:B:180:TYR:CG	1:B:181:PRO:HA	2.56	0.40
1:C:213:ARG:HB2	1:C:216:GLN:HG3	2.03	0.40
1:C:9:VAL:HB	1:C:362:MET:CE	2.52	0.40
1:D:14:THR:HG22	1:D:420:CYS:SG	2.61	0.40
1:E:103:ILE:HA	1:E:106:MET:CE	2.51	0.40
1:F:155:ASP:OD2	3:F:610:HOH:O	2.21	0.40
1:C:327:MET:HA	1:C:328:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/477 (96%)	442 (96%)	16 (4%)	0	100	100
1	B	458/477 (96%)	443 (97%)	15 (3%)	0	100	100
1	C	458/477 (96%)	442 (96%)	16 (4%)	0	100	100
1	D	458/477 (96%)	442 (96%)	16 (4%)	0	100	100
1	E	458/477 (96%)	443 (97%)	15 (3%)	0	100	100
1	F	458/477 (96%)	437 (95%)	20 (4%)	1 (0%)	51	71
All	All	2748/2862 (96%)	2649 (96%)	98 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	305	ARG

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	386/399 (97%)	372 (96%)	14 (4%)	40	65
1	B	386/399 (97%)	371 (96%)	15 (4%)	37	61
1	C	386/399 (97%)	369 (96%)	17 (4%)	33	55
1	D	386/399 (97%)	377 (98%)	9 (2%)	56	79
1	E	386/399 (97%)	374 (97%)	12 (3%)	45	71
1	F	386/399 (97%)	375 (97%)	11 (3%)	49	74
All	All	2316/2394 (97%)	2238 (97%)	78 (3%)	42	67

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	74	ARG
1	A	102	VAL
1	A	107	LEU
1	A	156	ARG
1	A	211	CYS
1	A	250	LEU
1	A	252	LEU
1	A	257	LEU
1	A	264	LEU
1	A	303	VAL
1	A	305	ARG
1	A	345	MET
1	A	399	LEU
1	B	37	THR
1	B	74	ARG
1	B	102	VAL
1	B	156	ARG
1	B	211	CYS
1	B	250	LEU
1	B	252	LEU
1	B	257	LEU

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Mol	Chain	Res	Type
1	B	265	VAL
1	B	270	MET
1	B	303	VAL
1	B	336	ARG
1	B	345	MET
1	B	363	ILE
1	B	399	LEU
1	C	14	THR
1	C	37	THR
1	C	40	GLU
1	C	57	ASP
1	C	74	ARG
1	C	88	THR
1	C	135	SER
1	C	250	LEU
1	C	257	LEU
1	C	264	LEU
1	C	309	SER
1	C	336	ARG
1	C	345	MET
1	C	350	ARG
1	C	354	LYS
1	C	399	LEU
1	C	407	SER
1	D	14	THR
1	D	211	CYS
1	D	250	LEU
1	D	264	LEU
1	D	270	MET
1	D	345	MET
1	D	392	MET
1	D	399	LEU
1	D	458	ARG
1	E	14	THR
1	E	25	LYS
1	E	88	THR
1	E	156	ARG
1	E	206	ARG
1	E	211	CYS
1	E	252	LEU
1	E	257	LEU
1	E	264	LEU

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Mol	Chain	Res	Type
1	E	305	ARG
1	E	345	MET
1	E	399	LEU
1	F	1	MET
1	F	25	LYS
1	F	74	ARG
1	F	135	SER
1	F	156	ARG
1	F	211	CYS
1	F	250	LEU
1	F	252	LEU
1	F	305	ARG
1	F	350	ARG
1	F	399	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	366	ASN
1	A	410	GLN
1	B	26	GLN
1	B	53	ASN
1	B	60	HIS
1	C	164	ASN
1	C	296	ASN
1	C	314	GLN
1	C	441	GLN
1	D	164	ASN
1	D	259	HIS
1	D	296	ASN
1	D	380	GLN
1	E	26	GLN
1	E	182	GLN
1	E	436	ASN
1	F	53	ASN
1	F	249	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CAS	A	292	1	6,8,9	0.75	0	2,9,11	1.04	0
1	CAS	B	292	1	6,8,9	0.92	0	2,9,11	2.37	1 (50%)
1	CAS	C	292	1	6,8,9	0.86	0	2,9,11	0.84	0
1	CAS	D	292	1	6,8,9	0.84	0	2,9,11	0.62	0
1	CAS	E	292	1	6,8,9	0.66	0	2,9,11	2.53	1 (50%)
1	CAS	F	292	1	6,8,9	0.99	0	2,9,11	0.61	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
1	CAS	A	292	1	-	0/0/7/9	0/0/0/0
1	CAS	B	292	1	-	0/0/7/9	0/0/0/0
1	CAS	C	292	1	-	0/0/7/9	0/0/0/0
1	CAS	D	292	1	-	0/0/7/9	0/0/0/0
1	CAS	E	292	1	-	0/0/7/9	0/0/0/0
1	CAS	F	292	1	-	0/0/7/9	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	CAS	CA-CB-SG	3.17	128.60	114.46
1	E	292	CAS	CA-CB-SG	3.44	129.82	114.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	292	CAS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	501	-	4,4,4	0.64	0	6,6,6	0.57	0
2	PO4	A	502	-	4,4,4	0.59	0	6,6,6	0.57	0
2	PO4	B	501	-	4,4,4	0.81	0	6,6,6	0.58	0
2	PO4	B	502	-	4,4,4	0.71	0	6,6,6	0.38	0
2	PO4	C	501	-	4,4,4	0.76	0	6,6,6	0.47	0
2	PO4	C	502	-	4,4,4	0.61	0	6,6,6	0.62	0
2	PO4	D	501	-	4,4,4	0.74	0	6,6,6	0.69	0
2	PO4	D	502	-	4,4,4	0.73	0	6,6,6	0.54	0
2	PO4	E	501	-	4,4,4	0.81	0	6,6,6	0.34	0
2	PO4	E	502	-	4,4,4	0.70	0	6,6,6	0.52	0
2	PO4	F	501	-	4,4,4	0.62	0	6,6,6	0.55	0
2	PO4	F	502	-	4,4,4	0.70	0	6,6,6	0.53	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	PO4	A	501	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	PO4	B	501	-	-	0/0/0/0	0/0/0/0
2	PO4	B	502	-	-	0/0/0/0	0/0/0/0
2	PO4	C	501	-	-	0/0/0/0	0/0/0/0
2	PO4	C	502	-	-	0/0/0/0	0/0/0/0
2	PO4	D	501	-	-	0/0/0/0	0/0/0/0
2	PO4	D	502	-	-	0/0/0/0	0/0/0/0
2	PO4	E	501	-	-	0/0/0/0	0/0/0/0
2	PO4	E	502	-	-	0/0/0/0	0/0/0/0
2	PO4	F	501	-	-	0/0/0/0	0/0/0/0
2	PO4	F	502	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PO4	1	0
2	C	502	PO4	1	0
2	E	502	PO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	460/477 (96%)	-0.41	0 100 100	14, 24, 44, 83	0
1	B	460/477 (96%)	-0.38	1 (0%) 94 95	14, 25, 45, 85	0
1	C	460/477 (96%)	-0.23	5 (1%) 80 81	16, 30, 56, 88	0
1	D	460/477 (96%)	-0.30	1 (0%) 94 95	16, 27, 49, 103	0
1	E	460/477 (96%)	-0.31	2 (0%) 92 92	17, 30, 53, 96	0
1	F	460/477 (96%)	-0.22	2 (0%) 92 92	17, 36, 63, 116	0
All	All	2760/2862 (96%)	-0.31	11 (0%) 92 92	14, 29, 53, 116	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	212	VAL	3.7
1	E	313	LEU	3.5
1	E	212	VAL	3.3
1	C	454	GLU	2.8
1	C	212	VAL	2.7
1	F	1	MET	2.4
1	C	459	ASN	2.3
1	C	457	GLU	2.2
1	B	212	VAL	2.1
1	D	1	MET	2.1
1	C	2	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	CAS	B	292	9/10	0.88	0.23	-	29,36,193,196	0
1	CAS	F	292	9/10	0.95	0.13	-	40,43,120,124	0
1	CAS	C	292	9/10	0.98	0.14	-	28,32,143,145	0
1	CAS	A	292	9/10	0.98	0.15	-	19,26,127,129	0
1	CAS	E	292	9/10	0.91	0.21	-	25,31,183,185	0
1	CAS	D	292	9/10	0.96	0.18	-	25,36,163,168	0

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(\AA^2)	Q<0.9
2	PO4	E	502	5/5	0.93	0.18	8.97	60,68,71,76	0
2	PO4	B	501	5/5	0.99	0.19	2.68	34,42,52,61	0
2	PO4	D	502	5/5	0.95	0.15	1.91	41,51,60,69	0
2	PO4	C	502	5/5	0.95	0.15	0.81	39,61,67,73	0
2	PO4	F	501	5/5	0.98	0.17	0.64	31,40,53,54	0
2	PO4	D	501	5/5	0.98	0.14	0.44	21,37,44,45	0
2	PO4	E	501	5/5	0.98	0.15	0.20	30,32,41,55	0
2	PO4	B	502	5/5	0.95	0.12	-0.13	42,54,61,67	0
2	PO4	A	501	5/5	0.99	0.12	-0.16	33,42,44,61	0
2	PO4	F	502	5/5	0.97	0.13	-0.24	47,53,63,71	0
2	PO4	C	501	5/5	0.98	0.13	-0.77	34,36,44,58	0
2	PO4	A	502	5/5	0.97	0.13	-1.67	31,39,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.