



# Full wwPDB X-ray Structure Validation Report i

Oct 22, 2024 – 10:24 pm BST

PDB ID : 8QX3  
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 R886G mutant  
Authors : Loris, R.; Haesaerts, S.; Larsen, P.B.  
Deposited on : 2023-10-21  
Resolution : 2.95 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  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

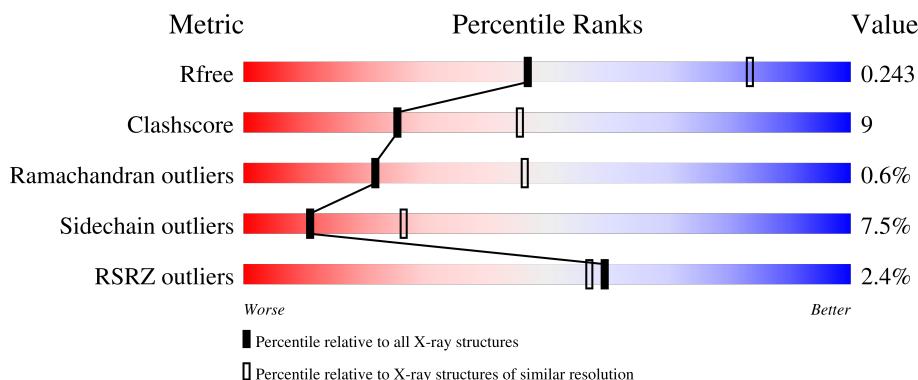
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

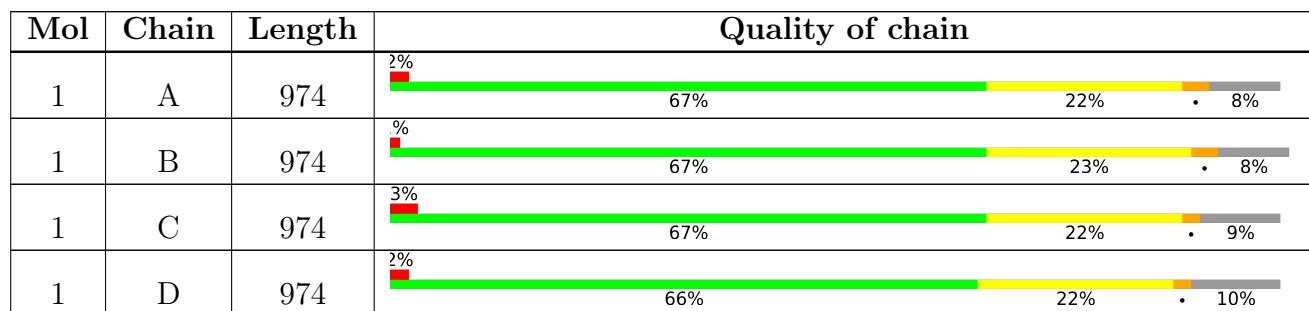
The reported resolution of this entry is 2.95 Å.

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))
$R_{free}$	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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.



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28637 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 Phosphoenolpyruvate carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	897	Total	C 7221	N 4581	O 1263	S 1348	29	0	0
1	B	899	Total	C 7233	N 4588	O 1263	S 1353	29	0	0
1	C	883	Total	C 7103	N 4507	O 1243	S 1324	29	0	0
1	D	877	Total	C 7052	N 4475	O 1228	S 1320	29	0	0

There are 32 discrepancies between the modelled and reference sequences:

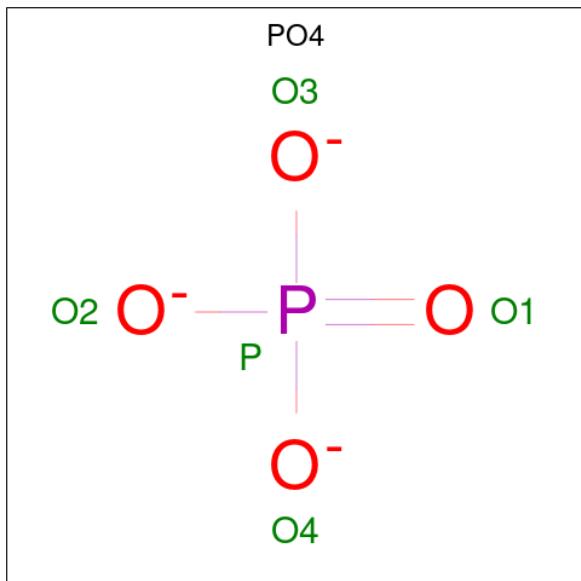
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
A	886	GLY	ARG	engineered mutation	UNP Q9MAH0
B	-6	MET	-	initiating methionine	UNP Q9MAH0
B	-5	HIS	-	expression tag	UNP Q9MAH0
B	-4	HIS	-	expression tag	UNP Q9MAH0
B	-3	HIS	-	expression tag	UNP Q9MAH0
B	-2	HIS	-	expression tag	UNP Q9MAH0
B	-1	HIS	-	expression tag	UNP Q9MAH0
B	0	HIS	-	expression tag	UNP Q9MAH0
B	886	GLY	ARG	engineered mutation	UNP Q9MAH0
C	-6	MET	-	initiating methionine	UNP Q9MAH0
C	-5	HIS	-	expression tag	UNP Q9MAH0
C	-4	HIS	-	expression tag	UNP Q9MAH0
C	-3	HIS	-	expression tag	UNP Q9MAH0
C	-2	HIS	-	expression tag	UNP Q9MAH0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP Q9MAH0
C	0	HIS	-	expression tag	UNP Q9MAH0
C	886	GLY	ARG	engineered mutation	UNP Q9MAH0
D	-6	MET	-	initiating methionine	UNP Q9MAH0
D	-5	HIS	-	expression tag	UNP Q9MAH0
D	-4	HIS	-	expression tag	UNP Q9MAH0
D	-3	HIS	-	expression tag	UNP Q9MAH0
D	-2	HIS	-	expression tag	UNP Q9MAH0
D	-1	HIS	-	expression tag	UNP Q9MAH0
D	0	HIS	-	expression tag	UNP Q9MAH0
D	886	GLY	ARG	engineered mutation	UNP Q9MAH0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

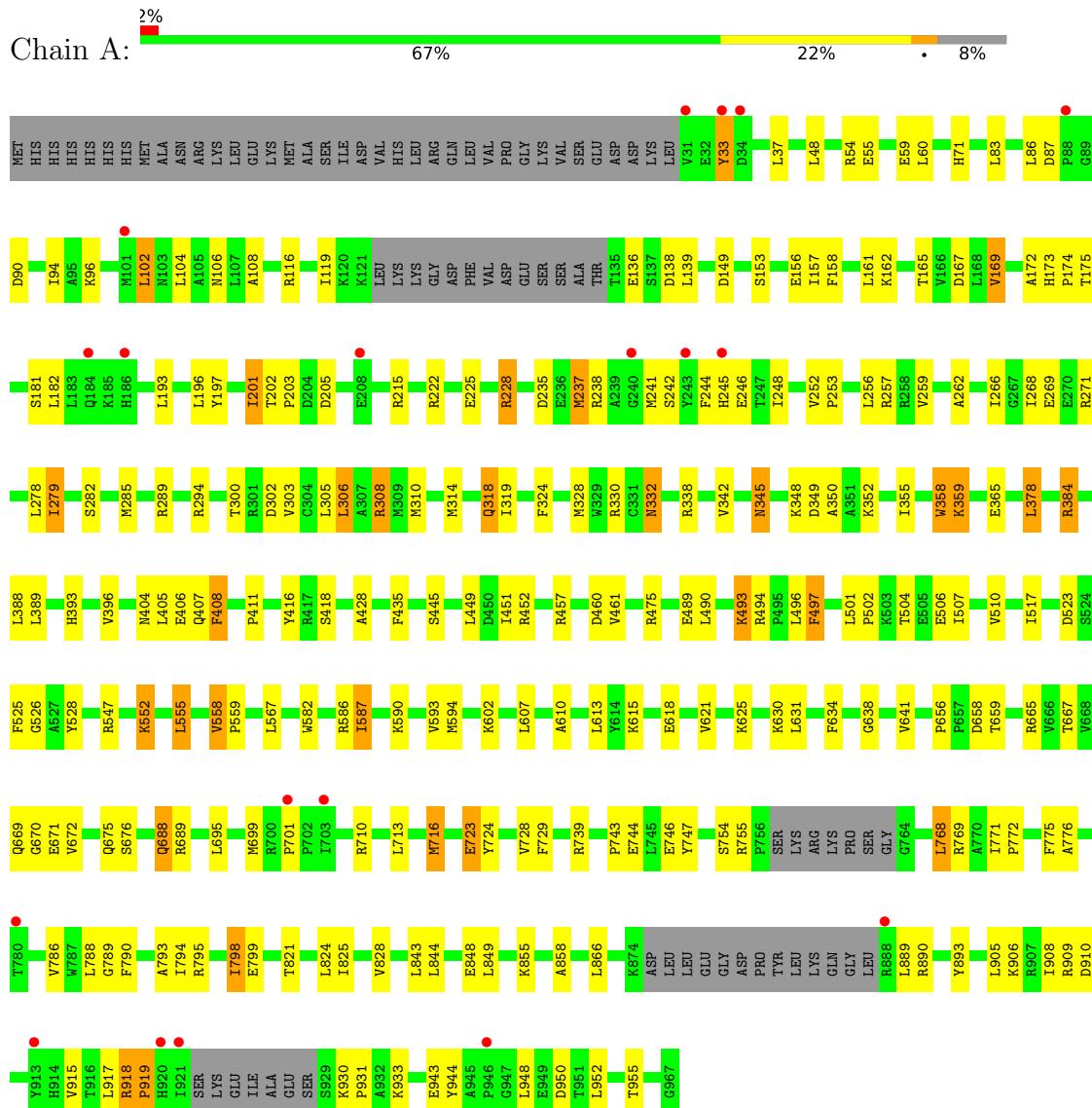
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	3	Total O 3 3	0	0

### 3 Residue-property plots [\(i\)](#)

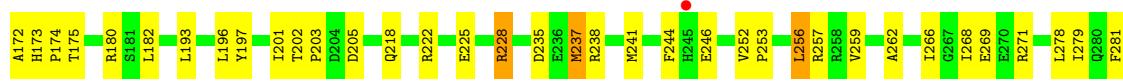
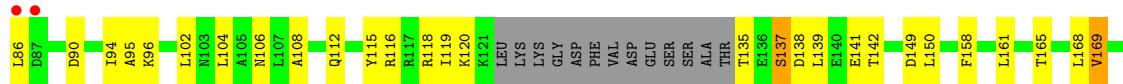
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphoenolpyruvate carboxylase 1

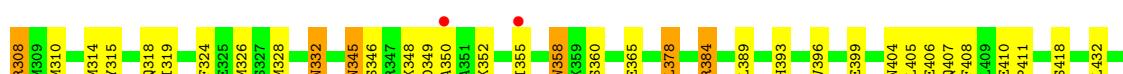
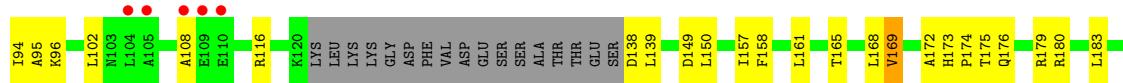
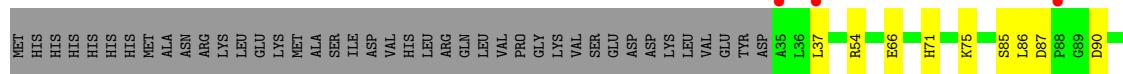


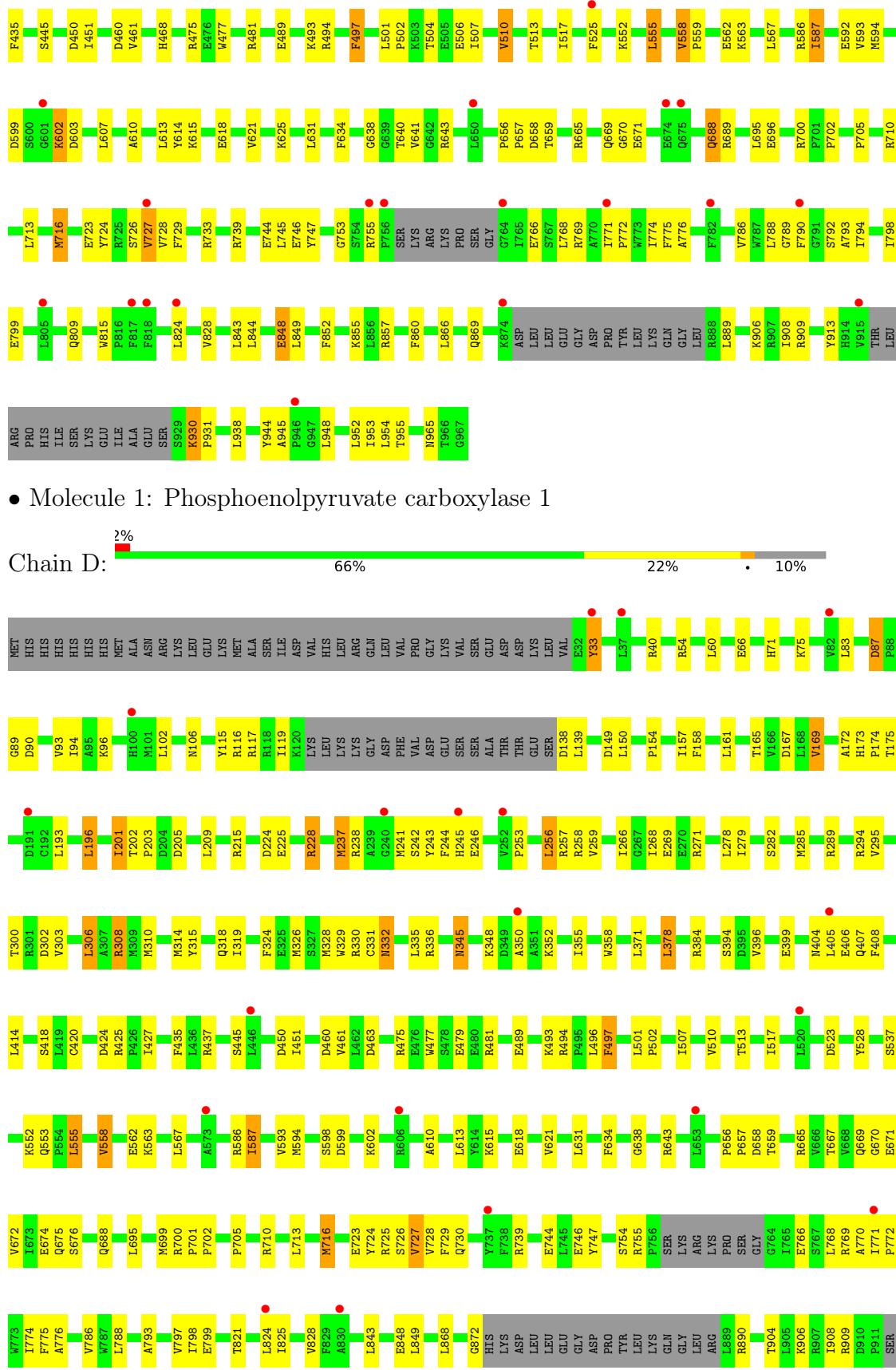
- Molecule 1: Phosphoenolpyruvate carboxylase 1

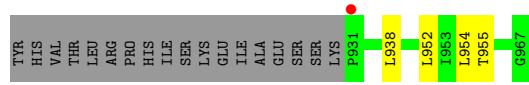




- Molecule 1: Phosphoenolpyruvate carboxylase 1







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.67 Å    159.16 Å    140.99 Å 90.00°    92.03°    90.00°	Depositor
Resolution (Å)	48.99 – 2.95 48.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.99-2.95) 99.7 (48.99-2.95)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.08 (at 2.96 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
$R$ , $R_{free}$	0.204 , 0.240 0.206 , 0.243	Depositor DCC
$R_{free}$ test set	6105 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.6	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 65.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.072 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	0.29	0/7377	0.47	1/9985 (0.0%)
1	B	0.29	0/7389	0.48	1/10001 (0.0%)
1	C	0.27	0/7256	0.45	2/9820 (0.0%)
1	D	0.26	0/7203	0.42	0/9750
All	All	0.28	0/29225	0.45	4/39556 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	689	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	C	689	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	768	LEU	CA-CB-CG	5.34	127.57	115.30
1	A	768	LEU	CA-CB-CG	5.29	127.46	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7221	0	7178	143	0
1	B	7233	0	7187	145	0
1	C	7103	0	7063	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	7052	0	7002	134	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	5	0	0	0	0
3	B	3	0	0	0	0
All	All	28637	0	28430	539	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 9.

All (539) 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:404:ASN:HB2	1:A:407:GLN:HB2	1.63	0.81
1:D:460:ASP:OD1	1:D:475:ARG:NH1	2.14	0.79
1:A:173:HIS:ND1	1:A:669:GLN:OE1	2.15	0.79
1:A:638:GLY:HA2	1:A:669:GLN:HG3	1.64	0.77
1:B:638:GLY:HA2	1:B:669:GLN:HG3	1.67	0.76
1:B:173:HIS:ND1	1:B:669:GLN:OE1	2.20	0.75
1:C:332:ASN:HD21	1:C:418:SER:HA	1.52	0.74
1:A:332:ASN:HD21	1:A:418:SER:HA	1.53	0.74
1:C:404:ASN:HB2	1:C:407:GLN:HB2	1.70	0.74
1:A:169:VAL:HB	1:A:282:SER:HB2	1.70	0.73
1:B:175:THR:HG23	1:B:671:GLU:H	1.53	0.73
1:C:345:ASN:OD1	1:C:345:ASN:N	2.21	0.73
1:D:656:PRO:HG2	1:D:659:THR:HG21	1.71	0.73
1:A:528:TYR:HB2	1:A:555:LEU:HD13	1.72	0.72
1:D:404:ASN:HB2	1:D:407:GLN:HB2	1.72	0.72
1:B:345:ASN:N	1:B:345:ASN:OD1	2.22	0.71
1:B:332:ASN:HD21	1:B:418:SER:HA	1.55	0.71
1:B:169:VAL:HB	1:B:282:SER:HB2	1.71	0.71
1:A:345:ASN:OD1	1:A:345:ASN:N	2.23	0.70
1:A:175:THR:HG23	1:A:671:GLU:H	1.58	0.69
1:C:460:ASP:OD1	1:C:475:ARG:NH1	2.25	0.69
1:A:384:ARG:HD2	1:A:396:VAL:HB	1.74	0.68
1:C:175:THR:HG23	1:C:671:GLU:H	1.56	0.68
1:D:638:GLY:HA2	1:D:669:GLN:HG3	1.76	0.67
1:C:656:PRO:HG2	1:C:659:THR:HG21	1.75	0.67
1:D:173:HIS:ND1	1:D:669:GLN:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:618:GLU:OE1	1:D:710:ARG:NH2	2.28	0.67
1:B:404:ASN:HB2	1:B:407:GLN:HB2	1.77	0.66
1:C:913:TYR:HB3	1:C:945:ALA:HB2	1.77	0.66
1:A:306:LEU:HD22	1:A:389:LEU:HD11	1.77	0.66
1:D:332:ASN:HD21	1:D:418:SER:HA	1.59	0.66
1:B:528:TYR:HB2	1:B:555:LEU:HD13	1.77	0.66
1:B:656:PRO:HG2	1:B:659:THR:HG21	1.77	0.66
1:D:175:THR:HG23	1:D:671:GLU:H	1.60	0.66
1:B:451:ILE:HG13	1:B:517:ILE:HD11	1.78	0.66
1:D:786:VAL:HG11	1:D:828:VAL:HG21	1.77	0.66
1:C:563:LYS:NZ	1:C:766:GLU:OE2	2.29	0.65
1:C:384:ARG:HD2	1:C:396:VAL:HB	1.77	0.65
1:D:345:ASN:N	1:D:345:ASN:OD1	2.29	0.65
1:B:106:ASN:OD1	1:B:890:ARG:NH2	2.29	0.64
1:D:302:ASP:O	1:D:306:LEU:HB2	1.98	0.64
1:A:451:ILE:HG13	1:A:517:ILE:HD11	1.80	0.64
1:A:716:MET:HG3	1:A:793:ALA:HB1	1.78	0.63
1:D:461:VAL:HG22	1:D:507:ILE:HG23	1.80	0.63
1:B:384:ARG:HD2	1:B:396:VAL:HB	1.80	0.63
1:D:106:ASN:OD1	1:D:890:ARG:NH2	2.32	0.63
1:A:332:ASN:ND2	1:A:418:SER:HA	2.14	0.62
1:C:772:PRO:HA	1:C:775:PHE:HB3	1.82	0.62
1:A:106:ASN:OD1	1:A:890:ARG:NH2	2.32	0.62
1:D:228:ARG:HH12	1:D:938:LEU:HB3	1.63	0.62
1:D:158:PHE:HB2	1:D:268:ILE:HD13	1.80	0.62
1:B:237:MET:HG2	1:B:303:VAL:HG12	1.80	0.62
1:C:594:MET:HA	1:C:634:PHE:HB3	1.80	0.62
1:A:656:PRO:HG2	1:A:659:THR:HG21	1.82	0.62
1:C:786:VAL:HG11	1:C:828:VAL:HG21	1.82	0.62
1:A:844:LEU:HD22	1:A:909:ARG:HH21	1.65	0.62
1:C:172:ALA:HB2	1:C:285:MET:HG3	1.82	0.62
1:D:384:ARG:HD2	1:D:396:VAL:HB	1.82	0.62
1:B:930:LYS:HG2	1:B:931:PRO:HD2	1.82	0.62
1:D:772:PRO:HA	1:D:775:PHE:HB3	1.82	0.62
1:A:158:PHE:HB2	1:A:268:ILE:HD13	1.82	0.61
1:C:161:LEU:HD13	1:C:695:LEU:HD22	1.82	0.61
1:A:237:MET:HG2	1:A:303:VAL:HG12	1.83	0.61
1:B:306:LEU:O	1:B:310:MET:HG3	2.00	0.61
1:A:618:GLU:OE1	1:A:710:ARG:NH2	2.34	0.61
1:B:593:VAL:HG12	1:B:631:LEU:HD11	1.82	0.61
1:C:696:GLU:HG2	1:C:700:ARG:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:O	1:A:310:MET:HG3	2.02	0.60
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.83	0.60
1:B:772:PRO:HA	1:B:775:PHE:HB3	1.84	0.60
1:D:169:VAL:HG13	1:D:667:THR:HA	1.82	0.60
1:A:772:PRO:HA	1:A:775:PHE:HB3	1.84	0.60
1:B:587:ILE:HG13	1:B:590:LYS:O	2.02	0.60
1:C:450:ASP:OD2	1:C:665:ARG:NH2	2.34	0.60
1:A:786:VAL:HG11	1:A:828:VAL:HG21	1.83	0.60
1:C:618:GLU:OE1	1:C:710:ARG:NH2	2.35	0.60
1:C:180:ARG:HA	1:C:183:LEU:HB2	1.82	0.60
1:C:739:ARG:NH1	1:C:744:GLU:OE1	2.35	0.59
1:C:638:GLY:HA2	1:C:669:GLN:HG3	1.84	0.59
1:B:908:ILE:HD11	1:B:948:LEU:HB3	1.84	0.59
1:D:237:MET:HG2	1:D:303:VAL:HG12	1.85	0.59
1:B:228:ARG:HH12	1:B:938:LEU:HB3	1.67	0.59
1:B:460:ASP:OD1	1:B:475:ARG:NH1	2.36	0.58
1:C:461:VAL:HG22	1:C:507:ILE:HG23	1.85	0.58
1:A:318:GLN:HB3	1:A:435:PHE:HE1	1.68	0.58
1:A:641:VAL:HG21	1:A:828:VAL:HG21	1.85	0.58
1:C:908:ILE:HD11	1:C:948:LEU:HB3	1.84	0.58
1:A:172:ALA:HB2	1:A:285:MET:HG3	1.84	0.57
1:B:332:ASN:ND2	1:B:418:SER:HA	2.18	0.57
1:D:237:MET:O	1:D:241:MET:HG2	2.03	0.57
1:A:794:ILE:O	1:A:798:ILE:HG12	2.04	0.57
1:B:641:VAL:HG21	1:B:828:VAL:HG21	1.86	0.57
1:B:37:LEU:HD13	1:B:104:LEU:HB3	1.86	0.57
1:D:253:PRO:O	1:D:257:ARG:HG3	2.05	0.57
1:D:501:LEU:HD12	1:D:502:PRO:HD2	1.86	0.57
1:A:289:ARG:NH2	1:A:300:THR:OG1	2.37	0.57
1:B:755:ARG:HD3	1:B:769:ARG:CZ	2.34	0.57
1:A:37:LEU:HD13	1:A:104:LEU:HB3	1.87	0.57
1:D:174:PRO:O	1:D:747:TYR:OH	2.21	0.57
1:A:201:ILE:H	1:A:201:ILE:HD13	1.69	0.57
1:A:489:GLU:O	1:A:547:ARG:NH2	2.37	0.57
1:A:460:ASP:OD1	1:A:475:ARG:NH1	2.37	0.56
1:A:930:LYS:HG2	1:A:931:PRO:HD2	1.87	0.56
1:B:174:PRO:O	1:B:747:TYR:OH	2.23	0.56
1:D:562:GLU:HG2	1:D:599:ASP:HB2	1.87	0.56
1:D:528:TYR:HB2	1:D:555:LEU:HD13	1.87	0.56
1:A:672:VAL:O	1:A:676:SER:OG	2.20	0.56
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:GLU:HG2	1:C:599:ASP:HB2	1.88	0.56
1:C:755:ARG:HD3	1:C:769:ARG:CZ	2.35	0.56
1:C:205:ASP:OD1	1:D:258:ARG:NH2	2.38	0.56
1:D:594:MET:HA	1:D:634:PHE:HB3	1.88	0.56
1:A:181:SER:OG	2:A:1001:PO4:O2	2.23	0.56
1:C:158:PHE:HB2	1:C:268:ILE:HD13	1.87	0.56
1:C:809:GLN:NE2	1:C:869:GLN:O	2.39	0.56
1:A:161:LEU:HD13	1:A:695:LEU:HD22	1.87	0.56
1:B:158:PHE:HB2	1:B:268:ILE:HD13	1.87	0.56
1:B:716:MET:HG3	1:B:793:ALA:HB1	1.86	0.56
1:C:228:ARG:HH12	1:C:938:LEU:HB3	1.70	0.56
1:B:350:ALA:HB1	1:B:352:LYS:HG3	1.88	0.56
1:B:37:LEU:HD11	1:B:108:ALA:HB2	1.89	0.55
1:A:308:ARG:HG3	1:A:445:SER:HB3	1.89	0.55
1:A:908:ILE:HD11	1:A:948:LEU:HB3	1.87	0.55
1:B:172:ALA:HB2	1:B:285:MET:HG3	1.88	0.55
1:D:306:LEU:O	1:D:310:MET:HG3	2.07	0.55
1:B:477:TRP:CD2	1:B:481:ARG:HD3	2.42	0.55
1:D:172:ALA:HB2	1:D:285:MET:HG3	1.88	0.55
1:B:180:ARG:N	2:B:1001:PO4:O4	2.40	0.55
1:D:201:ILE:HD13	1:D:201:ILE:H	1.72	0.55
1:A:723:GLU:HG2	1:A:789:GLY:HA2	1.87	0.55
1:A:746:GLU:HG3	1:A:952:LEU:HD21	1.88	0.55
1:A:139:LEU:HD11	1:A:259:VAL:HG22	1.89	0.55
1:B:672:VAL:HA	1:B:675:GLN:HB2	1.88	0.55
1:A:253:PRO:O	1:A:257:ARG:HG3	2.07	0.54
1:A:228:ARG:NH2	1:A:950:ASP:OD1	2.40	0.54
1:A:593:VAL:HG12	1:A:631:LEU:HD11	1.89	0.54
1:C:224:ASP:OD2	1:C:228:ARG:NH1	2.41	0.54
1:C:716:MET:HG3	1:C:793:ALA:HB1	1.88	0.54
1:A:302:ASP:O	1:A:306:LEU:HB2	2.08	0.54
1:A:525:PHE:HB3	1:A:555:LEU:HD23	1.90	0.54
1:A:638:GLY:HA2	1:A:669:GLN:CG	2.35	0.54
1:C:501:LEU:HD12	1:C:502:PRO:HD2	1.90	0.54
1:D:593:VAL:HG12	1:D:631:LEU:HD11	1.90	0.54
1:D:716:MET:HG3	1:D:793:ALA:HB1	1.89	0.53
1:A:501:LEU:HD12	1:A:502:PRO:HD2	1.90	0.53
1:C:824:LEU:O	1:C:828:VAL:HG23	2.08	0.53
1:B:237:MET:O	1:B:241:MET:HG2	2.08	0.53
1:D:89:GLY:O	1:D:93:VAL:HG23	2.09	0.53
1:D:739:ARG:NH1	1:D:744:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.91	0.53
1:D:167:ASP:HB3	1:D:665:ARG:HG3	1.91	0.53
1:B:33:TYR:CE2	1:B:193:LEU:HD22	2.44	0.53
1:B:86:LEU:HD13	1:B:94:ILE:HG13	1.90	0.53
1:B:618:GLU:OE1	1:B:710:ARG:NH2	2.42	0.53
1:B:723:GLU:HG2	1:B:789:GLY:HA2	1.91	0.53
1:C:238:ARG:NE	1:D:355:ILE:O	2.39	0.53
1:C:355:ILE:O	1:D:238:ARG:NE	2.41	0.52
1:B:39:ASP:OD1	1:B:40:ARG:N	2.42	0.52
1:C:318:GLN:HB3	1:C:435:PHE:HE1	1.74	0.52
1:C:173:HIS:ND1	1:C:669:GLN:OE1	2.42	0.52
1:B:48:LEU:HD22	1:B:222:ARG:NH1	2.24	0.52
1:C:174:PRO:O	1:C:747:TYR:OH	2.25	0.52
1:D:769:ARG:HB2	1:D:772:PRO:HD2	1.91	0.52
1:A:728:VAL:HG23	1:A:729:PHE:CD2	2.45	0.52
1:B:161:LEU:HD13	1:B:695:LEU:HD22	1.92	0.52
1:B:318:GLN:HB3	1:B:435:PHE:HE1	1.75	0.52
1:C:746:GLU:HG3	1:C:952:LEU:HD21	1.91	0.52
1:D:169:VAL:HB	1:D:282:SER:HB2	1.91	0.52
1:D:315:TYR:HB3	1:D:378:LEU:HD21	1.91	0.52
1:A:310:MET:O	1:A:314:MET:HG3	2.10	0.52
1:A:716:MET:CG	1:A:793:ALA:HB1	2.39	0.52
1:C:640:THR:HG22	1:C:965:ASN:HB3	1.92	0.52
1:A:672:VAL:HA	1:A:675:GLN:HB2	1.92	0.51
1:D:96:LYS:HE2	1:D:225:GLU:OE2	2.09	0.51
1:C:37:LEU:HD11	1:C:108:ALA:HB2	1.92	0.51
1:D:405:LEU:HD12	1:D:405:LEU:H	1.75	0.51
1:B:33:TYR:HE1	1:B:197:TYR:CG	2.29	0.51
1:B:638:GLY:HA2	1:B:669:GLN:CG	2.39	0.51
1:C:302:ASP:O	1:C:306:LEU:HB2	2.11	0.51
1:D:558:VAL:HG23	1:D:593:VAL:HA	1.93	0.51
1:B:728:VAL:HG23	1:B:729:PHE:CD2	2.45	0.51
1:B:746:GLU:HG3	1:B:952:LEU:HD21	1.92	0.51
1:D:746:GLU:HG3	1:D:952:LEU:HD21	1.93	0.51
1:A:449:LEU:O	1:A:526:GLY:N	2.38	0.51
1:A:358:TRP:CD2	1:B:238:ARG:NH2	2.78	0.51
1:C:306:LEU:HD22	1:C:389:LEU:HD11	1.93	0.51
1:A:558:VAL:HG23	1:A:593:VAL:HA	1.92	0.51
1:D:728:VAL:HG23	1:D:729:PHE:CD2	2.46	0.51
1:C:724:TYR:O	1:C:728:VAL:HG22	2.10	0.50
1:C:728:VAL:HG23	1:C:729:PHE:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:ARG:NH2	1:C:848:GLU:OE1	2.40	0.50
1:D:289:ARG:NH1	1:D:295:VAL:O	2.44	0.50
1:A:843:LEU:HD22	1:A:906:LYS:HD2	1.94	0.50
1:D:824:LEU:O	1:D:828:VAL:HG23	2.12	0.50
1:D:161:LEU:HD13	1:D:695:LEU:HD22	1.93	0.50
1:D:724:TYR:O	1:D:728:VAL:HG22	2.12	0.50
1:C:258:ARG:NH2	1:D:205:ASP:OD1	2.44	0.50
1:A:497:PHE:HD1	1:A:497:PHE:H	1.58	0.50
1:B:582:TRP:O	1:B:586:ARG:HD3	2.12	0.50
1:C:744:GLU:HB2	1:C:776:ALA:HB2	1.93	0.50
1:D:744:GLU:HB2	1:D:776:ALA:HB2	1.94	0.50
1:A:405:LEU:H	1:A:405:LEU:HD12	1.76	0.50
1:B:289:ARG:HG2	1:B:452:ARG:O	2.11	0.50
1:B:302:ASP:O	1:B:306:LEU:HB2	2.12	0.50
1:A:139:LEU:N	1:A:688:GLN:OE1	2.45	0.49
1:A:824:LEU:O	1:A:828:VAL:HG23	2.12	0.49
1:C:66:GLU:HB2	1:C:75:LYS:HE2	1.94	0.49
1:C:405:LEU:HD12	1:C:405:LEU:H	1.77	0.49
1:A:136:GLU:OE1	1:A:689:ARG:NE	2.32	0.49
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.93	0.49
1:A:908:ILE:HD12	1:A:944:TYR:CD2	2.48	0.49
1:B:494:ARG:NH2	1:D:489:GLU:OE2	2.42	0.49
1:B:844:LEU:HD22	1:B:909:ARG:HH21	1.77	0.49
1:C:253:PRO:O	1:C:257:ARG:HG3	2.12	0.49
1:C:724:TYR:CD1	1:C:788:LEU:HD23	2.47	0.49
1:C:857:ARG:O	1:C:860:PHE:HB3	2.11	0.49
1:C:139:LEU:HD11	1:C:259:VAL:HG22	1.93	0.49
1:B:115:TYR:O	1:B:119:ILE:HG22	2.13	0.49
1:B:603:ASP:OD1	1:B:603:ASP:N	2.43	0.49
1:C:306:LEU:O	1:C:310:MET:HG3	2.13	0.49
1:C:558:VAL:HG23	1:C:593:VAL:HA	1.93	0.49
1:C:844:LEU:HD22	1:C:909:ARG:HH21	1.78	0.49
1:D:724:TYR:CD1	1:D:788:LEU:HD23	2.46	0.49
1:B:306:LEU:HD22	1:B:389:LEU:HD11	1.95	0.49
1:C:96:LYS:HG3	1:C:954:LEU:HD21	1.94	0.49
1:C:332:ASN:ND2	1:C:418:SER:HA	2.25	0.49
1:D:424:ASP:HB3	1:D:427:ILE:HD12	1.94	0.49
1:A:294:ARG:HD3	1:A:754:SER:O	2.13	0.49
1:A:587:ILE:HD12	1:A:590:LYS:O	2.13	0.49
1:B:794:ILE:O	1:B:798:ILE:HG12	2.13	0.49
1:D:705:PRO:HG2	1:D:710:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PRO:O	1:B:257:ARG:HG3	2.12	0.49
1:B:262:ALA:O	1:B:266:ILE:HG12	2.12	0.49
1:C:346:SER:HG	1:C:360:SER:HG	1.60	0.49
1:A:724:TYR:CD1	1:A:788:LEU:HD23	2.48	0.49
1:A:86:LEU:HD13	1:A:94:ILE:HG13	1.94	0.48
1:D:672:VAL:O	1:D:676:SER:OG	2.29	0.48
1:A:457:ARG:NE	1:A:506:GLU:HB3	2.28	0.48
1:B:95:ALA:HB1	1:B:954:LEU:HB3	1.96	0.48
1:C:202:THR:O	1:C:205:ASP:N	2.45	0.48
1:A:37:LEU:HD11	1:A:108:ALA:HB2	1.95	0.48
1:A:238:ARG:NH2	1:B:358:TRP:CD2	2.79	0.48
1:B:457:ARG:NE	1:B:506:GLU:HB3	2.28	0.48
1:D:318:GLN:HB3	1:D:435:PHE:HE1	1.79	0.48
1:A:621:VAL:HG21	1:A:659:THR:HG22	1.95	0.48
1:C:257:ARG:HH22	1:D:215:ARG:NH2	2.11	0.48
1:B:310:MET:O	1:B:314:MET:HG3	2.14	0.48
1:D:66:GLU:HB2	1:D:75:LYS:HE2	1.95	0.48
1:D:610:ALA:HA	1:D:613:LEU:HD12	1.95	0.48
1:D:727:VAL:HG22	1:D:788:LEU:HD21	1.96	0.48
1:A:489:GLU:OE2	1:C:494:ARG:NH2	2.42	0.48
1:C:289:ARG:NH2	1:C:300:THR:OG1	2.47	0.48
1:D:384:ARG:HE	1:D:394:SER:HB3	1.78	0.48
1:A:844:LEU:HD13	1:A:909:ARG:NH2	2.29	0.48
1:A:174:PRO:O	1:A:747:TYR:OH	2.31	0.48
1:A:724:TYR:O	1:A:728:VAL:HG22	2.14	0.48
1:A:744:GLU:HB2	1:A:776:ALA:HB2	1.94	0.48
1:B:289:ARG:NH2	1:B:300:THR:OG1	2.40	0.48
1:C:174:PRO:HB3	1:C:753:GLY:HA3	1.94	0.48
1:C:289:ARG:NH1	1:C:295:VAL:O	2.47	0.48
1:C:602:LYS:NZ	1:C:766:GLU:O	2.47	0.48
1:D:308:ARG:HG3	1:D:445:SER:HB3	1.96	0.48
1:D:202:THR:O	1:D:205:ASP:N	2.46	0.47
1:A:96:LYS:HE2	1:A:225:GLU:OE2	2.14	0.47
1:C:638:GLY:HA2	1:C:669:GLN:CG	2.44	0.47
1:B:724:TYR:CE2	1:B:728:VAL:HG21	2.50	0.47
1:B:744:GLU:HB2	1:B:776:ALA:HB2	1.96	0.47
1:C:326:MET:HE1	1:C:432:LEU:HD22	1.97	0.47
1:C:769:ARG:HB2	1:C:772:PRO:HD2	1.96	0.47
1:D:157:ILE:O	1:D:161:LEU:HB2	2.14	0.47
1:C:739:ARG:HB3	1:C:745:LEU:HD11	1.95	0.47
1:A:33:TYR:CE2	1:A:193:LEU:HD22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD11	1:B:259:VAL:HG22	1.97	0.47
1:B:335:LEU:HD12	1:B:414:LEU:HG	1.96	0.47
1:A:405:LEU:HD11	1:A:523:ASP:HB3	1.95	0.47
1:D:138:ASP:OD1	1:D:139:LEU:N	2.47	0.47
1:D:450:ASP:OD2	1:D:665:ARG:NH2	2.48	0.47
1:B:202:THR:O	1:B:205:ASP:N	2.47	0.47
1:C:150:LEU:HD11	1:C:700:ARG:HB2	1.96	0.47
1:C:196:LEU:HD12	1:C:196:LEU:HA	1.81	0.47
1:B:150:LEU:HD11	1:B:700:ARG:HB2	1.96	0.46
1:B:672:VAL:O	1:B:676:SER:OG	2.32	0.46
1:C:497:PHE:HD1	1:C:497:PHE:H	1.62	0.46
1:C:615:LYS:HE3	1:C:615:LYS:HB3	1.71	0.46
1:A:490:LEU:HB3	1:A:582:TRP:CZ2	2.50	0.46
1:C:138:ASP:OD1	1:C:139:LEU:N	2.48	0.46
1:C:451:ILE:HG13	1:C:517:ILE:HD11	1.97	0.46
1:D:672:VAL:HA	1:D:675:GLN:HB2	1.96	0.46
1:C:727:VAL:HG22	1:C:788:LEU:HD21	1.98	0.46
1:D:477:TRP:HD1	1:D:481:ARG:HH21	1.63	0.46
1:B:716:MET:CG	1:B:793:ALA:HB1	2.45	0.46
1:A:48:LEU:HD22	1:A:222:ARG:NH1	2.31	0.46
1:B:405:LEU:HD12	1:B:405:LEU:H	1.81	0.46
1:A:202:THR:O	1:A:205:ASP:N	2.48	0.46
1:B:558:VAL:HG23	1:B:593:VAL:HA	1.97	0.46
1:B:572:ALA:O	1:B:576:ARG:HG3	2.15	0.46
1:B:724:TYR:CD1	1:B:788:LEU:HD23	2.50	0.46
1:C:157:ILE:O	1:C:161:LEU:HB2	2.15	0.46
1:C:593:VAL:HG12	1:C:631:LEU:HD11	1.98	0.46
1:D:420:CYS:SG	1:D:425:ARG:NH1	2.89	0.46
1:A:158:PHE:CE2	1:A:162:LYS:HD2	2.51	0.46
1:C:242:SER:HA	1:C:245:HIS:NE2	2.30	0.46
1:D:331:CYS:HB2	1:D:335:LEU:HB3	1.98	0.46
1:D:723:GLU:O	1:D:726:SER:OG	2.32	0.46
1:D:154:PRO:HG3	1:D:266:ILE:HG22	1.98	0.46
1:B:918:ARG:CB	1:B:919:PRO:HD3	2.47	0.45
1:D:169:VAL:HG11	1:D:634:PHE:CZ	2.52	0.45
1:C:350:ALA:HB1	1:C:352:LYS:HG3	1.98	0.45
1:D:96:LYS:HG3	1:D:954:LEU:HD21	1.98	0.45
1:B:716:MET:SD	1:B:797:VAL:HG21	2.57	0.45
1:A:238:ARG:NE	1:B:355:ILE:O	2.47	0.45
1:B:824:LEU:O	1:B:828:VAL:HG23	2.17	0.45
1:B:908:ILE:HD12	1:B:944:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:MET:O	1:C:241:MET:HG2	2.16	0.45
1:C:723:GLU:HG2	1:C:789:GLY:HA2	1.98	0.45
1:A:252:VAL:HG13	1:A:279:ILE:HD11	1.99	0.45
1:B:562:GLU:HG2	1:B:599:ASP:HB2	1.99	0.45
1:C:716:MET:CG	1:C:793:ALA:HB1	2.47	0.45
1:C:952:LEU:O	1:C:955:THR:OG1	2.28	0.45
1:D:621:VAL:HG21	1:D:659:THR:HG22	1.99	0.45
1:A:350:ALA:HB1	1:A:352:LYS:HG3	1.99	0.45
1:C:315:TYR:HB3	1:C:378:LEU:HD21	1.98	0.45
1:A:215:ARG:NH2	1:B:257:ARG:HH22	2.15	0.45
1:A:237:MET:HE3	1:A:303:VAL:HB	1.99	0.45
1:C:308:ARG:HG3	1:C:445:SER:HB3	1.99	0.45
1:A:582:TRP:O	1:A:586:ARG:HD3	2.16	0.45
1:D:332:ASN:ND2	1:D:418:SER:HA	2.29	0.45
1:D:821:THR:O	1:D:825:ILE:HG12	2.16	0.45
1:A:743:PRO:HB3	1:A:905:LEU:HD11	1.98	0.44
1:B:256:LEU:HD23	1:B:437:ARG:HD3	1.99	0.44
1:B:607:LEU:HB2	1:B:790:PHE:CE1	2.52	0.44
1:C:843:LEU:HD22	1:C:906:LYS:HD2	1.98	0.44
1:D:237:MET:HE3	1:D:303:VAL:HB	1.98	0.44
1:D:868:LEU:O	1:D:872:GLY:N	2.49	0.44
1:A:33:TYR:HE1	1:A:197:TYR:CG	2.34	0.44
1:A:222:ARG:NH2	1:B:422:CYS:O	2.50	0.44
1:A:237:MET:O	1:A:241:MET:HG2	2.16	0.44
1:B:244:PHE:C	1:B:246:GLU:H	2.20	0.44
1:B:563:LYS:NZ	1:B:766:GLU:OE2	2.50	0.44
1:C:358:TRP:CD2	1:D:238:ARG:NH2	2.84	0.44
1:C:603:ASP:OD1	1:C:603:ASP:N	2.48	0.44
1:A:795:ARG:HG3	1:A:866:LEU:HD11	1.99	0.44
1:B:218:GLN:O	1:B:222:ARG:HB2	2.18	0.44
1:B:739:ARG:NH1	1:B:744:GLU:OE1	2.51	0.44
1:A:552:LYS:H	1:A:552:LYS:HG2	1.46	0.44
1:C:201:ILE:HD13	1:C:201:ILE:H	1.81	0.44
1:D:621:VAL:HG21	1:D:659:THR:HA	2.00	0.44
1:A:855:LYS:O	1:A:858:ALA:HB3	2.18	0.44
1:A:244:PHE:C	1:A:246:GLU:H	2.21	0.44
1:B:287:GLY:HA3	1:B:450:ASP:O	2.17	0.44
1:D:326:MET:HG3	1:D:371:LEU:HD11	2.00	0.44
1:D:350:ALA:HB1	1:D:352:LYS:HG3	2.00	0.44
1:D:843:LEU:HD22	1:D:906:LYS:HD2	2.00	0.44
1:B:798:ILE:HG12	1:B:798:ILE:H	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LEU:HD23	1:D:437:ARG:HD3	1.99	0.44
1:D:310:MET:O	1:D:314:MET:HG3	2.17	0.44
1:A:153:SER:OG	1:A:156:GLU:HG3	2.18	0.44
1:A:338:ARG:O	1:A:342:VAL:HG23	2.17	0.44
1:B:96:LYS:HE2	1:B:225:GLU:OE2	2.18	0.44
1:B:165:THR:HG22	1:B:663:SER:HA	1.99	0.44
1:B:294:ARG:HD3	1:B:754:SER:O	2.18	0.44
1:D:224:ASP:OD2	1:D:228:ARG:NH1	2.51	0.44
1:B:329:TRP:CZ3	1:B:330:ARG:HG2	2.53	0.44
1:B:712:LEU:O	1:B:716:MET:HB2	2.18	0.44
1:C:587:ILE:HD13	1:C:587:ILE:HA	1.82	0.44
1:C:723:GLU:OE1	1:C:792:SER:OG	2.30	0.44
1:D:563:LYS:NZ	1:D:766:GLU:OE2	2.50	0.44
1:A:517:ILE:HA	1:A:525:PHE:CZ	2.53	0.43
1:B:138:ASP:OD1	1:B:139:LEU:N	2.51	0.43
1:A:262:ALA:O	1:A:266:ILE:HG12	2.18	0.43
1:A:416:TYR:CD2	1:A:428:ALA:HB1	2.53	0.43
1:A:610:ALA:HA	1:A:613:LEU:HD12	2.00	0.43
1:B:37:LEU:HD21	1:B:193:LEU:HD21	2.00	0.43
1:C:610:ALA:HA	1:C:613:LEU:HD12	1.98	0.43
1:A:37:LEU:HD21	1:A:193:LEU:HD21	2.01	0.43
1:A:724:TYR:CE2	1:A:728:VAL:HG21	2.53	0.43
1:C:477:TRP:HD1	1:C:481:ARG:HH21	1.65	0.43
1:B:416:TYR:CD2	1:B:428:ALA:HB1	2.53	0.43
1:C:87:ASP:OD1	1:C:87:ASP:N	2.52	0.43
1:C:310:MET:O	1:C:314:MET:HG3	2.18	0.43
1:D:87:ASP:N	1:D:87:ASP:OD1	2.50	0.43
1:A:493:LYS:HG2	1:C:468:HIS:CE1	2.53	0.43
1:A:590:LYS:HG2	1:A:630:LYS:HE2	2.01	0.43
1:A:594:MET:HA	1:A:634:PHE:HB3	2.00	0.43
1:A:933:LYS:HA	1:B:330:ARG:HD3	2.01	0.43
1:C:237:MET:HG2	1:C:303:VAL:HG12	2.01	0.43
1:A:60:LEU:HD21	1:A:83:LEU:HD21	2.00	0.43
1:B:252:VAL:HG11	1:B:441:THR:HG21	2.01	0.43
1:D:60:LEU:HD21	1:D:83:LEU:HD21	2.00	0.43
1:D:587:ILE:HD12	1:D:587:ILE:HA	1.77	0.43
1:A:330:ARG:HD3	1:B:933:LYS:HA	2.00	0.43
1:C:552:LYS:H	1:C:552:LYS:HG2	1.51	0.43
1:C:723:GLU:O	1:C:726:SER:OG	2.35	0.43
1:C:930:LYS:HG2	1:C:931:PRO:HD2	2.01	0.43
1:D:552:LYS:HG3	1:D:553:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:ARG:O	1:D:730:GLN:HG2	2.18	0.43
1:A:558:VAL:HA	1:A:559:PRO:HD3	1.90	0.43
1:B:168:LEU:O	1:B:281:PHE:HA	2.19	0.43
1:C:169:VAL:HB	1:C:282:SER:HB2	2.00	0.43
1:D:115:TYR:O	1:D:119:ILE:HG22	2.19	0.43
1:A:494:ARG:NH2	1:C:489:GLU:OE2	2.43	0.43
1:A:905:LEU:O	1:A:909:ARG:HG3	2.19	0.43
1:B:724:TYR:O	1:B:728:VAL:HG22	2.19	0.43
1:D:528:TYR:HB2	1:D:555:LEU:CD1	2.49	0.43
1:A:528:TYR:HB2	1:A:555:LEU:CD1	2.47	0.43
1:A:915:VAL:N	1:A:943:GLU:O	2.28	0.43
1:B:844:LEU:HD13	1:B:909:ARG:NH2	2.33	0.43
1:A:305:LEU:HD13	1:A:305:LEU:HA	1.86	0.42
1:C:621:VAL:HG21	1:C:659:THR:HA	2.01	0.42
1:C:641:VAL:HG21	1:C:828:VAL:HG21	2.01	0.42
1:D:331:CYS:SG	1:D:336:ARG:HD2	2.58	0.42
1:C:558:VAL:HA	1:C:559:PRO:HD3	1.91	0.42
1:D:196:LEU:HD12	1:D:196:LEU:HA	1.82	0.42
1:D:289:ARG:NH2	1:D:300:THR:OG1	2.52	0.42
1:D:513:THR:O	1:D:517:ILE:HG13	2.18	0.42
1:D:904:THR:O	1:D:908:ILE:HG12	2.19	0.42
1:A:607:LEU:HB2	1:A:790:PHE:CE1	2.54	0.42
1:B:137:SER:O	1:B:141:GLU:HB2	2.19	0.42
1:B:843:LEU:HD22	1:B:906:LYS:HD2	2.01	0.42
1:B:795:ARG:HG3	1:B:866:LEU:HD11	2.01	0.42
1:C:169:VAL:HG11	1:C:634:PHE:CZ	2.54	0.42
1:C:641:VAL:HG21	1:C:828:VAL:CG2	2.50	0.42
1:A:755:ARG:HD3	1:A:769:ARG:NH2	2.34	0.42
1:B:497:PHE:CD1	1:B:497:PHE:N	2.88	0.42
1:C:139:LEU:N	1:C:688:GLN:OE1	2.52	0.42
1:D:150:LEU:HD11	1:D:700:ARG:HD3	2.02	0.42
1:D:405:LEU:HD11	1:D:523:ASP:HB3	2.02	0.42
1:B:33:TYR:HB2	1:B:112:GLN:NE2	2.34	0.42
1:B:696:GLU:O	1:B:700:ARG:N	2.43	0.42
1:D:205:ASP:O	1:D:209:LEU:HG	2.20	0.42
1:B:496:LEU:HB3	1:B:497:PHE:H	1.66	0.42
1:C:284:TRP:CD1	1:C:450:ASP:HB2	2.54	0.42
1:D:242:SER:HA	1:D:245:HIS:NE2	2.35	0.42
1:D:716:MET:SD	1:D:797:VAL:HG21	2.59	0.42
1:B:305:LEU:HD13	1:B:305:LEU:HA	1.83	0.42
1:B:365:GLU:H	1:B:365:GLU:HG2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:ASP:HB2	1:D:475:ARG:HG3	2.02	0.42
1:D:952:LEU:O	1:D:955:THR:OG1	2.31	0.42
1:A:314:MET:HE2	1:A:314:MET:HB3	1.92	0.42
1:A:699:MET:O	1:A:701:PRO:HD3	2.20	0.42
1:A:918:ARG:CB	1:A:919:PRO:HD3	2.48	0.42
1:B:641:VAL:HG21	1:B:828:VAL:CG2	2.50	0.42
1:C:908:ILE:HD12	1:C:944:TYR:CD2	2.55	0.42
1:D:724:TYR:CE2	1:D:728:VAL:HG21	2.54	0.42
1:A:739:ARG:NH1	1:A:744:GLU:OE1	2.53	0.42
1:B:90:ASP:O	1:B:94:ILE:HG12	2.20	0.42
1:C:614:TYR:CZ	1:C:656:PRO:HB3	2.55	0.42
1:D:243:TYR:OH	1:D:674:GLU:HG2	2.20	0.42
1:B:615:LYS:HE3	1:B:615:LYS:HB3	1.77	0.41
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.89	0.41
1:D:33:TYR:CE2	1:D:193:LEU:HD22	2.55	0.41
1:D:256:LEU:HB3	1:D:437:ARG:CZ	2.50	0.41
1:B:60:LEU:HD21	1:B:83:LEU:HD21	2.02	0.41
1:B:139:LEU:N	1:B:688:GLN:OE1	2.53	0.41
1:C:226:ILE:HG23	1:C:953:ILE:HG21	2.01	0.41
1:C:510:VAL:O	1:C:513:THR:OG1	2.30	0.41
1:D:477:TRP:HA	1:D:481:ARG:NH2	2.35	0.41
1:D:496:LEU:HB3	1:D:497:PHE:H	1.65	0.41
1:D:638:GLY:HA2	1:D:669:GLN:CG	2.47	0.41
1:A:496:LEU:HB3	1:A:497:PHE:H	1.65	0.41
1:C:497:PHE:N	1:C:497:PHE:CD1	2.89	0.41
1:C:705:PRO:HG2	1:C:710:ARG:NH1	2.35	0.41
1:D:330:ARG:HD2	1:D:330:ARG:HA	1.92	0.41
1:D:755:ARG:HD3	1:D:769:ARG:CZ	2.50	0.41
1:A:167:ASP:HB3	1:A:665:ARG:HG3	2.02	0.41
1:A:359:LYS:HE3	1:B:235:ASP:OD1	2.20	0.41
1:B:546:GLN:OE1	1:B:555:LEU:N	2.50	0.41
1:C:506:GLU:O	1:C:510:VAL:HG12	2.21	0.41
1:C:525:PHE:HB3	1:C:555:LEU:HD23	2.01	0.41
1:C:729:PHE:CE1	1:C:766:GLU:HB2	2.55	0.41
1:D:245:HIS:CD2	1:D:245:HIS:H	2.38	0.41
1:D:294:ARG:HD3	1:D:754:SER:O	2.19	0.41
1:D:699:MET:O	1:D:701:PRO:HD3	2.20	0.41
1:B:492:GLY:O	1:B:547:ARG:NH2	2.53	0.41
1:C:410:GLU:HB3	1:C:411:PRO:HD3	2.02	0.41
1:C:607:LEU:HB2	1:C:790:PHE:CZ	2.55	0.41
1:C:643:ARG:HG3	1:C:774:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:PHE:O	1:C:855:LYS:HB2	2.21	0.41
1:D:451:ILE:HG13	1:D:517:ILE:HD11	2.02	0.41
1:B:489:GLU:OE2	1:D:494:ARG:NH2	2.44	0.41
1:C:86:LEU:HD13	1:C:94:ILE:HG13	2.01	0.41
1:A:242:SER:HA	1:A:245:HIS:NE2	2.35	0.41
1:A:408:PHE:O	1:A:411:PRO:HD2	2.21	0.41
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.92	0.41
1:B:607:LEU:HB2	1:B:790:PHE:CZ	2.56	0.41
1:C:168:LEU:O	1:C:281:PHE:HA	2.21	0.41
1:C:173:HIS:O	1:C:175:THR:N	2.54	0.41
1:C:705:PRO:HB3	1:C:815:TRP:CZ2	2.56	0.41
1:D:139:LEU:HD11	1:D:259:VAL:HG22	2.03	0.41
1:A:55:GLU:O	1:A:59:GLU:HG3	2.21	0.41
1:A:87:ASP:N	1:A:87:ASP:OD1	2.54	0.41
1:A:102:LEU:HD13	1:A:893:TYR:HD2	1.85	0.41
1:A:235:ASP:OD1	1:B:359:LYS:HE3	2.21	0.41
1:A:289:ARG:HG2	1:A:452:ARG:O	2.21	0.41
1:A:821:THR:O	1:A:825:ILE:HG12	2.20	0.41
1:B:314:MET:HB3	1:B:314:MET:HE2	1.95	0.41
1:B:318:GLN:HB3	1:B:435:PHE:CE1	2.56	0.41
1:B:669:GLN:O	1:B:672:VAL:N	2.51	0.41
1:B:918:ARG:HB2	1:B:919:PRO:HD3	2.03	0.41
1:C:621:VAL:HG21	1:C:659:THR:HG22	2.02	0.41
1:C:657:PRO:HB3	1:C:702:PRO:HD2	2.02	0.41
1:D:90:ASP:O	1:D:94:ILE:HG12	2.20	0.41
1:D:244:PHE:C	1:D:246:GLU:H	2.25	0.41
1:D:643:ARG:HG3	1:D:774:ILE:HG13	2.02	0.41
1:A:157:ILE:O	1:A:161:LEU:HB2	2.21	0.41
1:A:355:ILE:O	1:B:238:ARG:NE	2.48	0.41
1:B:594:MET:HA	1:B:634:PHE:HB3	2.02	0.41
1:C:95:ALA:HB1	1:C:954:LEU:HB3	2.03	0.41
1:A:252:VAL:HB	1:A:253:PRO:HD3	2.04	0.40
1:A:952:LEU:O	1:A:955:THR:OG1	2.27	0.40
1:D:335:LEU:HD12	1:D:414:LEU:HG	2.02	0.40
1:A:90:ASP:O	1:A:94:ILE:HG12	2.21	0.40
1:A:615:LYS:HB3	1:A:615:LYS:HE3	1.79	0.40
1:A:618:GLU:CD	1:A:710:ARG:HH22	2.25	0.40
1:C:176:GLN:NE2	1:C:671:GLU:HA	2.36	0.40
1:C:244:PHE:C	1:C:246:GLU:H	2.24	0.40
1:C:245:HIS:CD2	1:C:245:HIS:H	2.40	0.40
1:A:378:LEU:HA	1:A:378:LEU:HD12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.85	0.40
1:B:252:VAL:HB	1:B:253:PRO:HD3	2.02	0.40
1:C:179:ARG:HB2	2:C:1001:PO4:O1	2.21	0.40
1:C:794:ILE:HB	1:C:866:LEU:HD13	2.03	0.40
1:D:329:TRP:CZ3	1:D:330:ARG:HG2	2.56	0.40
1:D:598:SER:HB3	1:D:770:ALA:HB3	2.03	0.40
1:A:244:PHE:HA	1:A:248:ILE:HB	2.02	0.40
1:B:52:ASP:OD1	1:B:52:ASP:N	2.55	0.40
1:B:138:ASP:O	1:B:142:THR:OG1	2.30	0.40
1:B:610:ALA:HA	1:B:613:LEU:HD12	2.02	0.40
1:B:705:PRO:HB3	1:B:815:TRP:CZ2	2.56	0.40
1:C:90:ASP:O	1:C:94:ILE:HG12	2.21	0.40
1:C:592:GLU:OE2	1:C:665:ARG:NE	2.47	0.40
1:D:479:GLU:OE1	1:D:537:SER:HB3	2.21	0.40
1:D:657:PRO:HB3	1:D:702:PRO:HD2	2.04	0.40
1:A:634:PHE:CE1	1:A:667:THR:HG23	2.57	0.40
1:B:699:MET:O	1:B:701:PRO:HD3	2.21	0.40
1:B:720:ALA:HB2	1:B:793:ALA:HB2	2.02	0.40
1:D:169:VAL:HG11	1:D:634:PHE:CE1	2.57	0.40
1:D:378:LEU:HD12	1:D:378:LEU:HA	1.86	0.40
1:D:615:LYS:HB3	1:D:615:LYS:HE3	1.77	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	887/974 (91%)	843 (95%)	37 (4%)	7 (1%)	16 38
1	B	889/974 (91%)	842 (95%)	40 (4%)	7 (1%)	16 38
1	C	873/974 (90%)	833 (95%)	36 (4%)	4 (0%)	25 50
1	D	867/974 (89%)	826 (95%)	38 (4%)	3 (0%)	37 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3516/3896 (90%)	3344 (95%)	151 (4%)	21 (1%)	22 46

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	670	GLY
1	A	919	PRO
1	B	670	GLY
1	B	919	PRO
1	C	670	GLY
1	C	848	GLU
1	D	670	GLY
1	D	848	GLU
1	A	848	GLU
1	A	918	ARG
1	B	848	GLU
1	B	918	ARG
1	C	889	LEU
1	A	119	ILE
1	A	889	LEU
1	B	120	LYS
1	B	137	SER
1	C	203	PRO
1	B	203	PRO
1	D	203	PRO
1	A	203	PRO

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	780/848 (92%)	719 (92%)	61 (8%)	10 25
1	B	782/848 (92%)	721 (92%)	61 (8%)	10 25
1	C	766/848 (90%)	710 (93%)	56 (7%)	11 28
1	D	760/848 (90%)	707 (93%)	53 (7%)	12 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3088/3392 (91%)	2857 (92%)	231 (8%)	11 26

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	54	ARG
1	A	71	HIS
1	A	102	LEU
1	A	116	ARG
1	A	138	ASP
1	A	149	ASP
1	A	165	THR
1	A	169	VAL
1	A	182	LEU
1	A	196	LEU
1	A	201	ILE
1	A	228	ARG
1	A	237	MET
1	A	256	LEU
1	A	269	GLU
1	A	271	ARG
1	A	278	LEU
1	A	279	ILE
1	A	306	LEU
1	A	308	ARG
1	A	318	GLN
1	A	319	ILE
1	A	324	PHE
1	A	328	MET
1	A	332	ASN
1	A	345	ASN
1	A	348	LYS
1	A	349	ASP
1	A	358	TRP
1	A	359	LYS
1	A	365	GLU
1	A	378	LEU
1	A	384	ARG
1	A	388	LEU
1	A	393	HIS
1	A	406	GLU

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Mol	Chain	Res	Type
1	A	408	PHE
1	A	493	LYS
1	A	497	PHE
1	A	504	THR
1	A	510	VAL
1	A	552	LYS
1	A	555	LEU
1	A	558	VAL
1	A	567	LEU
1	A	587	ILE
1	A	602	LYS
1	A	625	LYS
1	A	658	ASP
1	A	688	GLN
1	A	713	LEU
1	A	716	MET
1	A	723	GLU
1	A	768	LEU
1	A	771	ILE
1	A	798	ILE
1	A	799	GLU
1	A	849	LEU
1	A	910	ASP
1	A	917	LEU
1	B	33	TYR
1	B	54	ARG
1	B	71	HIS
1	B	102	LEU
1	B	116	ARG
1	B	118	ARG
1	B	135	THR
1	B	149	ASP
1	B	169	VAL
1	B	182	LEU
1	B	196	LEU
1	B	201	ILE
1	B	228	ARG
1	B	237	MET
1	B	256	LEU
1	B	269	GLU
1	B	271	ARG
1	B	278	LEU

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Mol	Chain	Res	Type
1	B	279	ILE
1	B	306	LEU
1	B	308	ARG
1	B	318	GLN
1	B	319	ILE
1	B	324	PHE
1	B	328	MET
1	B	332	ASN
1	B	345	ASN
1	B	348	LYS
1	B	349	ASP
1	B	358	TRP
1	B	359	LYS
1	B	365	GLU
1	B	378	LEU
1	B	384	ARG
1	B	388	LEU
1	B	393	HIS
1	B	406	GLU
1	B	481	ARG
1	B	493	LYS
1	B	497	PHE
1	B	504	THR
1	B	510	VAL
1	B	555	LEU
1	B	558	VAL
1	B	567	LEU
1	B	587	ILE
1	B	602	LYS
1	B	625	LYS
1	B	632	THR
1	B	658	ASP
1	B	688	GLN
1	B	713	LEU
1	B	716	MET
1	B	723	GLU
1	B	768	LEU
1	B	771	ILE
1	B	798	ILE
1	B	799	GLU
1	B	849	LEU
1	B	874	LYS

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Mol	Chain	Res	Type
1	B	917	LEU
1	C	54	ARG
1	C	71	HIS
1	C	85	SER
1	C	102	LEU
1	C	116	ARG
1	C	149	ASP
1	C	165	THR
1	C	169	VAL
1	C	196	LEU
1	C	201	ILE
1	C	228	ARG
1	C	237	MET
1	C	256	LEU
1	C	269	GLU
1	C	271	ARG
1	C	278	LEU
1	C	279	ILE
1	C	306	LEU
1	C	308	ARG
1	C	319	ILE
1	C	324	PHE
1	C	328	MET
1	C	332	ASN
1	C	345	ASN
1	C	348	LYS
1	C	349	ASP
1	C	358	TRP
1	C	365	GLU
1	C	378	LEU
1	C	384	ARG
1	C	393	HIS
1	C	399	GLU
1	C	406	GLU
1	C	408	PHE
1	C	493	LYS
1	C	497	PHE
1	C	504	THR
1	C	510	VAL
1	C	555	LEU
1	C	558	VAL
1	C	567	LEU

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Mol	Chain	Res	Type
1	C	586	ARG
1	C	587	ILE
1	C	602	LYS
1	C	625	LYS
1	C	658	ASP
1	C	688	GLN
1	C	713	LEU
1	C	716	MET
1	C	727	VAL
1	C	768	LEU
1	C	771	ILE
1	C	798	ILE
1	C	799	GLU
1	C	849	LEU
1	C	930	LYS
1	D	33	TYR
1	D	40	ARG
1	D	54	ARG
1	D	71	HIS
1	D	87	ASP
1	D	102	LEU
1	D	116	ARG
1	D	117	ARG
1	D	149	ASP
1	D	165	THR
1	D	169	VAL
1	D	196	LEU
1	D	201	ILE
1	D	228	ARG
1	D	237	MET
1	D	256	LEU
1	D	269	GLU
1	D	271	ARG
1	D	278	LEU
1	D	279	ILE
1	D	306	LEU
1	D	308	ARG
1	D	319	ILE
1	D	324	PHE
1	D	328	MET
1	D	332	ASN
1	D	345	ASN

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Mol	Chain	Res	Type
1	D	348	LYS
1	D	358	TRP
1	D	378	LEU
1	D	399	GLU
1	D	406	GLU
1	D	408	PHE
1	D	493	LYS
1	D	497	PHE
1	D	510	VAL
1	D	555	LEU
1	D	558	VAL
1	D	567	LEU
1	D	586	ARG
1	D	587	ILE
1	D	602	LYS
1	D	658	ASP
1	D	688	GLN
1	D	713	LEU
1	D	716	MET
1	D	727	VAL
1	D	768	LEU
1	D	771	ILE
1	D	798	ILE
1	D	799	GLU
1	D	849	LEU
1	D	909	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	C	332	ASN
1	D	332	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

4 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	C	1001	-	4,4,4	0.91	0	6,6,6	0.46	0
2	PO4	B	1001	-	4,4,4	0.91	0	6,6,6	0.45	0
2	PO4	A	1001	-	4,4,4	0.86	0	6,6,6	0.46	0
2	PO4	D	1001	-	4,4,4	0.91	0	6,6,6	0.42	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	1001	PO4	1	0
2	B	1001	PO4	1	0
2	A	1001	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, 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	897/974 (92%)	-0.25	19 (2%) 63 61	49, 80, 131, 214	0
1	B	899/974 (92%)	-0.28	14 (1%) 70 68	51, 82, 135, 216	0
1	C	883/974 (90%)	0.06	33 (3%) 45 43	76, 140, 217, 268	0
1	D	877/974 (90%)	-0.03	20 (2%) 61 58	78, 133, 196, 277	0
All	All	3556/3896 (91%)	-0.13	86 (2%) 59 57	49, 105, 193, 277	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	LEU	6.0
1	B	245	HIS	5.2
1	A	245	HIS	4.5
1	A	31	VAL	4.5
1	C	105	ALA	3.8
1	B	921	ILE	3.7
1	A	913	TYR	3.7
1	B	889	LEU	3.6
1	C	193	LEU	3.5
1	D	37	LEU	3.5
1	A	184	GLN	3.4
1	C	110	GLU	3.4
1	B	87	ASP	3.3
1	D	245	HIS	3.3
1	A	88	PRO	3.2
1	A	921	ILE	3.2
1	B	34	ASP	3.2
1	D	240	GLY	3.2
1	C	37	LEU	3.1
1	D	931	PRO	3.1
1	C	350	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	674	GLU	3.1
1	C	771	ILE	3.1
1	C	109	GLU	3.0
1	B	31	VAL	3.0
1	B	33	TYR	3.0
1	D	33	TYR	2.9
1	A	34	ASP	2.9
1	C	245	HIS	2.9
1	C	525	PHE	2.8
1	D	824	LEU	2.8
1	A	240	GLY	2.8
1	A	33	TYR	2.6
1	A	186	HIS	2.6
1	B	919	PRO	2.6
1	C	756	PRO	2.6
1	D	252	VAL	2.6
1	C	601	GLY	2.5
1	B	913	TYR	2.5
1	C	824	LEU	2.5
1	D	606	ARG	2.5
1	C	650	LEU	2.5
1	D	573	ALA	2.5
1	D	830	ALA	2.5
1	C	755	ARG	2.4
1	D	350	ALA	2.4
1	A	243	TYR	2.4
1	D	82	VAL	2.4
1	A	780	THR	2.4
1	C	946	PRO	2.3
1	C	782	PHE	2.3
1	C	35	ALA	2.3
1	C	675	GLN	2.3
1	A	208	GLU	2.3
1	A	888	ARG	2.3
1	A	946	PRO	2.3
1	A	101	MET	2.3
1	A	701	PRO	2.3
1	B	959	ILE	2.2
1	D	771	ILE	2.2
1	B	920	HIS	2.2
1	D	737	TYR	2.2
1	C	727	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	36	LEU	2.2
1	C	108	ALA	2.2
1	B	86	LEU	2.2
1	C	104	LEU	2.2
1	C	88	PRO	2.2
1	A	703	ILE	2.2
1	C	915	VAL	2.2
1	D	520	LEU	2.1
1	D	191	ASP	2.1
1	B	755	ARG	2.1
1	C	221	PHE	2.1
1	C	818	PHE	2.1
1	D	446	LEU	2.1
1	C	355	ILE	2.1
1	C	764	GLY	2.1
1	C	874	LYS	2.1
1	C	805	LEU	2.0
1	C	790	PHE	2.0
1	C	817	PHE	2.0
1	A	920	HIS	2.0
1	D	653	LEU	2.0
1	D	405	LEU	2.0
1	D	100	HIS	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 monosaccharides 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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	D	1001	5/5	0.90	0.09	99,124,131,141	0
2	PO4	C	1001	5/5	0.91	0.08	119,125,133,135	0
2	PO4	A	1001	5/5	0.95	0.09	57,71,112,127	0
2	PO4	B	1001	5/5	0.98	0.06	57,89,98,105	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.