Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:39 PM GMT

PDB ID	:	1Q1L
Title	:	Crystal Structure of Chorismate Synthase
Authors	:	Viola, C.M.; Saridakis, V.; Christendat, D.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2003-07-21
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

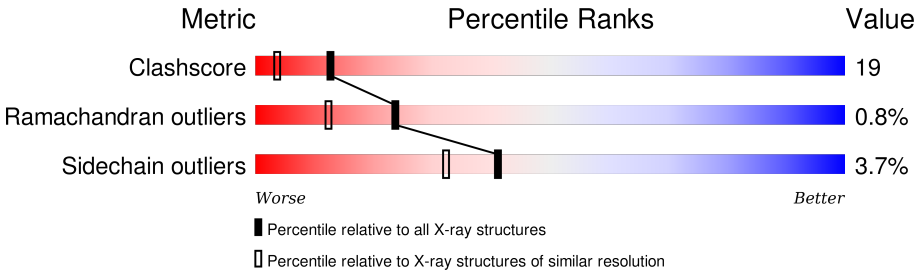
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	59% 23% • 16%
1	B	401	56% 25% • 16%
1	C	401	56% 25% • 17%
1	D	401	58% 23% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11091 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 Chorismate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	Se	0	1	0
			2635	1674	465	489	1	6			
1	B	336	Total	C	N	O	S	Se	0	2	0
			2640	1675	465	493	1	6			
1	C	333	Total	C	N	O	S	Se	0	2	0
			2622	1662	462	491	1	6			
1	D	334	Total	C	N	O	S	Se	0	3	0
			2634	1670	465	492	1	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP O66493
A	-1	SER	-	EXPRESSION TAG	UNP O66493
A	0	HIS	-	EXPRESSION TAG	UNP O66493
A	1	MSE	MET	MODIFIED RESIDUE	UNP O66493
A	257	MSE	MET	MODIFIED RESIDUE	UNP O66493
A	258	MSE	MET	MODIFIED RESIDUE	UNP O66493
A	312	MSE	MET	MODIFIED RESIDUE	UNP O66493
A	320	MSE	MET	MODIFIED RESIDUE	UNP O66493
A	363	MSE	MET	MODIFIED RESIDUE	UNP O66493
A	381	MSE	MET	MODIFIED RESIDUE	UNP O66493
B	-2	GLY	-	EXPRESSION TAG	UNP O66493
B	-1	SER	-	EXPRESSION TAG	UNP O66493
B	0	HIS	-	EXPRESSION TAG	UNP O66493
B	1	MSE	MET	MODIFIED RESIDUE	UNP O66493
B	257	MSE	MET	MODIFIED RESIDUE	UNP O66493
B	258	MSE	MET	MODIFIED RESIDUE	UNP O66493
B	312	MSE	MET	MODIFIED RESIDUE	UNP O66493
B	320	MSE	MET	MODIFIED RESIDUE	UNP O66493
B	363	MSE	MET	MODIFIED RESIDUE	UNP O66493
B	381	MSE	MET	MODIFIED RESIDUE	UNP O66493
C	-2	GLY	-	EXPRESSION TAG	UNP O66493

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP O66493
C	0	HIS	-	EXPRESSION TAG	UNP O66493
C	1	MSE	MET	MODIFIED RESIDUE	UNP O66493
C	257	MSE	MET	MODIFIED RESIDUE	UNP O66493
C	258	MSE	MET	MODIFIED RESIDUE	UNP O66493
C	312	MSE	MET	MODIFIED RESIDUE	UNP O66493
C	320	MSE	MET	MODIFIED RESIDUE	UNP O66493
C	363	MSE	MET	MODIFIED RESIDUE	UNP O66493
C	381	MSE	MET	MODIFIED RESIDUE	UNP O66493
D	-2	GLY	-	EXPRESSION TAG	UNP O66493
D	-1	SER	-	EXPRESSION TAG	UNP O66493
D	0	HIS	-	EXPRESSION TAG	UNP O66493
D	1	MSE	MET	MODIFIED RESIDUE	UNP O66493
D	257	MSE	MET	MODIFIED RESIDUE	UNP O66493
D	258	MSE	MET	MODIFIED RESIDUE	UNP O66493
D	312	MSE	MET	MODIFIED RESIDUE	UNP O66493
D	320	MSE	MET	MODIFIED RESIDUE	UNP O66493
D	363	MSE	MET	MODIFIED RESIDUE	UNP O66493
D	381	MSE	MET	MODIFIED RESIDUE	UNP O66493

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	157	Total O 157 157	0	0
2	B	137	Total O 137 137	0	0
2	C	127	Total O 127 127	0	0
2	D	139	Total O 139 139	0	0

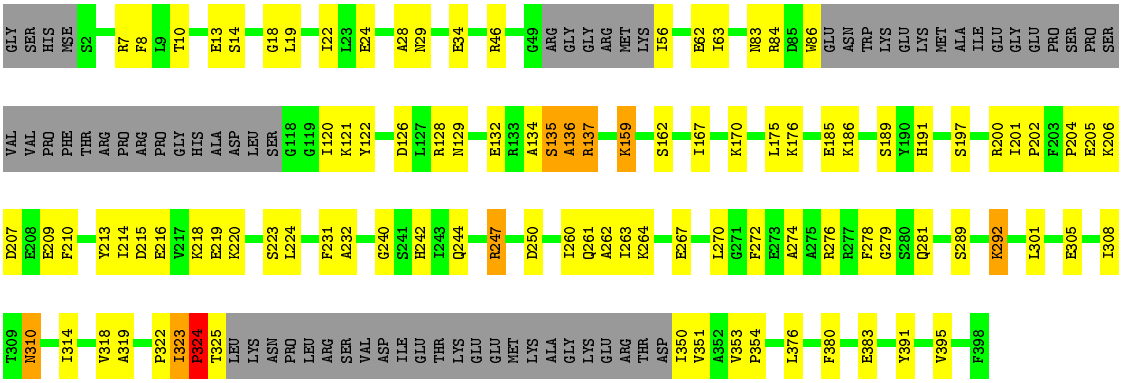
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

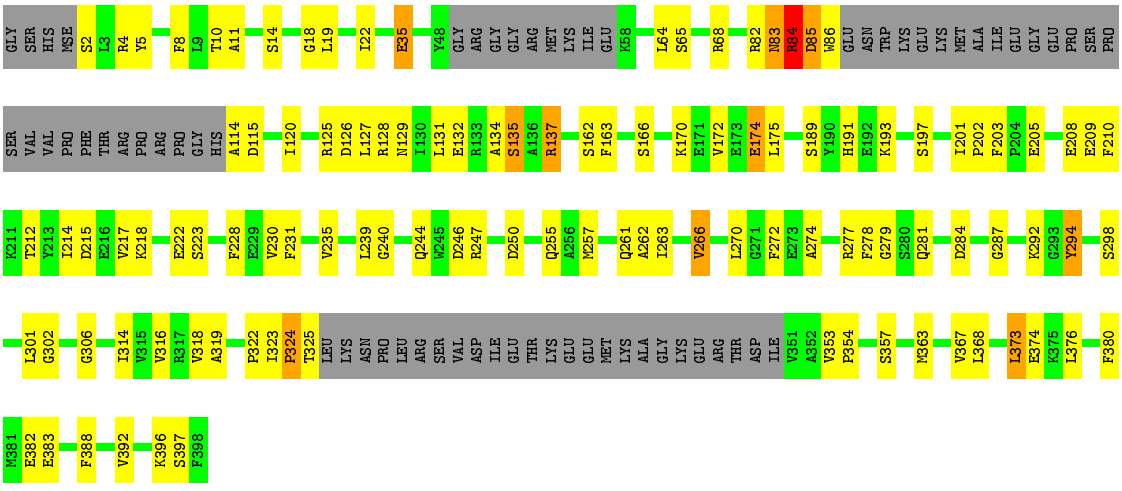
- Molecule 1: Chorismate synthase

Chain A:



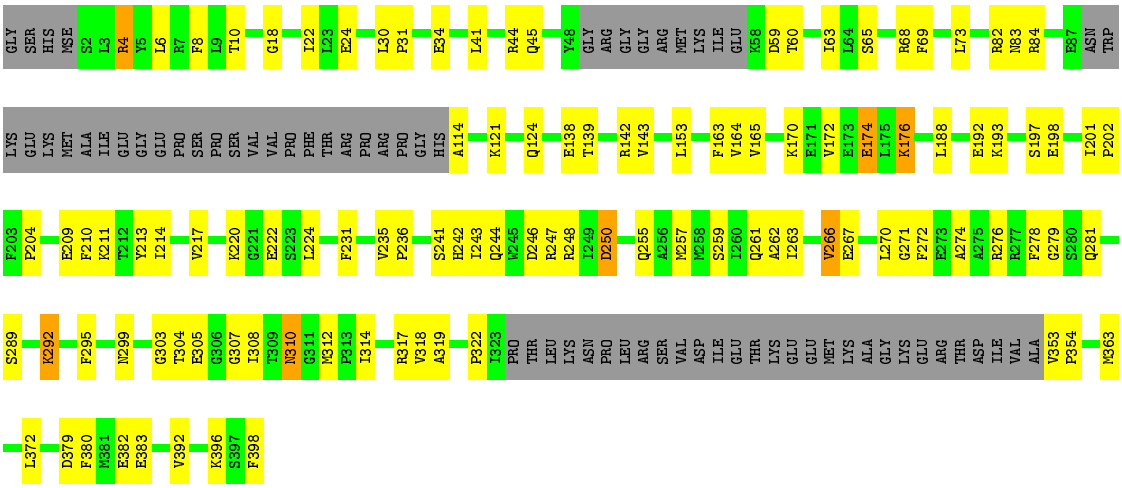
- Molecule 1: Chorismate synthase

Chain B:



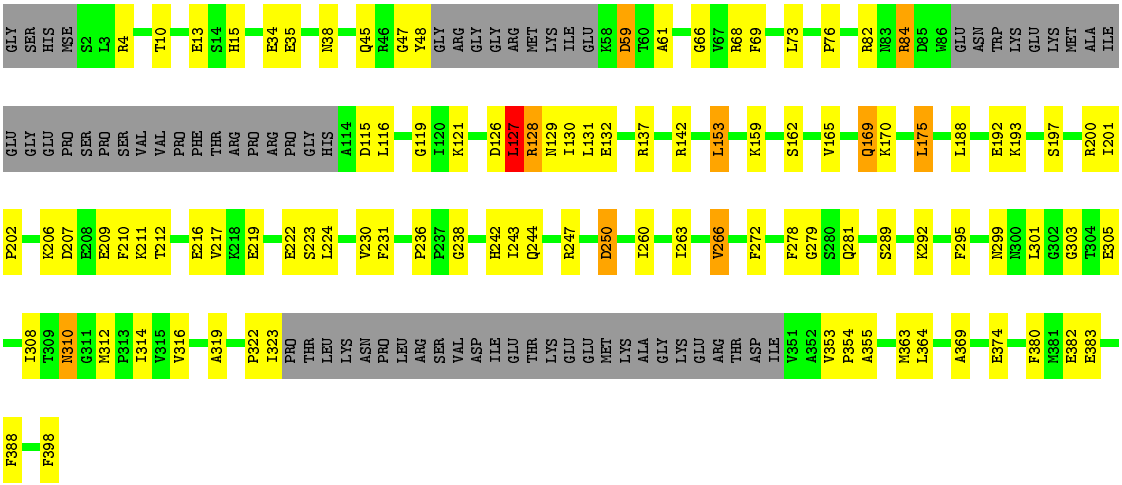
- Molecule 1: Chorismate synthase

Chain C:



- Molecule 1: Chorismate synthase

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.43Å 95.96Å 113.46Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	24.63 – 2.05	Depositor
% Data completeness (in resolution range)	81.2 (24.63-2.05)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11091	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.75	10/2675 (0.4%)	0.56	0/3579
1	B	1.15	16/2680 (0.6%)	0.52	0/3588
1	C	0.96	10/2661 (0.4%)	0.54	0/3560
1	D	1.11	24/2673 (0.9%)	0.53	0/3577
All	All	1.01	60/10689 (0.6%)	0.54	0/14304

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266[A]	VAL	CB-CG1	17.56	1.89	1.52
1	D	266[B]	VAL	CB-CG1	17.56	1.89	1.52
1	C	266[A]	VAL	CB-CG1	17.54	1.89	1.52
1	C	266[B]	VAL	CB-CG1	17.54	1.89	1.52
1	B	35[A]	GLU	CB-CG	17.36	1.85	1.52
1	B	35[B]	GLU	CB-CG	17.36	1.85	1.52
1	B	266[A]	VAL	CB-CG2	17.19	1.89	1.52
1	B	266[B]	VAL	CB-CG2	17.19	1.89	1.52
1	D	266[A]	VAL	CB-CG2	17.10	1.88	1.52
1	D	266[B]	VAL	CB-CG2	17.10	1.88	1.52
1	C	266[A]	VAL	CB-CG2	17.07	1.88	1.52
1	C	266[B]	VAL	CB-CG2	17.07	1.88	1.52
1	B	266[A]	VAL	CB-CG1	17.00	1.88	1.52
1	B	266[B]	VAL	CB-CG1	17.00	1.88	1.52
1	B	35[A]	GLU	CG-CD	14.53	1.73	1.51
1	B	35[B]	GLU	CG-CD	14.53	1.73	1.51
1	A	159[A]	LYS	CD-CE	13.54	1.85	1.51
1	A	159[B]	LYS	CD-CE	13.54	1.85	1.51
1	D	266[A]	VAL	CA-CB	13.48	1.83	1.54
1	D	266[B]	VAL	CA-CB	13.48	1.83	1.54
1	B	266[A]	VAL	CA-CB	13.38	1.82	1.54
1	B	266[B]	VAL	CA-CB	13.38	1.82	1.54
1	C	266[A]	VAL	CA-CB	13.28	1.82	1.54
1	C	266[B]	VAL	CA-CB	13.28	1.82	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159[A]	LYS	CB-CG	11.64	1.83	1.52
1	A	159[B]	LYS	CB-CG	11.64	1.83	1.52
1	D	169[A]	GLN	CB-CG	11.57	1.83	1.52
1	D	169[B]	GLN	CB-CG	11.57	1.83	1.52
1	C	250[A]	ASP	CB-CG	10.74	1.74	1.51
1	C	250[B]	ASP	CB-CG	10.74	1.74	1.51
1	D	250[A]	ASP	CB-CG	10.70	1.74	1.51
1	D	250[B]	ASP	CB-CG	10.70	1.74	1.51
1	B	35[A]	GLU	CD-OE2	10.59	1.37	1.25
1	B	35[B]	GLU	CD-OE2	10.59	1.37	1.25
1	B	35[A]	GLU	CD-OE1	10.40	1.37	1.25
1	B	35[B]	GLU	CD-OE1	10.40	1.37	1.25
1	D	169[A]	GLN	CG-CD	9.84	1.73	1.51
1	D	169[B]	GLN	CG-CD	9.84	1.73	1.51
1	A	159[A]	LYS	CG-CD	9.59	1.85	1.52
1	A	159[B]	LYS	CG-CD	9.59	1.85	1.52
1	A	159[A]	LYS	CE-NZ	9.17	1.72	1.49
1	A	159[B]	LYS	CE-NZ	9.17	1.72	1.49
1	B	35[A]	GLU	CA-CB	8.31	1.72	1.53
1	B	35[B]	GLU	CA-CB	8.31	1.72	1.53
1	A	159[A]	LYS	CA-CB	8.22	1.72	1.53
1	A	159[B]	LYS	CA-CB	8.22	1.72	1.53
1	D	169[A]	GLN	CA-CB	8.11	1.71	1.53
1	D	169[B]	GLN	CA-CB	8.11	1.71	1.53
1	C	250[A]	ASP	CA-CB	8.10	1.71	1.53
1	C	250[B]	ASP	CA-CB	8.10	1.71	1.53
1	D	250[A]	ASP	CA-CB	8.07	1.71	1.53
1	D	250[B]	ASP	CA-CB	8.07	1.71	1.53
1	D	169[A]	GLN	CD-NE2	5.68	1.47	1.32
1	D	169[B]	GLN	CD-NE2	5.68	1.47	1.32
1	D	169[A]	GLN	CD-OE1	5.62	1.36	1.24
1	D	169[B]	GLN	CD-OE1	5.62	1.36	1.24
1	D	250[A]	ASP	CG-OD2	5.06	1.36	1.25
1	D	250[B]	ASP	CG-OD2	5.06	1.36	1.25
1	D	250[A]	ASP	CG-OD1	5.02	1.36	1.25
1	D	250[B]	ASP	CG-OD1	5.02	1.36	1.25

There are no bond angle outliers.

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	2635	0	2653	104	0
1	B	2640	0	2648	115	0
1	C	2622	0	2624	111	0
1	D	2634	0	2639	127	0
2	A	157	0	0	1	0
2	B	137	0	0	4	0
2	C	127	0	0	6	0
2	D	139	0	0	5	0
All	All	11091	0	10564	407	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 19.

All (407) 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:B:266[A]:VAL:CA	1:B:266[A]:VAL:CB	1.82	1.56
1:B:266[B]:VAL:CA	1:B:266[B]:VAL:CB	1.82	1.56
1:C:266[A]:VAL:CB	1:C:266[A]:VAL:CA	1.82	1.55
1:C:266[B]:VAL:CA	1:C:266[B]:VAL:CB	1.82	1.55
1:A:159[B]:LYS:CG	1:A:159[B]:LYS:CB	1.84	1.54
1:A:159[A]:LYS:CB	1:A:159[A]:LYS:CG	1.84	1.54
1:D:169[A]:GLN:CB	1:D:169[A]:GLN:CG	1.83	1.53
1:A:159[A]:LYS:CG	1:A:159[A]:LYS:CD	1.85	1.53
1:A:159[B]:LYS:CG	1:A:159[B]:LYS:CD	1.85	1.53
1:D:266[B]:VAL:CA	1:D:266[B]:VAL:CB	1.83	1.52
1:D:266[A]:VAL:CB	1:D:266[A]:VAL:CA	1.83	1.52
1:D:169[B]:GLN:CB	1:D:169[B]:GLN:CG	1.84	1.52
1:A:159[B]:LYS:CE	1:A:159[B]:LYS:CD	1.85	1.51
1:A:159[A]:LYS:CE	1:A:159[A]:LYS:CD	1.85	1.51
1:B:35[A]:GLU:CB	1:B:35[A]:GLU:CG	1.85	1.50
1:B:35[B]:GLU:CB	1:B:35[B]:GLU:CG	1.85	1.50
1:B:266[A]:VAL:CB	1:B:266[A]:VAL:CG2	1.89	1.50
1:B:266[B]:VAL:CG2	1:B:266[B]:VAL:CB	1.89	1.50
1:D:266[A]:VAL:CG1	1:D:266[A]:VAL:CB	1.89	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266[B]:VAL:CG1	1:D:266[B]:VAL:CB	1.89	1.49
1:D:266[A]:VAL:CB	1:D:266[A]:VAL:CG2	1.88	1.48
1:D:266[B]:VAL:CG2	1:D:266[B]:VAL:CB	1.88	1.48
1:B:266[A]:VAL:CG1	1:B:266[A]:VAL:CB	1.88	1.48
1:B:266[B]:VAL:CG1	1:B:266[B]:VAL:CB	1.88	1.48
1:C:266[A]:VAL:CB	1:C:266[A]:VAL:CG2	1.88	1.48
1:C:266[B]:VAL:CG2	1:C:266[B]:VAL:CB	1.88	1.48
1:C:266[A]:VAL:CB	1:C:266[A]:VAL:CG1	1.89	1.48
1:C:266[B]:VAL:CG1	1:C:266[B]:VAL:CB	1.89	1.48
1:A:159[A]:LYS:NZ	1:A:159[A]:LYS:CE	1.72	1.48
1:A:159[B]:LYS:CE	1:A:159[B]:LYS:NZ	1.72	1.48
1:C:257:MSE:HE2	1:C:318:VAL:HG21	1.32	1.07
1:B:257:MSE:HE2	1:B:318:VAL:HG21	1.34	1.07
1:D:82:ARG:HB2	1:D:82:ARG:HH11	1.25	0.98
1:D:142:ARG:HB3	1:D:363:MSE:HE1	1.46	0.96
1:A:278:PHE:H	1:A:281:GLN:HE21	1.17	0.92
1:B:380:PHE:HD2	1:B:382:GLU:HG2	1.36	0.91
1:C:4:ARG:HH11	1:C:4:ARG:HB3	1.37	0.90
1:D:84:ARG:HA	1:D:84:ARG:HE	1.38	0.89
1:A:323:ILE:HG13	1:A:324:PRO:HD2	1.54	0.88
1:D:238:GLY:HA2	1:D:308:ILE:HD11	1.56	0.85
1:C:4:ARG:NH1	1:C:4:ARG:HB3	1.92	0.85
1:D:142:ARG:HB3	1:D:363:MSE:CE	2.10	0.81
1:B:324:PRO:HG2	1:B:325:THR:H	1.45	0.81
1:B:125:ARG:HB3	1:B:125:ARG:HH11	1.46	0.80
1:D:82:ARG:HB2	1:D:82:ARG:NH1	1.96	0.80
1:A:278:PHE:H	1:A:281:GLN:NE2	1.81	0.79
1:D:115:ASP:HB3	1:D:127:LEU:HD11	1.65	0.78
1:D:165:VAL:HG12	1:D:175:LEU:HD23	1.64	0.78
1:B:84:ARG:HD2	1:B:84:ARG:H	1.46	0.77
1:A:136:ALA:N	1:A:261:GLN:HE22	1.82	0.77
1:A:175:LEU:HD11	1:A:202:PRO:HG2	1.67	0.76
1:C:299:ASN:HD21	1:C:303:GLY:H	1.32	0.76
1:A:353:VAL:HG12	1:A:354:PRO:HD3	1.67	0.76
1:A:305:GLU:CD	1:A:310:ASN:HD21	1.89	0.76
1:D:38:ASN:HD21	1:D:61:ALA:H	1.32	0.75
1:B:380:PHE:CD2	1:B:382:GLU:HG2	2.20	0.75
1:B:125:ARG:NH1	1:B:125:ARG:HB3	2.02	0.74
1:B:170:LYS:HE2	1:B:209:GLU:HG2	1.68	0.73
1:B:214:ILE:HG22	1:B:218:LYS:HE2	1.70	0.73
1:B:353:VAL:HG12	1:B:354:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:H	1:A:191:HIS:HD2	1.37	0.72
1:D:243:ILE:HD11	1:D:247:ARG:HH11	1.52	0.72
1:A:247:ARG:HH11	1:A:247:ARG:HB3	1.55	0.71
1:B:68:ARG:HH11	1:D:129:ASN:ND2	1.88	0.71
1:A:132:GLU:HG3	1:C:68:ARG:HH12	1.56	0.71
1:D:243:ILE:HD11	1:D:247:ARG:NH1	2.04	0.71
1:D:84:ARG:NE	1:D:84:ARG:HA	2.04	0.71
1:D:45:GLN:CD	1:D:59:ASP:HB2	2.11	0.70
1:B:278:PHE:HB3	1:C:222:GLU:CG	2.21	0.70
1:A:278:PHE:N	1:A:281:GLN:HE21	1.90	0.70
1:D:13:GLU:HB3	1:D:132:GLU:CG	2.22	0.69
1:A:162:SER:OG	1:A:200:ARG:NH2	2.26	0.69
1:A:244:GLN:HE22	1:D:10:THR:H	1.40	0.69
1:C:83:ASN:HB3	2:C:415:HOH:O	1.93	0.69
1:D:116:LEU:H	1:D:127:LEU:HD21	1.56	0.68
1:D:170:LYS:HE3	1:D:209:GLU:HG2	1.74	0.68
1:D:13:GLU:HB3	1:D:132:GLU:HG3	1.73	0.68
1:D:238:GLY:HA2	1:D:308:ILE:CD1	2.25	0.67
1:B:14:SER:HA	1:B:137:ARG:HG2	1.76	0.67
1:D:4:ARG:HD2	1:D:247:ARG:HG2	1.77	0.67
1:C:170:LYS:HB2	1:C:170:LYS:NZ	2.10	0.67
1:C:4:ARG:HH21	1:C:247:ARG:HD2	1.61	0.66
1:B:162:SER:H	1:B:191:HIS:HD2	1.42	0.66
1:C:82:ARG:NH1	1:C:84:ARG:HG2	2.11	0.66
1:C:4:ARG:HE	1:C:247:ARG:HG2	1.61	0.66
1:D:175:LEU:HD21	1:D:202:PRO:HG2	1.77	0.66
1:A:170:LYS:HE2	1:A:209:GLU:HG2	1.78	0.66
1:A:323:ILE:CG1	1:A:324:PRO:HD2	2.25	0.66
1:C:312:MSE:HE3	2:C:417:HOH:O	1.96	0.65
1:D:45:GLN:OE1	1:D:59:ASP:HB2	1.97	0.65
1:C:45:GLN:HE22	1:C:59:ASP:H	1.46	0.64
1:B:380:PHE:CE2	1:B:383:GLU:HB2	2.33	0.64
1:D:353:VAL:HG12	1:D:354:PRO:HD3	1.81	0.63
1:D:353:VAL:CG1	1:D:354:PRO:HD3	2.27	0.63
1:A:13:GLU:HB3	1:A:132:GLU:HB3	1.79	0.63
1:A:301:LEU:HD13	1:A:305:GLU:HG2	1.80	0.62
1:C:257:MSE:HE2	1:C:318:VAL:CG2	2.20	0.62
1:B:257:MSE:HE2	1:B:318:VAL:CG2	2.22	0.62
1:D:38:ASN:ND2	1:D:61:ALA:H	1.97	0.62
1:A:270:LEU:HB3	1:A:274:ALA:HB2	1.79	0.62
1:B:244:GLN:HE22	1:C:10:THR:H	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HB3	1:D:222:GLU:CG	2.29	0.62
1:D:299:ASN:HD21	1:D:303:GLY:H	1.45	0.62
1:D:382:GLU:H	1:D:382:GLU:CD	2.03	0.62
1:A:278:PHE:HB2	1:A:281:GLN:HG2	1.82	0.61
1:B:5:TYR:CE2	1:B:373:LEU:HG	2.35	0.61
1:C:4:ARG:HH11	1:C:4:ARG:CB	2.11	0.61
1:C:188:LEU:O	1:C:192:GLU:HG2	1.99	0.61
1:B:270:LEU:HB3	1:B:274:ALA:HB2	1.82	0.61
1:C:267:GLU:HG2	1:C:317:ARG:HB2	1.81	0.61
1:A:121:LYS:HD2	1:D:308:ILE:CD1	2.31	0.61
1:C:34:GLU:HG2	1:C:63:ILE:HG13	1.82	0.61
1:C:142:ARG:HB3	1:C:363:MSE:CE	2.31	0.60
1:D:115:ASP:CB	1:D:127:LEU:HD11	2.32	0.60
1:A:204:PRO:HA	1:A:207:ASP:OD1	2.00	0.60
1:D:207:ASP:HB3	1:D:211:LYS:NZ	2.16	0.60
1:D:310:ASN:ND2	1:D:312:MSE:H	1.99	0.60
1:A:323:ILE:HG23	1:A:324:PRO:CD	2.31	0.60
1:A:29:ASN:HD21	1:C:124:GLN:HE22	1.50	0.60
1:C:45:GLN:NE2	1:C:59:ASP:HB2	2.16	0.60
1:A:323:ILE:HG23	1:A:324:PRO:HD2	1.84	0.60
1:B:84:ARG:CD	1:B:84:ARG:H	2.14	0.60
1:B:353:VAL:CG1	1:B:354:PRO:HD3	2.31	0.59
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.66	0.59
1:D:278:PHE:HB2	1:D:281:GLN:HG3	1.84	0.59
1:D:299:ASN:HD21	1:D:303:GLY:N	2.00	0.59
1:C:163:PHE:HB2	1:C:202:PRO:HG3	1.84	0.59
1:D:127:LEU:O	1:D:130:ILE:HG12	2.02	0.59
1:B:135:SER:C	1:B:137:ARG:H	2.06	0.59
1:C:170:LYS:HZ3	1:C:170:LYS:HB2	1.68	0.59
1:C:299:ASN:HD21	1:C:303:GLY:N	2.01	0.59
1:D:170:LYS:CE	1:D:209:GLU:HG2	2.32	0.59
1:B:197:SER:OG	1:B:201:ILE:HG12	2.03	0.58
1:B:174:GLU:H	1:B:174:GLU:CD	2.02	0.58
1:B:205:GLU:H	1:B:205:GLU:CD	2.07	0.58
1:B:277:ARG:HB3	1:B:281:GLN:CG	2.34	0.58
1:D:162:SER:OG	1:D:200:ARG:NH2	2.36	0.58
1:A:353:VAL:CG1	1:A:354:PRO:HD3	2.33	0.57
1:D:193:LYS:HE2	1:D:202:PRO:O	2.04	0.57
1:D:153:LEU:HD11	1:D:369:ALA:HA	1.86	0.57
1:C:18:GLY:HA2	1:C:83:ASN:ND2	2.20	0.57
1:C:174:GLU:CD	1:C:174:GLU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:GLU:H	1:C:382:GLU:CD	2.07	0.57
1:D:301:LEU:HD13	1:D:305:GLU:HG2	1.86	0.57
1:A:162:SER:H	1:A:191:HIS:CD2	2.22	0.57
1:C:267:GLU:CG	1:C:317:ARG:HB2	2.34	0.57
1:B:193:LYS:HE2	1:B:202:PRO:O	2.04	0.57
1:B:128:ARG:HG3	1:B:128:ARG:HH11	1.71	0.56
1:B:162:SER:H	1:B:191:HIS:CD2	2.23	0.56
1:D:380:PHE:CE2	1:D:383:GLU:HB2	2.40	0.56
1:C:380:PHE:CE2	1:C:383:GLU:HB2	2.40	0.56
1:D:4:ARG:NE	1:D:374:GLU:OE2	2.38	0.56
1:A:322:PRO:HB2	1:D:279:GLY:HA2	1.88	0.56
1:C:142:ARG:HB3	1:C:363:MSE:HE1	1.87	0.56
1:D:217:VAL:HG12	1:D:222:GLU:HB3	1.86	0.56
1:B:14:SER:N	1:B:132:GLU:O	2.34	0.56
1:D:126:ASP:OD1	1:D:128:ARG:HG2	2.06	0.56
1:B:120:ILE:HG12	1:C:398:PHE:CD2	2.41	0.56
1:B:84:ARG:C	1:B:86:TRP:H	2.09	0.55
1:C:217:VAL:HA	1:C:220:LYS:HE2	1.88	0.55
1:B:397:SER:HB3	2:B:452:HOH:O	2.07	0.55
1:D:206:LYS:HZ2	1:D:210:PHE:HE1	1.54	0.55
1:D:230:VAL:CG1	1:D:316:VAL:HB	2.36	0.55
1:D:15:HIS:HB2	1:D:132:GLU:OE1	2.06	0.55
1:B:128:ARG:O	1:B:132:GLU:HG2	2.07	0.55
1:A:272:PHE:CD1	1:D:319:ALA:HB2	2.42	0.55
1:A:121:LYS:HD2	1:D:308:ILE:HD11	1.89	0.55
1:D:127:LEU:O	1:D:127:LEU:HD13	2.07	0.54
1:C:213:TYR:O	1:C:217:VAL:HG12	2.07	0.54
1:D:128:ARG:H	1:D:128:ARG:HH11	1.53	0.54
1:B:208:GLU:O	1:B:212:THR:HG23	2.07	0.54
1:C:267:GLU:HB2	1:C:271:GLY:HA3	1.88	0.54
1:A:135:SER:C	1:A:137:ARG:H	2.10	0.54
1:B:4:ARG:HG2	1:B:4:ARG:HH11	1.72	0.54
1:C:45:GLN:HE22	1:C:59:ASP:N	2.05	0.54
1:D:310:ASN:C	1:D:310:ASN:HD22	2.11	0.54
1:A:263:ILE:HD12	1:A:318:VAL:HG12	1.90	0.54
1:B:83:ASN:O	1:B:85:ASP:N	2.41	0.54
1:D:116:LEU:N	1:D:127:LEU:HD21	2.22	0.54
1:A:122:TYR:CD1	1:C:379:ASP:HB3	2.43	0.54
1:C:353:VAL:CG1	1:C:354:PRO:HD3	2.38	0.54
1:A:84:ARG:C	1:A:86:TRP:H	2.10	0.54
1:A:10:THR:H	1:D:244:GLN:HE22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:CG2	1:B:218:LYS:HE2	2.37	0.53
1:C:4:ARG:HH21	1:C:247:ARG:CD	2.21	0.53
1:B:126:ASP:HB3	1:B:129:ASN:ND2	2.24	0.53
1:A:323:ILE:CB	1:A:324:PRO:HD2	2.39	0.52
1:C:295:PHE:HA	2:C:417:HOH:O	2.09	0.52
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.74	0.52
1:B:322:PRO:HB2	1:C:279:GLY:HA2	1.91	0.52
1:C:217:VAL:HG11	1:C:224:LEU:HD11	1.90	0.52
1:D:119:GLY:N	1:D:130:ILE:HD13	2.24	0.52
1:D:206:LYS:HB3	1:D:206:LYS:NZ	2.24	0.52
1:B:175:LEU:HD11	1:B:202:PRO:HG2	1.90	0.52
1:D:217:VAL:CG1	1:D:222:GLU:HB3	2.40	0.52
1:B:277:ARG:HB3	1:B:281:GLN:HG3	1.92	0.52
1:D:128:ARG:HG2	1:D:128:ARG:HH11	1.74	0.52
1:C:231:PHE:HA	1:C:314:ILE:O	2.09	0.51
1:C:44:ARG:HD2	1:C:143:VAL:HG21	1.93	0.51
1:D:380:PHE:CZ	1:D:383:GLU:HB2	2.45	0.51
1:B:18:GLY:HA2	1:B:83:ASN:HB2	1.92	0.51
1:D:231:PHE:HA	1:D:314:ILE:O	2.11	0.51
1:B:166:SER:OG	1:C:276:ARG:NH1	2.44	0.51
1:D:68:ARG:HG2	1:D:69:PHE:CD2	2.46	0.51
1:D:217:VAL:HG11	1:D:224:LEU:HD21	1.93	0.51
1:B:277:ARG:HD3	1:B:281:GLN:HG3	1.93	0.51
1:A:216:GLU:O	1:A:220:LYS:HE2	2.11	0.51
1:B:115:ASP:O	1:B:127:LEU:HD22	2.11	0.51
1:B:324:PRO:CG	1:B:325:THR:H	2.17	0.51
1:C:310:ASN:HD22	1:C:310:ASN:C	2.14	0.51
1:B:4:ARG:HG2	1:B:4:ARG:NH1	2.26	0.51
1:A:279:GLY:HA2	1:D:322:PRO:HB2	1.93	0.51
1:D:13:GLU:HB3	1:D:132:GLU:HG2	1.91	0.50
1:C:292:LYS:HE3	1:C:295:PHE:CD1	2.46	0.50
1:A:24:GLU:OE2	1:B:244:GLN:HB2	2.11	0.50
1:B:278:PHE:HB3	1:C:222:GLU:HG3	1.92	0.50
1:C:310:ASN:ND2	1:C:312:MSE:H	2.09	0.50
1:D:73:LEU:N	1:D:73:LEU:HD12	2.25	0.50
1:B:174:GLU:HG3	1:B:203:PHE:CZ	2.47	0.50
1:A:128:ARG:O	1:A:132:GLU:HG2	2.11	0.50
1:C:170:LYS:HG2	1:C:210:PHE:CE1	2.47	0.50
1:C:176:LYS:HD2	1:C:176:LYS:O	2.11	0.50
1:A:28:ALA:O	1:A:29:ASN:HB2	2.12	0.49
1:C:353:VAL:N	1:C:354:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ILE:HD12	1:C:318:VAL:HG12	1.93	0.49
1:D:115:ASP:OD1	1:D:131:LEU:HD13	2.12	0.49
1:A:29:ASN:ND2	1:C:124:GLN:HE22	2.10	0.49
1:B:272:PHE:CD2	1:C:319:ALA:HB2	2.47	0.49
1:A:121:LYS:HD2	1:D:308:ILE:HD12	1.94	0.49
1:C:198:GLU:OE2	1:C:211:LYS:HD2	2.13	0.49
1:D:301:LEU:CD1	1:D:305:GLU:HG2	2.42	0.49
1:A:205:GLU:HG2	1:A:206:LYS:N	2.26	0.49
1:A:214:ILE:O	1:A:218:LYS:HG2	2.13	0.49
1:D:238:GLY:CA	1:D:308:ILE:HD11	2.35	0.49
1:D:323:ILE:N	1:D:323:ILE:HD12	2.28	0.49
1:C:243:ILE:HD11	1:C:247:ARG:NH1	2.28	0.48
1:A:14:SER:HA	1:A:137:ARG:HG3	1.96	0.48
1:D:66:GLY:C	1:D:73:LEU:HD13	2.34	0.48
1:B:215:ASP:HA	1:B:218:LYS:HD2	1.95	0.48
1:B:82:ARG:HD3	2:B:462:HOH:O	2.12	0.48
1:C:312:MSE:HA	1:C:312:MSE:HE2	1.95	0.48
1:A:129:ASN:HB3	1:C:73:LEU:HD22	1.95	0.48
1:C:241:SER:HA	1:C:308:ILE:HD12	1.95	0.48
1:A:247:ARG:HH11	1:A:247:ARG:CB	2.25	0.48
1:C:304:THR:HG22	2:C:430:HOH:O	2.12	0.48
1:C:24:GLU:OE1	1:D:247:ARG:CZ	2.62	0.48
1:B:4:ARG:HD2	1:B:374:GLU:OE2	2.12	0.48
1:C:197:SER:OG	1:C:201:ILE:HG12	2.13	0.48
1:B:189:SER:O	1:B:193:LYS:HG3	2.14	0.48
1:D:115:ASP:O	1:D:116:LEU:HB3	2.14	0.48
1:D:128:ARG:NH1	1:D:128:ARG:HG2	2.28	0.48
1:B:261:GLN:OE1	1:C:248:ARG:NH2	2.47	0.48
1:D:34:GLU:HG3	2:D:457:HOH:O	2.13	0.48
1:C:220:LYS:HD3	2:C:514:HOH:O	2.14	0.47
1:D:236:PRO:HG2	1:D:388:PHE:HE1	1.80	0.47
1:B:125:ARG:CB	1:B:125:ARG:HH11	2.23	0.47
1:B:228:PHE:CE2	1:B:357:SER:HA	2.49	0.47
1:B:278:PHE:O	1:B:281:GLN:HG2	2.14	0.47
1:A:186:LYS:O	1:A:189:SER:HB3	2.14	0.47
1:B:134:ALA:HB2	1:C:242:HIS:CD2	2.50	0.47
1:B:135:SER:C	1:B:137:ARG:N	2.68	0.47
1:D:247:ARG:HD3	2:D:480:HOH:O	2.14	0.47
1:D:128:ARG:HD3	1:D:128:ARG:N	2.30	0.47
1:D:310:ASN:HD21	1:D:312:MSE:HB2	1.79	0.47
1:C:139:THR:O	1:C:143:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD13	1:C:31:PRO:O	2.14	0.47
1:B:292:LYS:NZ	1:B:292:LYS:HB3	2.29	0.47
1:D:48:TYR:CD2	1:D:48:TYR:N	2.82	0.47
1:A:323:ILE:CG2	1:A:324:PRO:HD2	2.45	0.47
1:C:41:LEU:O	1:C:45:GLN:HG3	2.15	0.47
1:C:261:GLN:O	1:C:262:ALA:HB3	2.15	0.47
1:A:380:PHE:CE2	1:A:383:GLU:HB2	2.49	0.47
1:A:7:ARG:HD3	1:A:24:GLU:OE1	2.15	0.46
1:A:170:LYS:HE3	1:A:210:PHE:CE1	2.50	0.46
1:A:19:LEU:HD11	1:A:137:ARG:HD3	1.97	0.46
1:D:236:PRO:HG2	1:D:388:PHE:CE1	2.50	0.46
1:A:135:SER:C	1:A:137:ARG:N	2.69	0.46
1:C:172:VAL:HG12	1:C:174:GLU:HG2	1.96	0.46
1:B:302:GLY:O	1:B:314:ILE:HA	2.15	0.46
1:D:217:VAL:CG1	1:D:224:LEU:HD21	2.46	0.46
1:A:350:ILE:HG22	1:A:350:ILE:O	2.16	0.46
1:A:126:ASP:OD2	1:A:128:ARG:HB3	2.16	0.46
1:D:162:SER:C	1:D:200:ARG:HH22	2.20	0.46
1:B:231:PHE:HA	1:B:314:ILE:O	2.16	0.46
1:A:319:ALA:HB2	1:D:272:PHE:CD1	2.50	0.45
1:A:167:ILE:HG12	1:A:353:VAL:HG11	1.96	0.45
1:D:207:ASP:HB3	1:D:211:LYS:HZ1	1.79	0.45
1:B:261:GLN:O	1:B:262:ALA:HB3	2.16	0.45
1:A:159[A]:LYS:O	1:A:232:ALA:HA	2.16	0.45
1:A:159[B]:LYS:O	1:A:232:ALA:HA	2.16	0.45
1:D:130:ILE:HG13	1:D:131:LEU:N	2.32	0.45
1:D:216:GLU:O	1:D:219:GLU:HB3	2.16	0.45
1:B:68:ARG:NH1	1:D:129:ASN:ND2	2.62	0.45
1:B:323:ILE:HA	1:B:324:PRO:HA	1.76	0.45
1:A:84:ARG:HG2	1:A:84:ARG:NH1	2.32	0.45
1:D:115:ASP:HA	1:D:130:ILE:CD1	2.47	0.45
1:C:8:PHE:HA	1:C:22:ILE:O	2.17	0.45
1:D:188:LEU:O	1:D:192:GLU:HG2	2.16	0.45
1:A:242:HIS:HD2	1:A:308:ILE:HD11	1.82	0.45
1:D:212:THR:O	1:D:216:GLU:HB2	2.16	0.45
1:B:10:THR:H	1:C:244:GLN:HE22	1.65	0.45
1:B:8:PHE:HA	1:B:22:ILE:O	2.16	0.45
1:A:264:LYS:HE3	1:D:301:LEU:HD22	1.99	0.45
1:B:4:ARG:NH2	1:B:246:ASP:CG	2.70	0.45
1:A:261:GLN:HG3	2:D:530:HOH:O	2.16	0.44
1:C:307:GLY:C	1:C:308:ILE:HD13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:GLY:C	1:D:355:ALA:HB2	2.36	0.44
1:C:45:GLN:NE2	1:C:59:ASP:H	2.12	0.44
1:A:214:ILE:HD13	1:A:351:VAL:HG21	1.98	0.44
1:A:323:ILE:O	1:A:324:PRO:O	2.35	0.44
1:A:162:SER:C	1:A:200:ARG:HH22	2.21	0.44
1:A:197:SER:OG	1:A:201:ILE:HG12	2.17	0.44
1:A:120:ILE:HG12	1:D:398:PHE:CD2	2.52	0.44
1:D:223:SER:C	1:D:224:LEU:HD22	2.37	0.44
1:A:34:GLU:HG2	1:A:63:ILE:HG13	1.98	0.44
1:D:289:SER:OG	1:D:292:LYS:HB3	2.17	0.44
1:B:4:ARG:NE	1:B:247:ARG:HD2	2.32	0.44
1:D:137:ARG:HG2	1:D:137:ARG:HH11	1.82	0.44
1:B:68:ARG:HD3	1:D:129:ASN:HD21	1.82	0.44
1:C:267:GLU:HB2	1:C:271:GLY:CA	2.46	0.44
1:B:223:SER:OG	1:C:279:GLY:HA3	2.17	0.44
1:B:263:ILE:HD12	1:B:318:VAL:HG12	2.00	0.44
1:C:138:GLU:OE1	1:C:142:ARG:HD2	2.17	0.44
1:C:380:PHE:CZ	1:C:383:GLU:HB2	2.52	0.44
1:A:289:SER:HB2	1:A:292:LYS:HB3	1.98	0.44
1:D:260:ILE:HB	1:D:263:ILE:HG13	2.00	0.44
1:A:18:GLY:HA2	1:A:83:ASN:ND2	2.33	0.44
1:B:278:PHE:CE2	1:C:224:LEU:HD21	2.52	0.43
1:C:289:SER:OG	1:C:292:LYS:HB3	2.18	0.43
1:D:206:LYS:HZ2	1:D:206:LYS:HB3	1.83	0.43
1:B:287:GLY:O	1:B:294:TYR:HA	2.18	0.43
1:A:301:LEU:CD1	1:A:305:GLU:HG2	2.48	0.43
1:A:13:GLU:OE2	1:C:65:SER:HB2	2.18	0.43
1:A:240:GLY:O	1:D:121:LYS:HE2	2.19	0.43
1:B:2:SER:OG	1:C:246:ASP:HB2	2.18	0.43
1:C:270:LEU:HB2	1:C:274:ALA:HB2	1.99	0.43
1:A:231:PHE:HA	1:A:314:ILE:O	2.19	0.43
1:C:34:GLU:HG3	2:C:481:HOH:O	2.19	0.43
1:B:4:ARG:HH22	1:B:246:ASP:CG	2.22	0.43
1:D:45:GLN:HG3	2:D:435:HOH:O	2.19	0.43
1:D:128:ARG:O	1:D:132:GLU:HB2	2.18	0.43
1:C:82:ARG:HH12	1:C:84:ARG:HG2	1.83	0.43
1:B:84:ARG:C	1:B:86:TRP:N	2.72	0.43
1:C:164:VAL:O	1:C:202:PRO:HD3	2.19	0.43
1:A:223:SER:OG	1:D:279:GLY:HA3	2.19	0.43
1:A:56:ILE:HG23	2:A:517:HOH:O	2.18	0.43
1:B:319:ALA:HB2	1:C:272:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ASN:ND2	1:D:310:ASN:C	2.71	0.43
1:B:114:ALA:N	1:C:305:GLU:HB3	2.33	0.43
1:A:134:ALA:HB2	1:D:242:HIS:CD2	2.54	0.43
1:A:185:GLU:H	1:A:185:GLU:CD	2.22	0.42
1:B:278:PHE:HB3	1:C:222:GLU:HG2	1.99	0.42
1:A:278:PHE:HB2	1:A:281:GLN:CG	2.49	0.42
1:A:353:VAL:N	1:A:354:PRO:CD	2.82	0.42
1:B:11:ALA:CB	1:D:76:PRO:HB2	2.50	0.42
1:A:324:PRO:O	1:A:325:THR:C	2.58	0.42
1:C:142:ARG:NH2	1:C:259:SER:OG	2.53	0.42
1:A:278:PHE:HB3	1:D:222:GLU:HG3	2.00	0.42
1:B:4:ARG:HH21	1:B:246:ASP:C	2.23	0.42
1:A:260:ILE:HB	1:A:263:ILE:HG13	2.02	0.42
1:B:235:VAL:CG1	1:B:239:LEU:HD22	2.50	0.42
1:B:210:PHE:O	1:B:214:ILE:HG13	2.20	0.42
1:A:267:GLU:OE1	1:A:272:PHE:N	2.40	0.42
1:B:306:GLY:HA3	1:C:114:ALA:N	2.35	0.42
1:B:353:VAL:N	1:B:354:PRO:CD	2.83	0.42
1:D:192:GLU:HA	1:D:192:GLU:OE2	2.20	0.42
1:B:131:LEU:HD23	1:B:131:LEU:C	2.39	0.42
1:D:116:LEU:H	1:D:130:ILE:HD11	1.84	0.41
1:B:132:GLU:HG3	1:D:68:ARG:NH2	2.35	0.41
1:B:284:ASP:HB3	1:B:298:SER:O	2.20	0.41
1:B:217:VAL:HG12	1:B:222:GLU:HB2	2.02	0.41
1:B:324:PRO:CG	1:B:325:THR:N	2.80	0.41
1:C:170:LYS:HE2	1:C:209:GLU:HG2	2.03	0.41
1:D:292:LYS:HD2	1:D:295:PHE:CD2	2.55	0.41
1:C:68:ARG:HG2	1:C:69:PHE:CD2	2.55	0.41
1:C:267:GLU:OE1	1:C:271:GLY:HA3	2.20	0.41
1:C:353:VAL:HG12	1:C:354:PRO:HD3	2.01	0.41
1:D:159:LYS:HD2	2:D:415:HOH:O	2.19	0.41
1:B:392:VAL:HG12	1:B:396:LYS:HE2	2.01	0.41
1:A:213:TYR:O	1:A:216:GLU:HB3	2.20	0.41
1:A:391:TYR:O	1:A:395:VAL:HG23	2.21	0.41
1:B:240:GLY:O	1:C:121:LYS:HE2	2.21	0.41
1:D:353:VAL:N	1:D:354:PRO:CD	2.83	0.41
1:B:163:PHE:HB2	1:B:202:PRO:HG3	2.03	0.41
1:C:278:PHE:HD1	1:C:281:GLN:OE1	2.04	0.41
1:B:172:VAL:HG12	1:B:174:GLU:HG2	2.02	0.41
1:C:163:PHE:CB	1:C:202:PRO:HG3	2.50	0.41
1:D:292:LYS:O	1:D:292:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:SER:OG	1:D:201:ILE:HG12	2.20	0.41
1:C:193:LYS:HB3	1:C:204:PRO:HD3	2.02	0.41
1:A:261:GLN:O	1:A:262:ALA:HB3	2.20	0.41
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.85	0.41
1:B:64:LEU:O	1:B:65:SER:HB3	2.20	0.41
1:A:34:GLU:OE2	1:A:62:GLU:HA	2.20	0.41
1:B:363:MSE:O	1:B:367:VAL:HG23	2.21	0.40
1:B:68:ARG:HH11	1:D:129:ASN:HD21	1.62	0.40
1:C:214:ILE:O	1:C:217:VAL:HG13	2.21	0.40
1:B:388:PHE:O	1:B:392:VAL:HG23	2.20	0.40
1:A:215:ASP:O	1:A:219:GLU:HG3	2.21	0.40
1:B:255:GLN:HB2	1:C:255:GLN:HB2	2.02	0.40
1:B:230:VAL:CG1	1:B:316:VAL:HB	2.52	0.40
1:B:279:GLY:HA2	1:C:322:PRO:HB2	2.03	0.40
1:C:235:VAL:HA	1:C:236:PRO:HD3	1.89	0.40
1:B:35[A]:GLU:HG2	2:B:479:HOH:O	2.21	0.40
1:B:35[B]:GLU:HG2	2:B:479:HOH:O	2.21	0.40
1:A:8:PHE:HA	1:A:22:ILE:O	2.21	0.40
1:C:392:VAL:CG1	1:C:396:LYS:HE3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	329/401 (82%)	313 (95%)	12 (4%)	4 (1%)	16 6
1	B	330/401 (82%)	312 (94%)	13 (4%)	5 (2%)	13 3
1	C	327/401 (82%)	316 (97%)	10 (3%)	1 (0%)	46 36
1	D	329/401 (82%)	320 (97%)	8 (2%)	1 (0%)	46 36
All	All	1315/1604 (82%)	1261 (96%)	43 (3%)	11 (1%)	24 12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	PRO
1	B	84	ARG
1	B	324	PRO
1	A	292	LYS
1	B	135	SER
1	B	294	TYR
1	A	136	ALA
1	B	85	ASP
1	C	292	LYS
1	D	127	LEU
1	A	135	SER

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	274/322 (85%)	264 (96%)	10 (4%)	42	34
1	B	275/322 (85%)	265 (96%)	10 (4%)	42	34
1	C	273/322 (85%)	262 (96%)	11 (4%)	38	29
1	D	274/322 (85%)	263 (96%)	11 (4%)	38	29
All	All	1096/1288 (85%)	1054 (96%)	42 (4%)	41	31

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	137	ARG
1	A	176	LYS
1	A	224	LEU
1	A	247	ARG
1	A	250	ASP
1	A	310	ASN
1	A	323	ILE
1	A	324	PRO

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Mol	Chain	Res	Type
1	A	376	LEU
1	B	19	LEU
1	B	83	ASN
1	B	84	ARG
1	B	137	ARG
1	B	174	GLU
1	B	250	ASP
1	B	301	LEU
1	B	368	LEU
1	B	373	LEU
1	B	376	LEU
1	C	4	ARG
1	C	6	LEU
1	C	60	THR
1	C	153	LEU
1	C	165	VAL
1	C	174	GLU
1	C	176	LYS
1	C	250[A]	ASP
1	C	250[B]	ASP
1	C	310	ASN
1	C	372	LEU
1	D	35	GLU
1	D	59	ASP
1	D	84	ARG
1	D	127	LEU
1	D	128	ARG
1	D	153	LEU
1	D	175	LEU
1	D	250[A]	ASP
1	D	250[B]	ASP
1	D	310	ASN
1	D	364	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	191	HIS
1	A	242	HIS
1	A	244	GLN
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	281	GLN
1	A	297	HIS
1	A	310	ASN
1	A	393	ASN
1	A	394	HIS
1	B	15	HIS
1	B	83	ASN
1	B	169	GLN
1	B	191	HIS
1	B	244	GLN
1	B	255	GLN
1	C	45	GLN
1	C	83	ASN
1	C	244	GLN
1	C	255	GLN
1	C	299	ASN
1	C	300	ASN
1	C	310	ASN
1	D	38	ASN
1	D	124	GLN
1	D	129	ASN
1	D	244	GLN
1	D	299	ASN
1	D	300	ASN
1	D	310	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.