Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2023 – 01:03 PM EST

PDB ID	:	4RHV
Title	:	THE USE OF MOLECULAR-REPLACEMENT PHASES FOR THE REFINEMENT OF THE HUMAN RHINOVIRUS 14 STRUCTURE
Authors	:	Arnold, E.; Rossmann, M.G.
Deposited on	:	1988-01-25
Resolution	:	3.00 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
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.

The following versions of software and data (see references (1)) were used in the production of this report:

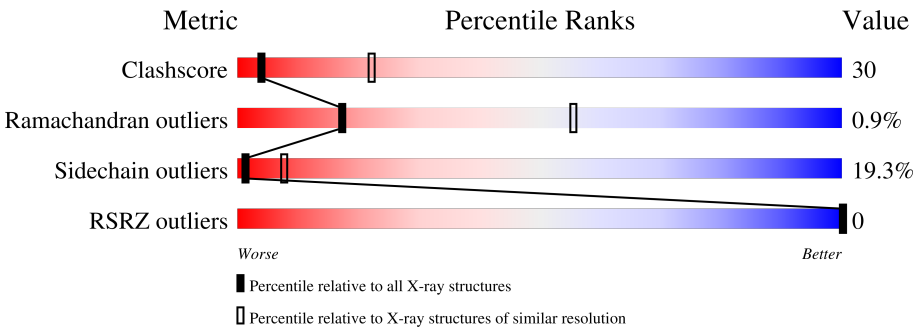
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 >=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 <=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	1	289	34% 38% 16% 6% 6%
2	2	262	45% 34% 13% 6% •
3	3	236	43% 36% 15% 6%
4	4	68	18% 21% 12% 9% 41%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6542 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 HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	273	2170	1373	375	414	8	0	0	0

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	255	1952	1238	330	372	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	conflict	UNP P03303

- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	236	1849	1184	305	353	7	0	0	0

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	40	297	186	47	62	2	0	0	0

- Molecule 5 is water.

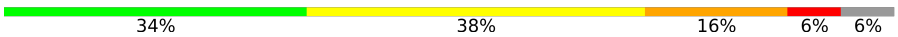
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	1	100	100	100	0	0
			Total	O		
5	2	84	84	84	0	0
			Total	O		
5	3	81	81	81	0	0
			Total	O		
5	4	9	9	9	0	0

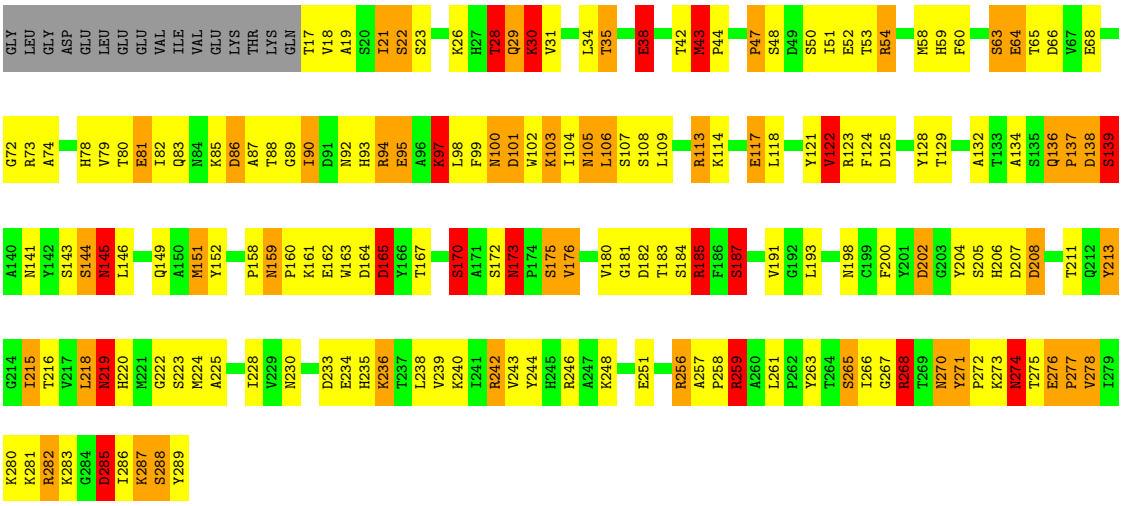
3 Residue-property plots (i)

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: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

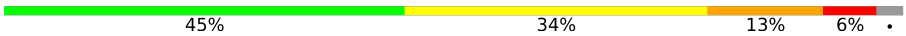
Chain 1:





• Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

Chain 2:



• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

Chain 3: 43% 36% 15% 6%

G1 T15 T16 D17 D18 R19 Q20 S21 P26 N27 Y28 E29 P30 T31 P32 R33 I34 H35 I36 P37 G38 N42 L43 L44 E45 I46 I47 D50 I53 P54 N55 N56 N57 T58 H59 T60 K61 D62 E63 V64 N65 S66 Y67 L68 N74 R75 Q76 N77 E78 Q79 V80 F81 F86

D89 G90 V91 F92 K93 T94 T95 G98 E99 T100 V101 Q102 Y103 Y104 S108 R112 F113 S114 L115 M116 Y117 T118 A121 A125 L129 A130 Y131 R137 G138 P139 Q140 D141 R142 R143 E144 A145 M146 L147 G148 T149 H150 V151 I155 G156 L157 Q158 S159 T160 I161 V162 M163

T164 I165 P166 W167 Q172 F173 R174 Y175 T176 D177 P178 D179 T180 Y181 T182 S183 F186 W190 Y191 Q192 T193 S194 L195 I196 L197 P198 P199 E200 T201 V205 L208 S209 F210 I211 S212 A213 C214 P215 D216 F217 K218 L219 R220 L221 M222 K223 D224 T225 Q226 T227 I228 S229 Q230 T231

T235 E236

- Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4)

Chain 4: 18% 21% 12% 9% 41%

GLY ALA GLN VAL SER THR GLN LYS SER GLY SER HIS GLU ASN GLN ASN ILE LEU THR ASN GLY SER ASN GLN THR PHE THR VAL I29 N30 Y31 Y32 K33 A36 S37 T38 S39 S40 A41 G42 Q43 S44 L45 S46 M47 D48 P49 S50 K51 E54 K57 D58 L59 M60 L61 K62 G63

L67 N68

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00 49.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-3.00) 55.8 (49.76-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.61Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.160 , (Not available) 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6542	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	1	1.97	44/2228 (2.0%)	2.47	137/3031 (4.5%)
2	2	1.85	32/2001 (1.6%)	2.17	78/2735 (2.9%)
3	3	1.77	21/1898 (1.1%)	2.18	75/2597 (2.9%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.89	110/6429 (1.7%)	2.29	311/8769 (3.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
2	2	0	2
All	All	0	4

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	170	SER	CB-OG	-14.28	1.23	1.42
1	1	285	ASP	CA-CB	11.80	1.79	1.53
4	4	42	GLY	N-CA	11.71	1.63	1.46
4	4	40	SER	CB-OG	10.77	1.56	1.42
2	2	256	SER	CB-OG	10.18	1.55	1.42
1	1	95	GLU	CB-CG	10.15	1.71	1.52
4	4	44	SER	CB-OG	9.91	1.55	1.42
1	1	117	GLU	CD-OE2	9.40	1.35	1.25
4	4	41	ALA	C-O	9.40	1.41	1.23
1	1	175	SER	CB-OG	-9.13	1.30	1.42
1	1	38	GLU	CB-CG	-9.05	1.34	1.52
1	1	187	SER	CB-OG	-8.87	1.30	1.42
3	3	21	SER	CA-CB	8.74	1.66	1.52
1	1	63	SER	CB-OG	-8.73	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	248	CYS	CB-SG	-8.67	1.67	1.82
3	3	57	ASN	CA-CB	8.43	1.75	1.53
2	2	40	GLU	CD-OE2	8.22	1.34	1.25
1	1	288	SER	CA-CB	8.04	1.65	1.52
2	2	52	LYS	CE-NZ	7.92	1.68	1.49
3	3	1	GLY	N-CA	7.83	1.57	1.46
3	3	63	GLU	CD-OE2	7.73	1.34	1.25
2	2	219	SER	CA-CB	-7.70	1.41	1.52
1	1	283	LYS	N-CA	7.66	1.61	1.46
1	1	105	ASN	CA-CB	7.56	1.72	1.53
2	2	136	GLU	CB-CG	7.56	1.66	1.52
3	3	108	SER	CB-OG	7.47	1.51	1.42
4	4	33	LYS	CE-NZ	7.42	1.67	1.49
1	1	282	ARG	CD-NE	7.39	1.59	1.46
1	1	234	GLU	CD-OE2	7.38	1.33	1.25
1	1	139	SER	CB-OG	7.26	1.51	1.42
2	2	152	ARG	CD-NE	7.20	1.58	1.46
1	1	187	SER	N-CA	7.16	1.60	1.46
2	2	152	ARG	CZ-NH2	7.03	1.42	1.33
2	2	194	ASN	CA-CB	6.97	1.71	1.53
4	4	46	SER	CB-OG	6.93	1.51	1.42
3	3	164	THR	C-O	6.86	1.36	1.23
4	4	51	LYS	CE-NZ	6.78	1.66	1.49
1	1	143	SER	CB-OG	6.76	1.51	1.42
3	3	61	LYS	CE-NZ	6.73	1.65	1.49
2	2	256	SER	C-O	6.68	1.36	1.23
1	1	161	LYS	CE-NZ	6.61	1.65	1.49
1	1	72	GLY	C-O	6.52	1.34	1.23
1	1	30	LYS	CE-NZ	6.48	1.65	1.49
1	1	81	GLU	CD-OE2	6.42	1.32	1.25
2	2	12	ARG	NE-CZ	6.42	1.41	1.33
2	2	8	GLY	N-CA	6.39	1.55	1.46
1	1	283	LYS	CE-NZ	6.37	1.65	1.49
1	1	52	GLU	C-O	6.34	1.35	1.23
2	2	87	LYS	CB-CG	-6.29	1.35	1.52
1	1	30	LYS	CD-CE	6.29	1.67	1.51
3	3	138	GLY	N-CA	6.26	1.55	1.46
3	3	194	SER	CB-OG	-6.19	1.34	1.42
4	4	33	LYS	CD-CE	6.11	1.66	1.51
3	3	50	ASP	CA-CB	-6.08	1.40	1.53
1	1	144	SER	N-CA	6.01	1.58	1.46
1	1	94	ARG	CD-NE	6.00	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	108	SER	CA-CB	-5.99	1.44	1.52
4	4	54	GLU	CD-OE2	5.94	1.32	1.25
3	3	99	GLU	CB-CG	-5.92	1.41	1.52
2	2	102	GLY	N-CA	5.89	1.54	1.46
1	1	105	ASN	C-O	5.87	1.34	1.23
1	1	285	ASP	N-CA	-5.79	1.34	1.46
2	2	11	ASP	CA-CB	5.69	1.66	1.53
2	2	168	ASP	C-O	5.66	1.34	1.23
1	1	175	SER	CA-CB	-5.65	1.44	1.52
4	4	37	SER	CB-OG	-5.64	1.34	1.42
3	3	172	GLN	CG-CD	-5.63	1.38	1.51
4	4	63	GLY	N-CA	5.63	1.54	1.46
1	1	97	LYS	CD-CE	5.62	1.65	1.51
2	2	187	GLN	N-CA	5.61	1.57	1.46
3	3	45	GLU	CD-OE2	5.59	1.31	1.25
2	2	235	THR	C-N	-5.58	1.23	1.34
3	3	222	MET	CG-SD	5.57	1.95	1.81
4	4	45	LEU	C-N	5.56	1.46	1.34
1	1	139	SER	CA-CB	5.56	1.61	1.52
2	2	219	SER	CB-OG	-5.49	1.35	1.42
1	1	73	ARG	C-O	5.43	1.33	1.23
2	2	236	PRO	C-O	5.43	1.34	1.23
1	1	276	GLU	CD-OE2	5.42	1.31	1.25
2	2	54	SER	CA-CB	-5.41	1.44	1.52
4	4	50	SER	CB-OG	5.40	1.49	1.42
2	2	262	GLN	CD-OE1	5.39	1.35	1.24
2	2	187	GLN	CB-CG	-5.38	1.38	1.52
1	1	267	GLY	C-O	5.36	1.32	1.23
1	1	94	ARG	NE-CZ	5.33	1.40	1.33
2	2	40	GLU	CB-CG	5.28	1.62	1.52
1	1	117	GLU	CD-OE1	-5.27	1.19	1.25
2	2	68	SER	CB-OG	-5.26	1.35	1.42
1	1	246	ARG	CZ-NH2	5.25	1.39	1.33
1	1	175	SER	N-CA	5.25	1.56	1.46
3	3	118	THR	CB-OG1	5.24	1.53	1.43
1	1	251	GLU	CA-CB	-5.24	1.42	1.53
3	3	33	ARG	CZ-NH2	5.22	1.39	1.33
2	2	120	GLY	N-CA	5.21	1.53	1.46
2	2	74	GLY	C-O	5.17	1.31	1.23
1	1	143	SER	C-O	5.16	1.33	1.23
2	2	161	GLU	CA-CB	-5.16	1.42	1.53
2	2	12	ARG	CZ-NH2	5.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	202	ASP	CA-CB	-5.12	1.42	1.53
3	3	38	GLY	CA-C	-5.12	1.43	1.51
1	1	283	LYS	CD-CE	5.11	1.64	1.51
1	1	68	GLU	CD-OE1	-5.10	1.20	1.25
1	1	26	LYS	CB-CG	-5.08	1.38	1.52
3	3	77	ASN	C-O	5.08	1.33	1.23
1	1	288	SER	C-O	5.07	1.32	1.23
2	2	58	THR	C-O	5.06	1.32	1.23
3	3	86	PHE	CA-CB	-5.04	1.42	1.53
2	2	136	GLU	CD-OE2	5.04	1.31	1.25
2	2	38	TRP	CG-CD1	5.04	1.43	1.36
3	3	30	PRO	N-CD	-5.04	1.40	1.47

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	246	ARG	NE-CZ-NH1	22.42	131.51	120.30
1	1	256	ARG	NE-CZ-NH2	20.42	130.51	120.30
1	1	123	ARG	NE-CZ-NH1	19.20	129.90	120.30
2	2	255	ARG	NE-CZ-NH2	-18.51	111.04	120.30
2	2	87	LYS	CA-CB-CG	17.64	152.21	113.40
1	1	285	ASP	CB-CG-OD2	-17.60	102.46	118.30
1	1	256	ARG	NE-CZ-NH1	-16.93	111.83	120.30
3	3	137	ARG	NE-CZ-NH1	-16.86	111.87	120.30
1	1	94	ARG	NE-CZ-NH2	-16.51	112.05	120.30
3	3	216	ASP	CB-CG-OD1	16.15	132.84	118.30
1	1	282	ARG	NE-CZ-NH2	-14.17	113.22	120.30
2	2	255	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	1	165	ASP	CB-CG-OD1	13.05	130.04	118.30
2	2	168	ASP	CB-CG-OD2	-12.82	106.76	118.30
1	1	185	ARG	NE-CZ-NH1	12.29	126.45	120.30
3	3	50	ASP	CA-CB-CG	12.24	140.33	113.40
1	1	94	ARG	CD-NE-CZ	-12.04	106.75	123.60
2	2	11	ASP	CB-CG-OD1	-11.72	107.75	118.30
2	2	194	ASN	N-CA-CB	-11.56	89.79	110.60
1	1	105	ASN	N-CA-CB	-11.54	89.84	110.60
2	2	193	THR	C-N-CA	11.38	150.15	121.70
3	3	174	ARG	NE-CZ-NH2	-11.33	114.64	120.30
1	1	170	SER	CA-CB-OG	11.12	141.21	111.20
3	3	215	PRO	C-N-CA	11.00	149.20	121.70
2	2	152	ARG	NE-CZ-NH2	-10.99	114.81	120.30
4	4	41	ALA	CA-C-N	10.88	137.96	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	48	ASP	CB-CG-OD2	-10.87	108.52	118.30
3	3	19	ARG	NE-CZ-NH2	10.79	125.69	120.30
3	3	33	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	1	285	ASP	CB-CG-OD1	10.59	127.83	118.30
1	1	285	ASP	CA-CB-CG	-10.46	90.39	113.40
3	3	50	ASP	CB-CG-OD1	10.43	127.69	118.30
2	2	151	GLU	CA-CB-CG	10.36	136.19	113.40
1	1	246	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	1	187	SER	CB-CA-C	10.07	129.24	110.10
1	1	282	ARG	CD-NE-CZ	-10.05	109.53	123.60
1	1	246	ARG	CD-NE-CZ	10.01	137.62	123.60
1	1	113	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	1	208	ASP	CB-CG-OD2	-9.83	109.45	118.30
3	3	57	ASN	N-CA-CB	-9.82	92.92	110.60
3	3	146	MET	CG-SD-CE	9.81	115.90	100.20
3	3	216	ASP	CB-CG-OD2	-9.77	109.51	118.30
2	2	88	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	1	242	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	1	54	ARG	CD-NE-CZ	-9.39	110.45	123.60
1	1	219	ASN	CB-CA-C	-9.37	91.65	110.40
1	1	105	ASN	CB-CA-C	-9.21	91.98	110.40
1	1	66	ASP	CB-CG-OD2	-9.19	110.03	118.30
3	3	57	ASN	CB-CA-C	-9.02	92.36	110.40
2	2	11	ASP	CA-CB-CG	-8.98	93.64	113.40
1	1	38	GLU	CA-CB-CG	8.88	132.93	113.40
3	3	112	ARG	NE-CZ-NH2	-8.83	115.88	120.30
3	3	137	ARG	NE-CZ-NH2	8.76	124.68	120.30
3	3	182	THR	CA-CB-CG2	8.55	124.37	112.40
1	1	165	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	1	285	ASP	N-CA-CB	-8.52	95.26	110.60
1	1	268	ARG	CD-NE-CZ	-8.46	111.76	123.60
1	1	175	SER	CB-CA-C	8.41	126.07	110.10
1	1	123	ARG	CD-NE-CZ	8.38	135.33	123.60
1	1	63	SER	CB-CA-C	-8.37	94.20	110.10
1	1	165	ASP	CB-CA-C	-8.35	93.70	110.40
2	2	250	GLU	CA-CB-CG	8.32	131.72	113.40
1	1	285	ASP	CB-CA-C	-8.29	93.81	110.40
3	3	172	GLN	CB-CG-CD	8.25	133.05	111.60
1	1	187	SER	N-CA-CB	-8.20	98.20	110.50
2	2	152	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	1	251	GLU	CA-CB-CG	8.18	131.38	113.40
4	4	45	LEU	N-CA-CB	-8.13	94.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	224	ASP	CB-CG-OD2	-8.11	111.00	118.30
2	2	255	ARG	CA-CB-CG	8.03	131.07	113.40
3	3	181	TYR	CB-CG-CD2	-8.03	116.18	121.00
2	2	11	ASP	OD1-CG-OD2	8.03	138.55	123.30
4	4	48	ASP	OD1-CG-OD2	8.02	138.54	123.30
1	1	95	GLU	OE1-CD-OE2	8.01	132.91	123.30
1	1	38	GLU	CB-CG-CD	7.99	135.78	114.20
1	1	224	MET	CA-CB-CG	7.91	126.74	113.30
4	4	47	MET	CA-CB-CG	-7.85	99.95	113.30
2	2	219	SER	CA-CB-OG	7.85	132.39	111.20
3	3	174	ARG	CD-NE-CZ	-7.84	112.62	123.60
1	1	145	ASN	OD1-CG-ND2	7.80	139.84	121.90
2	2	155	ASP	CB-CG-OD2	-7.70	111.37	118.30
3	3	21	SER	CB-CA-C	-7.69	95.50	110.10
1	1	121	TYR	CB-CG-CD1	-7.68	116.39	121.00
3	3	78	GLU	OE1-CD-OE2	7.63	132.46	123.30
2	2	187	GLN	CA-CB-CG	7.58	130.09	113.40
1	1	277	PRO	N-CD-CG	-7.54	91.88	103.20
2	2	11	ASP	C-N-CA	7.54	140.54	121.70
1	1	123	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	1	173	ASN	N-CA-CB	-7.51	97.08	110.60
2	2	170	LEU	CA-CB-CG	7.51	132.57	115.30
2	2	187	GLN	CB-CA-C	7.50	125.39	110.40
1	1	182	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	1	105	ASN	CA-CB-CG	-7.43	97.06	113.40
1	1	223	SER	N-CA-CB	-7.38	99.42	110.50
3	3	112	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	1	259	ARG	CA-CB-CG	-7.36	97.22	113.40
2	2	214	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	1	117	GLU	CG-CD-OE1	7.26	132.82	118.30
1	1	282	ARG	NH1-CZ-NH2	7.26	127.38	119.40
1	1	219	ASN	CA-CB-CG	-7.25	97.45	113.40
1	1	219	ASN	N-CA-CB	-7.22	97.60	110.60
3	3	142	ARG	CA-CB-CG	7.21	129.25	113.40
2	2	194	ASN	CA-CB-CG	-7.13	97.71	113.40
2	2	190	ASN	CA-CB-CG	7.08	128.98	113.40
2	2	168	ASP	N-CA-CB	-7.06	97.90	110.60
3	3	137	ARG	CD-NE-CZ	-7.04	113.74	123.60
1	1	185	ARG	NH1-CZ-NH2	-7.04	111.66	119.40
1	1	113	ARG	NE-CZ-NH1	7.03	123.82	120.30
3	3	121	ALA	CB-CA-C	-7.03	99.55	110.10
3	3	28	TYR	CB-CG-CD1	-7.03	116.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	256	SER	CA-C-O	-7.01	105.38	120.10
1	1	68	GLU	CG-CD-OE1	6.99	132.29	118.30
3	3	174	ARG	NH1-CZ-NH2	6.98	127.07	119.40
4	4	41	ALA	CA-C-O	-6.97	105.46	120.10
1	1	28	THR	CB-CA-C	-6.93	92.89	111.60
1	1	42	THR	CA-CB-CG2	6.90	122.06	112.40
1	1	26	LYS	CA-CB-CG	6.88	128.53	113.40
1	1	125	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	1	219	ASN	OD1-CG-ND2	6.83	137.60	121.90
2	2	136	GLU	CG-CD-OE2	-6.78	104.75	118.30
4	4	37	SER	CB-CA-C	6.77	122.96	110.10
3	3	194	SER	N-CA-CB	-6.73	100.40	110.50
3	3	163	MET	CA-CB-CG	-6.72	101.87	113.30
1	1	191	VAL	CG1-CB-CG2	6.68	121.59	110.90
2	2	146	PHE	CB-CG-CD1	-6.68	116.13	120.80
3	3	216	ASP	N-CA-CB	-6.65	98.63	110.60
2	2	103	ARG	CD-NE-CZ	-6.63	114.31	123.60
1	1	265	SER	N-CA-CB	-6.63	100.55	110.50
1	1	104	ILE	C-N-CA	6.63	138.27	121.70
3	3	57	ASN	CA-CB-CG	-6.61	98.86	113.40
3	3	45	GLU	CG-CD-OE1	6.59	131.47	118.30
2	2	87	LYS	CB-CG-CD	6.58	128.70	111.60
3	3	27	ASN	CB-CA-C	-6.57	97.26	110.40
1	1	94	ARG	NH1-CZ-NH2	6.56	126.62	119.40
1	1	276	GLU	OE1-CD-OE2	6.56	131.17	123.30
1	1	68	GLU	CG-CD-OE2	-6.55	105.20	118.30
1	1	53	THR	CA-CB-OG1	-6.53	95.30	109.00
1	1	288	SER	CB-CA-C	-6.52	97.71	110.10
2	2	203	TYR	CB-CG-CD1	6.51	124.91	121.00
4	4	45	LEU	CB-CA-C	6.49	122.53	110.20
3	3	74	ASN	CA-CB-CG	-6.49	99.13	113.40
1	1	144	SER	N-CA-CB	-6.47	100.79	110.50
1	1	22	SER	N-CA-CB	-6.46	100.80	110.50
1	1	288	SER	N-CA-CB	-6.46	100.80	110.50
3	3	183	SER	N-CA-CB	-6.45	100.82	110.50
1	1	176	VAL	CB-CA-C	-6.45	99.14	111.40
1	1	274	ASN	O-C-N	6.44	133.01	122.70
3	3	55	MET	CA-CB-CG	-6.42	102.39	113.30
2	2	168	ASP	OD1-CG-OD2	6.41	135.49	123.30
3	3	29	GLU	CB-CG-CD	6.41	131.52	114.20
1	1	138	ASP	CB-CG-OD1	6.35	124.01	118.30
1	1	106	LEU	CA-CB-CG	6.34	129.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	218	LEU	C-N-CA	6.34	137.54	121.70
2	2	97	PHE	CB-CG-CD1	-6.33	116.37	120.80
3	3	16	THR	N-CA-CB	-6.32	98.30	110.30
3	3	65	ASN	CA-CB-CG	-6.32	99.51	113.40
1	1	95	GLU	CB-CG-CD	-6.28	97.25	114.20
4	4	44	SER	CA-C-N	-6.26	103.43	117.20
2	2	38	TRP	N-CA-CB	-6.25	99.34	110.60
3	3	27	ASN	CA-CB-CG	-6.25	99.66	113.40
3	3	19	ARG	CA-CB-CG	6.24	127.13	113.40
3	3	63	GLU	CG-CD-OE2	-6.24	105.83	118.30
1	1	145	ASN	CA-CB-CG	-6.22	99.71	113.40
1	1	271	TYR	CB-CG-CD2	6.22	124.73	121.00
2	2	203	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	1	122	VAL	N-CA-CB	-6.18	97.90	111.50
2	2	136	GLU	CB-CG-CD	-6.15	97.59	114.20
2	2	69	LYS	CA-CB-CG	6.14	126.91	113.40
1	1	97	LYS	CD-CE-NZ	-6.11	97.65	111.70
1	1	117	GLU	CG-CD-OE2	-6.11	106.08	118.30
2	2	219	SER	CB-CA-C	6.10	121.69	110.10
3	3	222	MET	CG-SD-CE	-6.09	90.46	100.20
3	3	66	SER	CB-CA-C	6.07	121.63	110.10
1	1	86	ASP	CB-CG-OD2	6.06	123.75	118.30
3	3	219	LEU	CA-CB-CG	6.05	129.22	115.30
2	2	235	THR	CA-CB-CG2	-6.05	103.93	112.40
1	1	118	LEU	CA-CB-CG	6.05	129.21	115.30
1	1	164	ASP	C-N-CA	6.05	136.82	121.70
2	2	119	SER	N-CA-CB	6.05	119.57	110.50
1	1	213	TYR	CB-CG-CD1	6.04	124.62	121.00
2	2	12	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	2	67	ASP	CA-CB-CG	-6.02	100.15	113.40
2	2	103	ARG	CA-CB-CG	6.01	126.62	113.40
2	2	247	MET	CB-CA-C	6.00	122.39	110.40
4	4	48	ASP	CB-CG-OD1	-5.98	112.92	118.30
4	4	61	LEU	CB-CG-CD2	-5.98	100.84	111.00
3	3	1	GLY	N-CA-C	5.96	128.01	113.10
1	1	101	ASP	CB-CG-OD2	-5.92	112.97	118.30
3	3	58	THR	CA-CB-CG2	-5.91	104.12	112.40
1	1	35	THR	N-CA-CB	-5.89	99.11	110.30
1	1	94	ARG	CG-CD-NE	-5.89	99.43	111.80
1	1	257	ALA	N-CA-CB	-5.89	101.86	110.10
1	1	256	ARG	CD-NE-CZ	-5.88	115.37	123.60
2	2	214	ARG	NE-CZ-NH2	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	45	GLU	CG-CD-OE2	-5.87	106.55	118.30
2	2	256	SER	CA-C-N	5.86	130.10	117.20
4	4	30	ASN	CA-CB-CG	-5.86	100.50	113.40
1	1	236	LYS	CD-CE-NZ	-5.84	98.26	111.70
1	1	268	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	2	238	LEU	N-CA-CB	-5.81	98.78	110.40
2	2	31	ALA	N-CA-CB	5.81	118.23	110.10
4	4	33	LYS	CD-CE-NZ	-5.81	98.35	111.70
1	1	224	MET	CB-CA-C	5.79	121.98	110.40
3	3	27	ASN	O-C-N	5.78	131.95	122.70
1	1	233	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	2	255	ARG	CB-CG-CD	5.78	126.61	111.60
2	2	73	THR	CA-CB-OG1	-5.77	96.89	109.00
1	1	28	THR	OG1-CB-CG2	5.76	123.25	110.00
3	3	77	ASN	CA-C-N	5.75	129.85	117.20
2	2	68	SER	N-CA-CB	-5.75	101.88	110.50
1	1	274	ASN	N-CA-CB	5.74	120.92	110.60
1	1	95	GLU	CA-CB-CG	-5.72	100.82	113.40
3	3	1	GLY	O-C-N	-5.71	113.57	122.70
3	3	147	LEU	CA-CB-CG	5.71	128.43	115.30
2	2	52	LYS	CD-CE-NZ	-5.70	98.59	111.70
2	2	75	SER	N-CA-CB	-5.70	101.95	110.50
1	1	213	TYR	CA-CB-CG	5.69	124.21	113.40
2	2	161	GLU	CA-CB-CG	5.68	125.90	113.40
1	1	48	SER	CA-C-O	-5.67	108.19	120.10
1	1	246	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
3	3	177	ASP	CB-CG-OD2	-5.66	113.21	118.30
3	3	164	THR	N-CA-CB	-5.63	99.61	110.30
4	4	44	SER	O-C-N	5.62	131.70	122.70
1	1	100	ASN	N-CA-CB	-5.60	100.52	110.60
3	3	94	THR	O-C-N	5.59	131.65	122.70
2	2	210	ASP	N-CA-CB	-5.58	100.56	110.60
1	1	151	MET	CG-SD-CE	-5.56	91.30	100.20
3	3	186	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	1	202	ASP	CA-CB-CG	5.53	125.56	113.40
1	1	122	VAL	CB-CA-C	5.53	121.90	111.40
2	2	9	TYR	CB-CA-C	5.50	121.41	110.40
2	2	12	ARG	CD-NE-CZ	-5.50	115.89	123.60
4	4	44	SER	C-N-CA	-5.50	107.96	121.70
1	1	109	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	1	81	GLU	CG-CD-OE2	-5.49	107.33	118.30
1	1	233	ASP	CB-CG-OD1	5.49	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	112	ARG	CA-CB-CG	5.48	125.45	113.40
1	1	43	MET	CG-SD-CE	5.47	108.96	100.20
1	1	244	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	2	84	ASP	CB-CG-OD2	-5.47	113.38	118.30
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
1	1	26	LYS	CD-CE-NZ	-5.46	99.15	111.70
1	1	270	ASN	O-C-N	5.43	131.39	122.70
1	1	193	LEU	CA-CB-CG	5.43	127.78	115.30
3	3	60	THR	CA-CB-OG1	-5.42	97.61	109.00
2	2	174	ASN	CA-C-N	5.41	127.02	116.20
4	4	44	SER	N-CA-CB	5.40	118.60	110.50
3	3	115	LEU	CA-CB-CG	5.40	127.71	115.30
1	1	123	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
2	2	44	ASP	CA-CB-CG	5.38	125.24	113.40
3	3	161	ILE	CA-CB-CG1	-5.38	100.79	111.00
1	1	152	TYR	CB-CG-CD1	5.37	124.22	121.00
3	3	65	ASN	N-CA-CB	-5.37	100.94	110.60
3	3	231	THR	CA-CB-OG1	-5.36	97.74	109.00
1	1	202	ASP	CB-CA-C	5.35	121.11	110.40
2	2	262	GLN	CA-C-O	-5.35	108.86	120.10
2	2	169	VAL	CB-CA-C	-5.34	101.25	111.40
1	1	105	ASN	OD1-CG-ND2	5.34	134.17	121.90
3	3	42	ASN	CB-CG-OD1	-5.33	110.93	121.60
1	1	64	GLU	CA-CB-CG	5.33	125.12	113.40
1	1	205	SER	O-C-N	5.32	131.22	122.70
2	2	259	ILE	CB-CG1-CD1	-5.31	99.03	113.90
2	2	88	ASP	CA-CB-CG	-5.29	101.77	113.40
2	2	143	LYS	CD-CE-NZ	-5.26	99.59	111.70
3	3	116	MET	CB-CG-SD	-5.26	96.63	112.40
1	1	242	ARG	CD-NE-CZ	-5.25	116.25	123.60
3	3	33	ARG	CB-CG-CD	-5.25	97.96	111.60
3	3	78	GLU	CA-CB-CG	5.23	124.91	113.40
1	1	149	GLN	CB-CG-CD	5.23	125.19	111.60
1	1	128	TYR	CB-CG-CD2	5.23	124.14	121.00
2	2	38	TRP	CA-CB-CG	-5.23	103.77	113.70
3	3	74	ASN	OD1-CG-ND2	5.22	133.90	121.90
2	2	170	LEU	CB-CG-CD2	5.21	119.87	111.00
1	1	275	THR	CA-C-O	-5.21	109.17	120.10
3	3	222	MET	CB-CG-SD	-5.20	96.80	112.40
1	1	271	TYR	CB-CG-CD1	-5.20	117.88	121.00
2	2	203	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	1	275	THR	CA-C-N	5.19	128.61	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	219	SER	N-CA-CB	5.18	118.28	110.50
4	4	48	ASP	CA-CB-CG	-5.18	102.00	113.40
2	2	11	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	1	282	ARG	CG-CD-NE	-5.17	100.95	111.80
2	2	14	GLN	OE1-CD-NE2	5.17	133.78	121.90
1	1	21	ILE	CA-CB-CG1	-5.16	101.19	111.00
4	4	36	ALA	C-N-CA	-5.16	108.80	121.70
1	1	164	ASP	CB-CG-OD1	5.15	122.94	118.30
1	1	50	SER	CA-C-N	5.14	128.52	117.20
2	2	52	LYS	CA-C-N	5.14	128.51	117.20
4	4	31	TYR	CG-CD2-CE2	-5.13	117.20	121.30
2	2	14	GLN	CA-CB-CG	-5.11	102.15	113.40
4	4	58	ASP	O-C-N	5.11	130.88	122.70
1	1	141	ASN	CA-CB-CG	-5.11	102.15	113.40
2	2	203	TYR	CG-CD1-CE1	5.10	125.38	121.30
2	2	221	MET	CA-CB-CG	-5.10	104.63	113.30
1	1	162	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	1	274	ASN	CA-C-N	-5.08	106.03	117.20
2	2	18	LEU	CB-CA-C	5.07	119.84	110.20
3	3	144	GLU	CA-CB-CG	5.07	124.54	113.40
4	4	39	SER	O-C-N	5.07	130.80	122.70
3	3	175	TYR	N-CA-CB	-5.06	101.49	110.60
3	3	141	ASP	CB-CG-OD2	5.06	122.85	118.30
1	1	270	ASN	CB-CA-C	-5.05	100.29	110.40
3	3	86	PHE	CB-CA-C	5.05	120.49	110.40
1	1	282	ARG	CB-CA-C	-5.04	100.31	110.40
1	1	17	THR	CA-CB-CG2	-5.04	105.34	112.40
2	2	170	LEU	CB-CA-C	5.04	119.77	110.20
3	3	172	GLN	CG-CD-NE2	5.03	128.77	116.70
1	1	121	TYR	CB-CG-CD2	5.03	124.02	121.00
1	1	160	PRO	N-CD-CG	-5.02	95.67	103.20
3	3	146	MET	CB-CA-C	5.02	120.43	110.40
3	3	178	PRO	O-C-N	5.01	130.72	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	Sidechain

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	1	2170	0	2104	154	0
2	2	1952	0	1926	119	0
3	3	1849	0	1831	140	0
4	4	297	0	294	31	0
5	1	100	0	0	9	0
5	2	84	0	0	7	0
5	3	81	0	0	5	0
5	4	9	0	0	1	0
All	All	6542	0	6155	377	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 30.

All (377) 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)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.79	1.54
3:3:179:ASP:OD1	3:3:182:THR:HB	1.41	1.16
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP:OD2	2.00	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.06
2:2:217:ASN:HB3	5:2:274:HOH:O	1.55	1.06
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.05
2:2:12:ARG:NH1	2:2:12:ARG:HG3	1.69	1.05
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.03
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	1.02
1:1:145:ASN:HB2	5:1:336:HOH:O	1.62	0.98
3:3:57:ASN:CB	3:3:57:ASN:N	2.28	0.97
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.97
5:1:341:HOH:O	3:3:58:THR:HA	1.63	0.97
1:1:136:GLN:HE21	1:1:235:HIS:CD2	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:58:MET:HE1	3:3:216:ASP:HA	1.49	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
3:3:57:ASN:CB	3:3:57:ASN:C	2.37	0.92
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.91
1:1:285:ASP:CA	1:1:285:ASP:CG	2.37	0.91
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
2:2:12:ARG:HG3	2:2:12:ARG:HH11	1.27	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.53	0.90
1:1:92:ASN:ND2	1:1:95:GLU:HB2	1.87	0.89
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.89
1:1:285:ASP:OD2	1:1:285:ASP:HA	1.73	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.87
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.85
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.57	0.85
1:1:151:MET:CE	1:1:170:SER:HB2	2.06	0.84
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.82
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.82
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.81
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
1:1:151:MET:HE3	1:1:170:SER:HB2	1.62	0.81
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.80
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.80
1:1:107:SER:HB2	1:1:113:ARG:HD2	1.63	0.80
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.79
1:1:58:MET:HE1	3:3:216:ASP:CA	2.13	0.78
1:1:136:GLN:NE2	1:1:235:HIS:NE2	2.32	0.78
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.77
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.68	0.74
3:3:179:ASP:OD1	3:3:182:THR:CB	2.31	0.74
1:1:204:TYR:CE2	1:1:213:TYR:HB2	2.21	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
3:3:236:GLU:OE1	5:3:268:HOH:O	2.06	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
2:2:9:TYR:HA	5:2:315:HOH:O	1.88	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.73
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.73
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.72
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.71
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.71
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.71
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.70
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.70
1:1:97:LYS:HE3	5:1:352:HOH:O	1.90	0.70
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.70
2:2:195:ASN:OD1	2:2:196:THR:HG23	1.92	0.69
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.69
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.69
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.68
4:4:29:ILE:HG22	4:4:29:ILE:O	1.94	0.68
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.67
3:3:61:LYS:HD3	3:3:63:GLU:OE1	1.95	0.67
1:1:278:VAL:HG12	3:3:62:ASP:OD1	1.95	0.67
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.67
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.66
1:1:151:MET:CE	1:1:173:ASN:HD22	2.08	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
1:1:204:TYR:HE2	1:1:213:TYR:HB2	1.61	0.65
1:1:151:MET:HE1	1:1:173:ASN:ND2	2.12	0.65
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
1:1:107:SER:HB2	1:1:113:ARG:CD	2.26	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.64
3:3:200:GLU:CG	5:3:258:HOH:O	2.46	0.64
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.63
2:2:155:ASP:OD2	2:2:155:ASP:C	2.37	0.62
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
1:1:151:MET:HA	1:1:175:SER:HB2	1.82	0.61
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
1:1:187:SER:HB3	3:3:21:SER:CB	2.31	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
3:3:55:MET:HG3	3:3:55:MET:O	1.99	0.61
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.61
1:1:151:MET:HE2	1:1:173:ASN:HB3	1.84	0.60
3:3:175:TYR:H	3:3:182:THR:HG21	1.66	0.60
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
3:3:200:GLU:HG2	5:3:258:HOH:O	2.00	0.60
1:1:103:LYS:HG3	1:1:103:LYS:O	2.00	0.60
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.59
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.59
1:1:58:MET:HE1	3:3:216:ASP:C	2.23	0.59
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.59
1:1:94:ARG:NH1	1:1:94:ARG:CG	2.60	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE2	2.38	0.59
1:1:281:LYS:HE3	5:1:341:HOH:O	2.03	0.58
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.58
2:2:192:ARG:NH2	5:2:278:HOH:O	2.17	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:87:ALA:HB2	1:1:98:LEU:HD11	1.86	0.58
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.57
2:2:64:TYR:CD2	2:2:89:MET:HB3	2.39	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57
1:1:159:ASN:ND2	5:1:362:HOH:O	2.38	0.57
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
3:3:179:ASP:OD1	3:3:182:THR:CG2	2.53	0.57
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
3:3:175:TYR:H	3:3:182:THR:CG2	2.19	0.56
1:1:82:ILE:HG22	1:1:100:ASN:HB2	1.86	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
1:1:136:GLN:NE2	1:1:235:HIS:CD2	2.64	0.56
1:1:117:GLU:HB3	1:1:200:PHE:HZ	1.70	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
2:2:192:ARG:NH1	5:2:294:HOH:O	2.02	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.56
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.55
1:1:38:GLU:CD	3:3:116:MET:HE1	2.27	0.55
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.55
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.55
1:1:151:MET:CE	1:1:173:ASN:ND2	2.68	0.55
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.55
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.55
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
1:1:107:SER:CB	1:1:113:ARG:HD2	2.36	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
1:1:151:MET:HE2	1:1:170:SER:HB2	1.89	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.54
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:117:TYR:CD2	3:3:155:ILE:HD13	2.44	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
2:2:158:SER:HG	2:2:167:LYS:HE2	1.69	0.53
2:2:192:ARG:HD3	5:2:294:HOH:O	2.08	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
3:3:18:ASP:OD1	4:4:40:SER:HB2	2.09	0.53
1:1:220:HIS:CE1	1:1:222:GLY:H	2.27	0.53
1:1:108:SER:HB2	1:1:266:ILE:HD11	1.90	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.52
3:3:57:ASN:HB3	3:3:57:ASN:C	2.28	0.52
1:1:88:THR:O	1:1:90:ILE:HD13	2.10	0.52
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:151:MET:HE2	1:1:173:ASN:HD22	1.75	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:187:SER:HB3	3:3:21:SER:HB2	1.92	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
1:1:216:THR:O	1:1:219:ASN:HB2	2.10	0.52
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE1	2.41	0.51
1:1:43:MET:HE3	1:1:43:MET:HA	1.92	0.51
1:1:117:GLU:HB3	1:1:200:PHE:CZ	2.46	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
1:1:87:ALA:CB	1:1:98:LEU:HD11	2.41	0.51
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.51
3:3:174:ARG:NH2	5:3:315:HOH:O	2.43	0.50
3:3:182:THR:CG2	5:3:257:HOH:O	2.60	0.50
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.50
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.50
1:1:58:MET:CE	3:3:216:ASP:O	2.60	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE1	2.44	0.50
1:1:58:MET:HE1	3:3:216:ASP:O	2.12	0.50
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.50
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.94	0.49
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.49
2:2:158:SER:HG	2:2:167:LYS:CE	2.24	0.48
2:2:217:ASN:ND2	5:2:268:HOH:O	2.45	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
1:1:99:PHE:C	1:1:99:PHE:CD2	2.86	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD2	2.13	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.28	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.47
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47
4:4:29:ILE:O	4:4:29:ILE:CG2	2.62	0.47
4:4:45:LEU:N	5:4:71:HOH:O	2.40	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.14	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.47
2:2:63:PHE:CD2	2:2:245:ALA:HB2	2.50	0.47
4:4:44:SER:C	4:4:46:SER:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:ASN:CB	5:1:336:HOH:O	2.36	0.47
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.47
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.43	0.46
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.62	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.46
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.97	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.81	0.45
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.45
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.44
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.44
1:1:198:ASN:HB3	1:1:200:PHE:O	2.17	0.44
1:1:207:ASP:HA	2:2:144:TYR:CE1	2.52	0.44
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.17	0.44
1:1:101:ASP:HA	1:1:225:ALA:HA	1.98	0.44
1:1:289:TYR:CE1	3:3:138:GLY:HA3	2.53	0.44
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.99	0.44
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
1:1:289:TYR:CD1	3:3:138:GLY:HA3	2.53	0.44
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.43
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
2:2:10:SER:CB	2:2:12:ARG:HB2	2.48	0.43
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.43
1:1:102:TRP:CZ3	1:1:243:VAL:HG11	2.53	0.42
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.42
1:1:137:PRO:HD2	5:1:348:HOH:O	2.19	0.42
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.99	0.42
1:1:206:HIS:HB2	5:1:339:HOH:O	2.18	0.42
1:1:216:THR:CG2	1:1:218:LEU:HB2	2.50	0.42
1:1:187:SER:HB3	3:3:21:SER:HB3	2.01	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.42
3:3:174:ARG:HD2	3:3:182:THR:O	2.19	0.42
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	0.42
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.42
1:1:107:SER:CA	1:1:113:ARG:HD2	2.49	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD1	2.55	0.41
1:1:286:ILE:HD13	1:1:286:ILE:HG21	1.77	0.41
5:1:356:HOH:O	4:4:44:SER:HB2	2.19	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
3:3:113:PHE:CE1	3:3:115:LEU:HD13	2.55	0.41
1:1:86:ASP:OD2	1:1:88:THR:HB	2.21	0.41
2:2:187:GLN:HE21	2:2:187:GLN:HB2	1.57	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.91	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.02	0.41
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:38:GLU:CD	3:3:116:MET:CE	2.88	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
3:3:64:VAL:HG12	3:3:64:VAL:O	2.21	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
3:3:157:LEU:HD23	3:3:157:LEU:O	2.21	0.41
1:1:215:ILE:HG21	1:1:215:ILE:HD12	1.84	0.40
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
2:2:195:ASN:OD1	2:2:195:ASN:C	2.59	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40
2:2:168:ASP:HB3	5:2:329:HOH:O	2.20	0.40
3:3:101:VAL:HG13	3:3:176:THR:HB	2.04	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	1	271/289 (94%)	254 (94%)	15 (6%)	2 (1%)	22	60
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	19	57
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	17	55
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	5	27
All	All	796/855 (93%)	738 (93%)	51 (6%)	7 (1%)	17	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
1	1	165	ASP
2	2	255	ARG
2	2	257	LYS
4	4	47	MET

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	1	239/253 (94%)	195 (82%)	44 (18%)	1	9
2	2	223/229 (97%)	181 (81%)	42 (19%)	1	8
3	3	209/209 (100%)	172 (82%)	37 (18%)	2	9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	568 (81%)	136 (19%)	1	8

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL

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Mol	Chain	Res	Type
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	28	THR
1	1	29	GLN
1	1	30	LYS
1	1	38	GLU
1	1	43	MET
1	1	47	PRO
1	1	63	SER
1	1	81	GLU
1	1	90	ILE
1	1	97	LYS
1	1	103	LYS
1	1	105	ASN
1	1	106	LEU
1	1	122	VAL
1	1	136	GLN
1	1	137	PRO
1	1	138	ASP
1	1	139	SER
1	1	144	SER
1	1	145	ASN
1	1	159	ASN
1	1	165	ASP
1	1	170	SER
1	1	172	SER
1	1	173	ASN
1	1	176	VAL
1	1	183	THR
1	1	184	SER
1	1	185	ARG
1	1	187	SER
1	1	202	ASP
1	1	215	ILE
1	1	219	ASN
1	1	240	LYS
1	1	256	ARG
1	1	268	ARG
1	1	274	ASN
1	1	278	VAL
1	1	285	ASP

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Mol	Chain	Res	Type
1	1	287	LYS
2	2	11	ASP
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	49	ASP
2	2	52	LYS
2	2	66	LEU
2	2	69	LYS
2	2	73	THR
2	2	76	LYS
2	2	81	LYS
2	2	87	LYS
2	2	88	ASP
2	2	103	ARG
2	2	116	LYS
2	2	119	SER
2	2	136	GLU
2	2	141	SER
2	2	145	THR
2	2	152	ARG
2	2	165	PRO
2	2	168	ASP
2	2	169	VAL
2	2	170	LEU
2	2	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	209	ILE
2	2	211	SER
2	2	217	ASN
2	2	221	MET
2	2	225	ILE
2	2	232	THR
2	2	236	PRO
2	2	238	LEU
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG
2	2	256	SER

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Mol	Chain	Res	Type
2	2	262	GLN
3	3	16	THR
3	3	33	ARG
3	3	46	ILE
3	3	55	MET
3	3	60	THR
3	3	61	LYS
3	3	65	ASN
3	3	91	VAL
3	3	94	THR
3	3	101	VAL
3	3	112	ARG
3	3	114	SER
3	3	115	LEU
3	3	137	ARG
3	3	146	MET
3	3	157	LEU
3	3	158	GLN
3	3	159	SER
3	3	164	THR
3	3	172	GLN
3	3	174	ARG
3	3	179	ASP
3	3	182	THR
3	3	192	GLN
3	3	194	SER
3	3	196	ILE
3	3	201	THR
3	3	208	LEU
3	3	211	ILE
3	3	217	PHE
3	3	218	LYS
3	3	219	LEU
3	3	220	ARG
3	3	223	LYS
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE
4	4	33	LYS
4	4	40	SER
4	4	43	GLN

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Mol	Chain	Res	Type
4	4	45	LEU
4	4	46	SER
4	4	47	MET
4	4	50	SER
4	4	51	LYS
4	4	59	LEU
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	136	GLN
1	1	159	ASN
1	1	173	ASN
1	1	219	ASN
2	2	20	ASN
2	2	174	ASN
2	2	217	ASN
2	2	262	GLN
3	3	41	HIS
3	3	102	GLN
3	3	140	GLN
3	3	172	GLN
3	3	192	GLN
3	3	226	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	1	273/289 (94%)	-0.83	0	100	100	8, 14, 30, 42	0
2	2	255/262 (97%)	-0.82	0	100	100	7, 12, 24, 42	0
3	3	236/236 (100%)	-0.88	0	100	100	8, 12, 23, 31	0
4	4	40/68 (58%)	-0.51	0	100	100	13, 24, 37, 38	0
All	All	804/855 (94%)	-0.82	0	100	100	7, 13, 28, 42	0

There are no RSRZ outliers to report.

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.