Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:42 AM GMT

PDB ID	:	2RR1
Title	:	STRUCTURAL ANALYSIS OF ANTIVIRAL AGENTS THAT INTERACT WITH THE CAPSID OF HUMAN RHINOVIRUSES
Authors	:	Badger, J.; Smith, T.J.; Rossmann, M.G.
Deposited on	:	1988-10-03
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

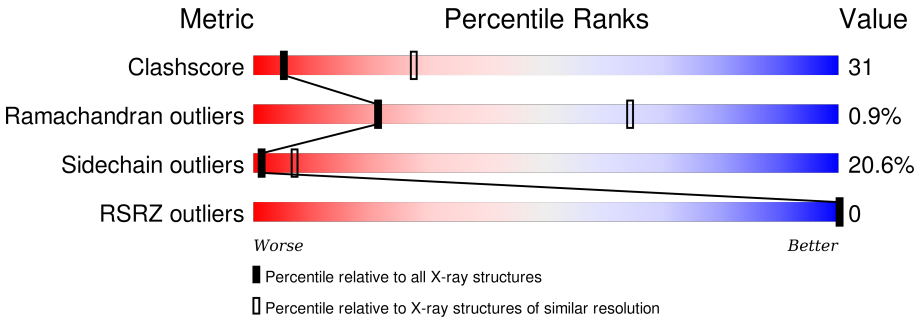
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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.

Mol	Chain	Length	Quality of chain
1	1	289	37% 36% 16% 6% 6%
2	2	262	42% 36% 13% 6% •
3	3	236	42% 37% 16% 5%
4	4	68	18% 16% 16% 9% 41%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6301 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
1	1	273	Total	C	N	O	S	0	0	0
			2170	1373	375	414	8			

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

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

There is a discrepancy between the modelled and reference sequences:

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

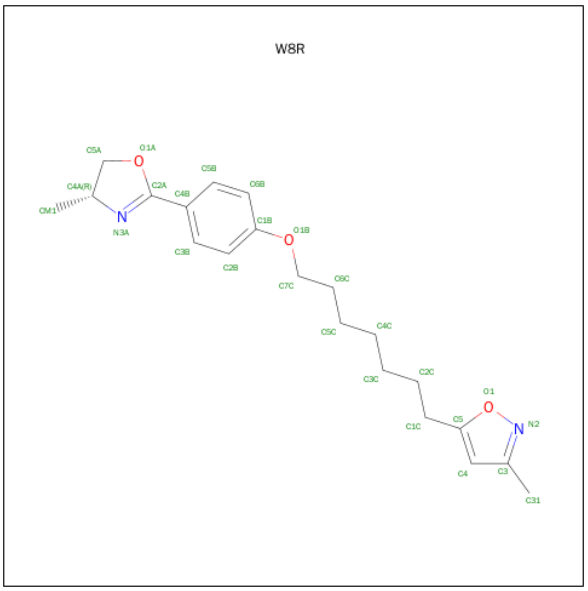
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

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

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

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

- Molecule 5 is 5-(7-(5-HYDRO-4-METHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (three-letter code: W8R) (formula: $C_{21}H_{28}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1	1	Total C N O 26 21 2 3	0	0

- Molecule 6 is water.

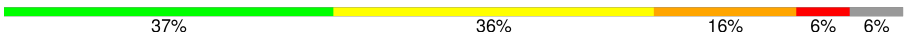
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	6	Total O 6 6	0	0
6	2	1	Total O 1 1	0	0

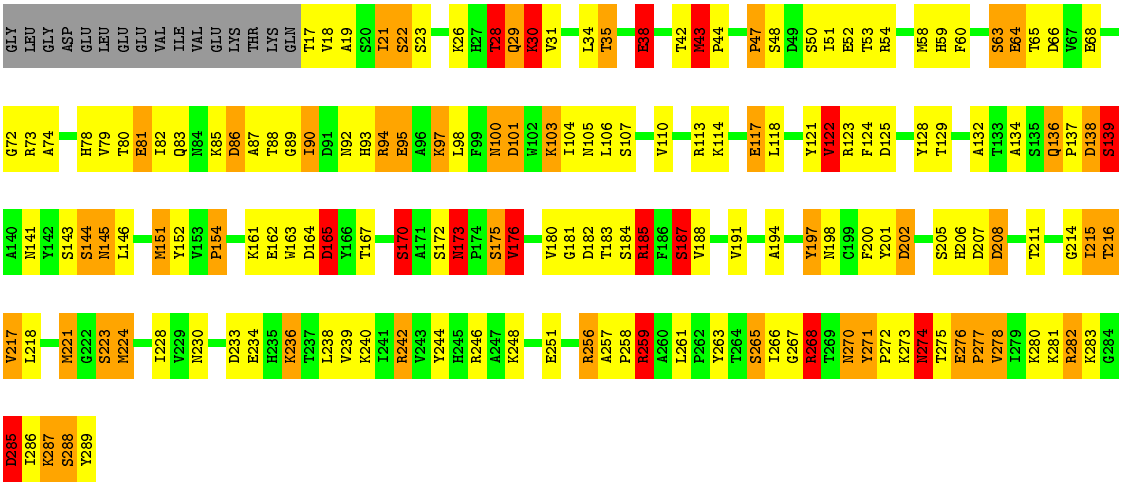
3 Residue-property plots (i)

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.

- Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

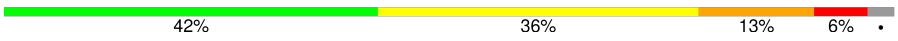
Chain 1:

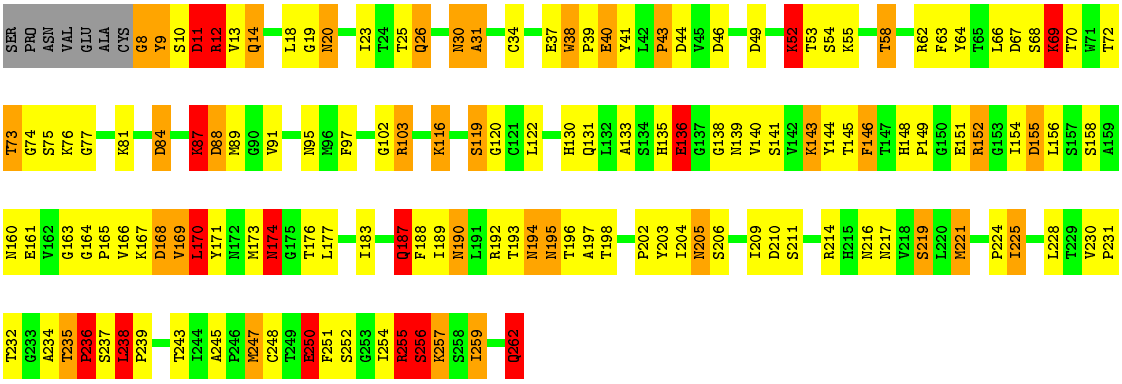




- Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

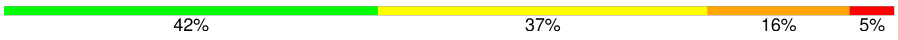
Chain 2:

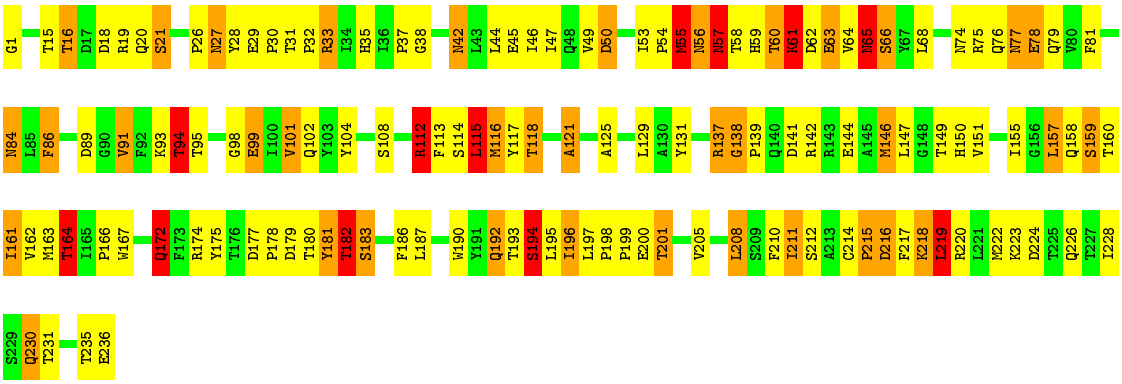




- Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

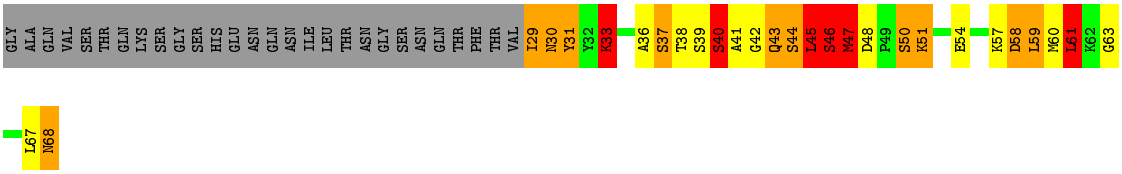
Chain 3:





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

Chain 4:



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)	(Not available) – 3.00 49.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 27.1 (49.46-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.81 (at 3.01Å)	Xtriage
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	(Not available) , (Not available) 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.0	EDS
Estimated twinning fraction	0.079 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 156662 reflections	Xtriage
F_o,F_c correlation	0.09	EDS
Total number of atoms	6301	wwPDB-VP
Average B, all atoms (Å^2)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W8R

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	1.86	39/2228 (1.8%)	2.37	120/3031 (4.0%)
2	2	1.85	32/2001 (1.6%)	2.17	78/2735 (2.9%)
3	3	1.77	21/1898 (1.1%)	2.16	70/2597 (2.7%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.85	105/6429 (1.6%)	2.25	289/8769 (3.3%)

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 (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	170	SER	CB-OG	-14.31	1.23	1.42
1	1	285	ASP	CA-CB	11.82	1.79	1.53
4	4	42	GLY	N-CA	11.70	1.63	1.46
4	4	40	SER	CB-OG	10.74	1.56	1.42
2	2	256	SER	CB-OG	10.20	1.55	1.42
1	1	95	GLU	CB-CG	10.13	1.71	1.52
4	4	44	SER	CB-OG	9.94	1.55	1.42
4	4	41	ALA	C-O	9.37	1.41	1.23
1	1	117	GLU	CD-OE2	9.36	1.35	1.25
1	1	38	GLU	CB-CG	-9.07	1.34	1.52
1	1	187	SER	CB-OG	-8.87	1.30	1.42
1	1	63	SER	CB-OG	-8.78	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	21	SER	CA-CB	8.71	1.66	1.52
2	2	248	CYS	CB-SG	-8.67	1.67	1.82
3	3	57	ASN	CA-CB	8.44	1.75	1.53
2	2	40	GLU	CD-OE2	8.22	1.34	1.25
1	1	288	SER	CA-CB	8.05	1.65	1.52
2	2	52	LYS	CE-NZ	7.91	1.68	1.49
3	3	1	GLY	N-CA	7.85	1.57	1.46
2	2	219	SER	CA-CB	-7.69	1.41	1.52
3	3	63	GLU	CD-OE2	7.69	1.34	1.25
1	1	283	LYS	N-CA	7.66	1.61	1.46
2	2	136	GLU	CB-CG	7.53	1.66	1.52
3	3	108	SER	CB-OG	7.45	1.51	1.42
4	4	33	LYS	CE-NZ	7.42	1.67	1.49
1	1	234	GLU	CD-OE2	7.38	1.33	1.25
1	1	282	ARG	CD-NE	7.35	1.58	1.46
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	7.04	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	6.89	1.36	1.23
4	4	51	LYS	CE-NZ	6.78	1.66	1.49
1	1	143	SER	CB-OG	6.75	1.51	1.42
3	3	61	LYS	CE-NZ	6.70	1.65	1.49
2	2	256	SER	C-O	6.69	1.36	1.23
1	1	72	GLY	C-O	6.55	1.34	1.23
1	1	30	LYS	CE-NZ	6.49	1.65	1.49
1	1	81	GLU	CD-OE2	6.42	1.32	1.25
2	2	8	GLY	N-CA	6.41	1.55	1.46
2	2	12	ARG	NE-CZ	6.37	1.41	1.33
1	1	283	LYS	CE-NZ	6.36	1.65	1.49
1	1	52	GLU	C-O	6.32	1.35	1.23
3	3	138	GLY	N-CA	6.32	1.55	1.46
2	2	87	LYS	CB-CG	-6.31	1.35	1.52
1	1	30	LYS	CD-CE	6.28	1.67	1.51
3	3	194	SER	CB-OG	-6.26	1.34	1.42
4	4	33	LYS	CD-CE	6.12	1.66	1.51
3	3	50	ASP	CA-CB	-6.08	1.40	1.53
1	1	144	SER	N-CA	6.03	1.58	1.46
1	1	94	ARG	CD-NE	6.02	1.56	1.46
3	3	108	SER	CA-CB	-6.02	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	54	GLU	CD-OE2	5.97	1.32	1.25
2	2	102	GLY	N-CA	5.93	1.54	1.46
3	3	99	GLU	CB-CG	-5.90	1.41	1.52
1	1	285	ASP	N-CA	-5.83	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
4	4	37	SER	CB-OG	-5.64	1.34	1.42
3	3	45	GLU	CD-OE2	5.64	1.31	1.25
3	3	172	GLN	CG-CD	-5.62	1.38	1.51
2	2	235	THR	C-N	-5.62	1.23	1.34
1	1	97	LYS	CD-CE	5.60	1.65	1.51
4	4	63	GLY	N-CA	5.60	1.54	1.46
2	2	187	GLN	N-CA	5.59	1.57	1.46
3	3	222	MET	CG-SD	5.56	1.95	1.81
1	1	139	SER	CA-CB	5.56	1.61	1.52
4	4	45	LEU	C-N	5.54	1.46	1.34
2	2	219	SER	CB-OG	-5.49	1.35	1.42
2	2	236	PRO	C-O	5.43	1.34	1.23
1	1	276	GLU	CD-OE2	5.41	1.31	1.25
2	2	262	GLN	CD-OE1	5.41	1.35	1.24
2	2	187	GLN	CB-CG	-5.38	1.38	1.52
1	1	73	ARG	C-O	5.38	1.33	1.23
2	2	54	SER	CA-CB	-5.37	1.44	1.52
4	4	50	SER	CB-OG	5.37	1.49	1.42
1	1	267	GLY	C-O	5.36	1.32	1.23
1	1	94	ARG	NE-CZ	5.31	1.40	1.33
2	2	40	GLU	CB-CG	5.29	1.62	1.52
1	1	246	ARG	CZ-NH2	5.28	1.40	1.33
1	1	251	GLU	CA-CB	-5.26	1.42	1.53
3	3	118	THR	CB-OG1	5.25	1.53	1.43
2	2	68	SER	CB-OG	-5.23	1.35	1.42
3	3	33	ARG	CZ-NH2	5.22	1.39	1.33
2	2	120	GLY	N-CA	5.21	1.53	1.46
1	1	117	GLU	CD-OE1	-5.20	1.20	1.25
2	2	161	GLU	CA-CB	-5.17	1.42	1.53
2	2	74	GLY	C-O	5.17	1.31	1.23
2	2	12	ARG	CZ-NH2	5.13	1.39	1.33
1	1	143	SER	C-O	5.12	1.33	1.23
1	1	68	GLU	CD-OE1	-5.12	1.20	1.25
1	1	283	LYS	CD-CE	5.11	1.64	1.51
3	3	38	GLY	CA-C	-5.11	1.43	1.51
3	3	77	ASN	C-O	5.09	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	136	GLU	CD-OE2	5.09	1.31	1.25
1	1	26	LYS	CB-CG	-5.08	1.38	1.52
1	1	154	PRO	CA-C	-5.08	1.42	1.52
1	1	202	ASP	CA-CB	-5.08	1.42	1.53
2	2	38	TRP	CG-CD1	5.05	1.43	1.36
2	2	58	THR	C-O	5.05	1.32	1.23
3	3	86	PHE	CA-CB	-5.04	1.42	1.53
1	1	288	SER	C-O	5.04	1.32	1.23
3	3	30	PRO	N-CD	-5.02	1.40	1.47

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	246	ARG	NE-CZ-NH1	22.45	131.52	120.30
1	1	256	ARG	NE-CZ-NH2	20.38	130.49	120.30
1	1	123	ARG	NE-CZ-NH1	19.14	129.87	120.30
2	2	255	ARG	NE-CZ-NH2	-18.62	110.99	120.30
2	2	87	LYS	CA-CB-CG	17.62	152.17	113.40
1	1	285	ASP	CB-CG-OD2	-17.61	102.45	118.30
3	3	137	ARG	NE-CZ-NH1	-16.95	111.83	120.30
1	1	256	ARG	NE-CZ-NH1	-16.89	111.86	120.30
1	1	94	ARG	NE-CZ-NH2	-16.57	112.01	120.30
3	3	216	ASP	CB-CG-OD1	16.11	132.80	118.30
1	1	282	ARG	NE-CZ-NH2	-14.11	113.25	120.30
2	2	255	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	1	165	ASP	CB-CG-OD1	13.06	130.05	118.30
1	1	197	TYR	N-CA-CB	-12.94	87.31	110.60
2	2	168	ASP	CB-CG-OD2	-12.82	106.76	118.30
1	1	185	ARG	NE-CZ-NH1	12.34	126.47	120.30
3	3	50	ASP	CA-CB-CG	12.24	140.32	113.40
1	1	94	ARG	CD-NE-CZ	-12.06	106.72	123.60
1	1	197	TYR	CA-CB-CG	11.85	135.91	113.40
2	2	11	ASP	CB-CG-OD1	-11.72	107.75	118.30
2	2	194	ASN	N-CA-CB	-11.55	89.81	110.60
2	2	193	THR	C-N-CA	11.38	150.16	121.70
1	1	170	SER	CA-CB-OG	11.12	141.22	111.20
3	3	215	PRO	C-N-CA	11.00	149.19	121.70
2	2	152	ARG	NE-CZ-NH2	-11.00	114.80	120.30
4	4	41	ALA	CA-C-N	10.88	137.96	116.20
4	4	48	ASP	CB-CG-OD2	-10.86	108.52	118.30
3	3	19	ARG	NE-CZ-NH2	10.82	125.71	120.30
3	3	33	ARG	NE-CZ-NH2	-10.66	114.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	285	ASP	CB-CG-OD1	10.59	127.83	118.30
1	1	285	ASP	CA-CB-CG	-10.46	90.38	113.40
3	3	50	ASP	CB-CG-OD1	10.43	127.68	118.30
2	2	151	GLU	CA-CB-CG	10.39	136.26	113.40
1	1	187	SER	CB-CA-C	10.07	129.24	110.10
1	1	246	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	1	246	ARG	CD-NE-CZ	10.03	137.65	123.60
1	1	282	ARG	CD-NE-CZ	-10.03	109.56	123.60
1	1	208	ASP	CB-CG-OD2	-9.86	109.43	118.30
3	3	57	ASN	N-CA-CB	-9.83	92.91	110.60
3	3	146	MET	CG-SD-CE	9.80	115.88	100.20
3	3	216	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	1	113	ARG	NE-CZ-NH2	-9.71	115.44	120.30
2	2	88	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	1	242	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	1	54	ARG	CD-NE-CZ	-9.38	110.48	123.60
1	1	66	ASP	CB-CG-OD2	-9.17	110.05	118.30
3	3	57	ASN	CB-CA-C	-9.04	92.32	110.40
2	2	11	ASP	CA-CB-CG	-8.99	93.62	113.40
1	1	38	GLU	CA-CB-CG	8.89	132.97	113.40
3	3	137	ARG	NE-CZ-NH2	8.88	124.74	120.30
3	3	112	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	1	165	ASP	CB-CG-OD2	-8.57	110.59	118.30
3	3	182	THR	CA-CB-CG2	8.56	124.39	112.40
1	1	285	ASP	N-CA-CB	-8.52	95.27	110.60
1	1	268	ARG	CD-NE-CZ	-8.44	111.78	123.60
1	1	123	ARG	CD-NE-CZ	8.38	135.34	123.60
1	1	63	SER	CB-CA-C	-8.36	94.22	110.10
1	1	165	ASP	CB-CA-C	-8.34	93.72	110.40
2	2	250	GLU	CA-CB-CG	8.33	131.73	113.40
1	1	285	ASP	CB-CA-C	-8.31	93.79	110.40
3	3	172	GLN	CB-CG-CD	8.23	133.01	111.60
1	1	187	SER	N-CA-CB	-8.19	98.21	110.50
1	1	251	GLU	CA-CB-CG	8.19	131.41	113.40
2	2	152	ARG	NE-CZ-NH1	8.17	124.39	120.30
4	4	45	LEU	N-CA-CB	-8.16	94.08	110.40
3	3	224	ASP	CB-CG-OD2	-8.09	111.02	118.30
2	2	255	ARG	CA-CB-CG	8.04	131.08	113.40
2	2	11	ASP	OD1-CG-OD2	8.02	138.54	123.30
4	4	48	ASP	OD1-CG-OD2	8.02	138.53	123.30
3	3	181	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	1	38	GLU	CB-CG-CD	7.98	135.74	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	95	GLU	OE1-CD-OE2	7.98	132.87	123.30
2	2	219	SER	CA-CB-OG	7.83	132.35	111.20
4	4	47	MET	CA-CB-CG	-7.83	99.99	113.30
1	1	145	ASN	OD1-CG-ND2	7.79	139.83	121.90
3	3	21	SER	CB-CA-C	-7.68	95.50	110.10
1	1	121	TYR	CB-CG-CD1	-7.67	116.39	121.00
2	2	155	ASP	CB-CG-OD2	-7.64	111.43	118.30
2	2	187	GLN	CA-CB-CG	7.59	130.09	113.40
3	3	78	GLU	OE1-CD-OE2	7.58	132.40	123.30
2	2	11	ASP	C-N-CA	7.54	140.56	121.70
1	1	277	PRO	N-CD-CG	-7.54	91.90	103.20
1	1	173	ASN	N-CA-CB	-7.52	97.06	110.60
2	2	170	LEU	CA-CB-CG	7.51	132.57	115.30
2	2	187	GLN	CB-CA-C	7.49	125.39	110.40
1	1	123	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	1	182	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	1	259	ARG	CA-CB-CG	-7.35	97.23	113.40
2	2	214	ARG	NE-CZ-NH1	7.33	123.96	120.30
3	3	112	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	1	282	ARG	NH1-CZ-NH2	7.27	127.39	119.40
1	1	117	GLU	CG-CD-OE1	7.25	132.80	118.30
3	3	142	ARG	CA-CB-CG	7.21	129.27	113.40
2	2	194	ASN	CA-CB-CG	-7.15	97.68	113.40
2	2	190	ASN	CA-CB-CG	7.09	129.00	113.40
1	1	185	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
1	1	197	TYR	CB-CA-C	7.05	124.51	110.40
2	2	168	ASP	N-CA-CB	-7.03	97.95	110.60
3	3	121	ALA	CB-CA-C	-7.02	99.56	110.10
3	3	137	ARG	CD-NE-CZ	-7.02	113.78	123.60
2	2	256	SER	CA-C-O	-7.01	105.38	120.10
1	1	68	GLU	CG-CD-OE1	7.00	132.29	118.30
3	3	28	TYR	CB-CG-CD1	-6.99	116.81	121.00
4	4	41	ALA	CA-C-O	-6.97	105.47	120.10
1	1	113	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	1	28	THR	CB-CA-C	-6.91	92.95	111.60
1	1	42	THR	CA-CB-CG2	6.91	122.07	112.40
1	1	125	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	1	26	LYS	CA-CB-CG	6.86	128.50	113.40
2	2	136	GLU	CG-CD-OE2	-6.78	104.74	118.30
4	4	37	SER	CB-CA-C	6.76	122.95	110.10
3	3	194	SER	N-CA-CB	-6.75	100.38	110.50
3	3	163	MET	CA-CB-CG	-6.73	101.87	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	216	ASP	N-CA-CB	-6.67	98.60	110.60
2	2	103	ARG	CD-NE-CZ	-6.64	114.31	123.60
2	2	146	PHE	CB-CG-CD1	-6.63	116.16	120.80
1	1	265	SER	N-CA-CB	-6.63	100.56	110.50
3	3	57	ASN	CA-CB-CG	-6.63	98.82	113.40
3	3	45	GLU	CG-CD-OE1	6.61	131.51	118.30
2	2	87	LYS	CB-CG-CD	6.59	128.74	111.60
3	3	27	ASN	CB-CA-C	-6.57	97.25	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	-6.56	105.19	118.30
1	1	288	SER	CB-CA-C	-6.54	97.67	110.10
1	1	53	THR	CA-CB-OG1	-6.52	95.31	109.00
2	2	203	TYR	CB-CG-CD1	6.52	124.91	121.00
1	1	151	MET	CG-SD-CE	6.50	110.60	100.20
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	288	SER	N-CA-CB	-6.48	100.78	110.50
1	1	22	SER	N-CA-CB	-6.46	100.80	110.50
1	1	144	SER	N-CA-CB	-6.46	100.81	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	221	MET	CG-SD-CE	6.44	110.50	100.20
3	3	55	MET	CA-CB-CG	-6.43	102.37	113.30
1	1	274	ASN	O-C-N	6.42	132.97	122.70
2	2	168	ASP	OD1-CG-OD2	6.42	135.50	123.30
3	3	29	GLU	CB-CG-CD	6.42	131.52	114.20
1	1	101	ASP	CB-CA-C	-6.41	97.58	110.40
2	2	97	PHE	CB-CG-CD1	-6.34	116.36	120.80
3	3	16	THR	N-CA-CB	-6.30	98.32	110.30
3	3	65	ASN	CA-CB-CG	-6.30	99.54	113.40
1	1	138	ASP	CB-CG-OD1	6.30	123.97	118.30
1	1	95	GLU	CB-CG-CD	-6.28	97.25	114.20
4	4	44	SER	CA-C-N	-6.25	103.44	117.20
2	2	38	TRP	N-CA-CB	-6.25	99.35	110.60
1	1	271	TYR	CB-CG-CD2	6.25	124.75	121.00
3	3	19	ARG	CA-CB-CG	6.23	127.11	113.40
3	3	63	GLU	CG-CD-OE2	-6.23	105.84	118.30
3	3	27	ASN	CA-CB-CG	-6.23	99.70	113.40
1	1	145	ASN	CA-CB-CG	-6.22	99.71	113.40
1	1	122	VAL	N-CA-CB	-6.17	97.92	111.50
2	2	69	LYS	CA-CB-CG	6.14	126.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	136	GLU	CB-CG-CD	-6.14	97.62	114.20
2	2	203	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	1	97	LYS	CD-CE-NZ	-6.11	97.66	111.70
3	3	222	MET	CG-SD-CE	-6.09	90.45	100.20
1	1	117	GLU	CG-CD-OE2	-6.09	106.11	118.30
2	2	219	SER	CB-CA-C	6.09	121.66	110.10
3	3	66	SER	CB-CA-C	6.06	121.62	110.10
3	3	219	LEU	CA-CB-CG	6.06	129.24	115.30
1	1	86	ASP	CB-CG-OD2	6.05	123.74	118.30
1	1	164	ASP	C-N-CA	6.05	136.82	121.70
2	2	235	THR	CA-CB-CG2	-6.04	103.94	112.40
1	1	118	LEU	CA-CB-CG	6.04	129.19	115.30
2	2	119	SER	N-CA-CB	6.04	119.56	110.50
2	2	67	ASP	CA-CB-CG	-6.02	100.15	113.40
2	2	247	MET	CB-CA-C	6.01	122.41	110.40
2	2	103	ARG	CA-CB-CG	6.00	126.60	113.40
4	4	61	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	1	224	MET	CG-SD-CE	5.97	109.75	100.20
4	4	48	ASP	CB-CG-OD1	-5.97	112.93	118.30
3	3	1	GLY	N-CA-C	5.96	128.01	113.10
2	2	12	ARG	NE-CZ-NH2	-5.92	117.34	120.30
3	3	58	THR	CA-CB-CG2	-5.92	104.11	112.40
1	1	257	ALA	N-CA-CB	-5.91	101.83	110.10
1	1	256	ARG	CD-NE-CZ	-5.90	115.34	123.60
1	1	35	THR	N-CA-CB	-5.90	99.10	110.30
3	3	45	GLU	CG-CD-OE2	-5.89	106.53	118.30
1	1	94	ARG	CG-CD-NE	-5.87	99.47	111.80
2	2	256	SER	CA-C-N	5.87	130.11	117.20
4	4	30	ASN	CA-CB-CG	-5.87	100.49	113.40
1	1	236	LYS	CD-CE-NZ	-5.84	98.27	111.70
1	1	268	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	2	238	LEU	N-CA-CB	-5.83	98.75	110.40
2	2	214	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	2	31	ALA	N-CA-CB	5.82	118.24	110.10
4	4	33	LYS	CD-CE-NZ	-5.82	98.33	111.70
3	3	27	ASN	O-C-N	5.80	131.97	122.70
1	1	28	THR	OG1-CB-CG2	5.78	123.29	110.00
2	2	255	ARG	CB-CG-CD	5.75	126.56	111.60
2	2	73	THR	CA-CB-OG1	-5.75	96.93	109.00
3	3	77	ASN	CA-C-N	5.74	129.84	117.20
2	2	68	SER	N-CA-CB	-5.74	101.89	110.50
1	1	233	ASP	CB-CG-OD2	-5.74	113.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	95	GLU	CA-CB-CG	-5.72	100.81	113.40
1	1	274	ASN	N-CA-CB	5.72	120.90	110.60
3	3	147	LEU	CA-CB-CG	5.71	128.44	115.30
1	1	246	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
3	3	1	GLY	O-C-N	-5.70	113.59	122.70
1	1	48	SER	CA-C-O	-5.69	108.15	120.10
2	2	52	LYS	CD-CE-NZ	-5.69	98.61	111.70
2	2	161	GLU	CA-CB-CG	5.69	125.91	113.40
2	2	75	SER	N-CA-CB	-5.68	101.98	110.50
3	3	164	THR	N-CA-CB	-5.63	99.60	110.30
3	3	177	ASP	CB-CG-OD2	-5.62	113.24	118.30
4	4	44	SER	O-C-N	5.61	131.67	122.70
2	2	210	ASP	N-CA-CB	-5.57	100.58	110.60
3	3	94	THR	O-C-N	5.56	131.60	122.70
2	2	84	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	1	122	VAL	CB-CA-C	5.53	121.91	111.40
1	1	202	ASP	CA-CB-CG	5.52	125.54	113.40
1	1	154	PRO	O-C-N	5.50	131.55	121.10
2	2	9	TYR	CB-CA-C	5.50	121.40	110.40
4	4	44	SER	C-N-CA	-5.49	107.97	121.70
3	3	186	PHE	CB-CG-CD1	-5.48	116.96	120.80
2	2	12	ARG	CD-NE-CZ	-5.48	115.93	123.60
3	3	112	ARG	CA-CB-CG	5.47	125.44	113.40
1	1	43	MET	CG-SD-CE	5.47	108.95	100.20
1	1	244	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	2	43	PRO	N-CD-CG	-5.47	95.00	103.20
1	1	26	LYS	CD-CE-NZ	-5.47	99.13	111.70
1	1	233	ASP	CB-CG-OD1	5.47	123.22	118.30
1	1	81	GLU	CG-CD-OE2	-5.46	107.38	118.30
1	1	270	ASN	O-C-N	5.43	131.39	122.70
3	3	60	THR	CA-CB-OG1	-5.42	97.61	109.00
2	2	174	ASN	CA-C-N	5.42	127.03	116.20
3	3	161	ILE	CA-CB-CG1	-5.40	100.74	111.00
4	4	44	SER	N-CA-CB	5.39	118.59	110.50
2	2	44	ASP	CA-CB-CG	5.39	125.26	113.40
3	3	115	LEU	CA-CB-CG	5.39	127.69	115.30
1	1	123	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	1	175	SER	CB-CA-C	5.37	120.30	110.10
2	2	169	VAL	CB-CA-C	-5.36	101.21	111.40
2	2	262	GLN	CA-C-O	-5.36	108.84	120.10
3	3	231	THR	CA-CB-OG1	-5.36	97.74	109.00
3	3	65	ASN	N-CA-CB	-5.35	100.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	64	GLU	CA-CB-CG	5.35	125.17	113.40
1	1	202	ASP	CB-CA-C	5.34	121.08	110.40
2	2	259	ILE	CB-CG1-CD1	-5.31	99.03	113.90
1	1	128	TYR	CB-CG-CD2	5.31	124.18	121.00
1	1	205	SER	O-C-N	5.31	131.19	122.70
3	3	42	ASN	CB-CG-OD1	-5.31	110.99	121.60
2	2	88	ASP	CA-CB-CG	-5.29	101.76	113.40
2	2	143	LYS	CD-CE-NZ	-5.28	99.56	111.70
3	3	116	MET	CB-CG-SD	-5.26	96.61	112.40
3	3	33	ARG	CB-CG-CD	-5.25	97.94	111.60
2	2	38	TRP	CA-CB-CG	-5.22	103.78	113.70
1	1	242	ARG	CD-NE-CZ	-5.22	116.29	123.60
2	2	170	LEU	CB-CG-CD2	5.21	119.86	111.00
3	3	74	ASN	OD1-CG-ND2	5.21	133.89	121.90
1	1	275	THR	CA-C-N	5.21	128.66	117.20
3	3	78	GLU	CA-CB-CG	5.21	124.85	113.40
1	1	275	THR	CA-C-O	-5.20	109.19	120.10
4	4	48	ASP	CA-CB-CG	-5.20	101.96	113.40
1	1	271	TYR	CB-CG-CD1	-5.20	117.88	121.00
3	3	222	MET	CB-CG-SD	-5.19	96.82	112.40
2	2	219	SER	N-CA-CB	5.19	118.29	110.50
2	2	203	TYR	CD1-CE1-CZ	-5.18	115.14	119.80
4	4	36	ALA	C-N-CA	-5.17	108.77	121.70
1	1	21	ILE	CA-CB-CG1	-5.17	101.18	111.00
1	1	282	ARG	CG-CD-NE	-5.16	100.95	111.80
2	2	14	GLN	OE1-CD-NE2	5.16	133.77	121.90
4	4	31	TYR	CG-CD2-CE2	-5.16	117.17	121.30
2	2	11	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	2	52	LYS	CA-C-N	5.15	128.52	117.20
1	1	50	SER	CA-C-N	5.14	128.50	117.20
1	1	162	GLU	OE1-CD-OE2	5.12	129.44	123.30
2	2	203	TYR	CG-CD1-CE1	5.12	125.39	121.30
2	2	221	MET	CA-CB-CG	-5.11	104.61	113.30
1	1	141	ASN	CA-CB-CG	-5.11	102.16	113.40
1	1	164	ASP	CB-CG-OD1	5.11	122.90	118.30
2	2	14	GLN	CA-CB-CG	-5.10	102.17	113.40
3	3	144	GLU	CA-CB-CG	5.09	124.59	113.40
4	4	58	ASP	O-C-N	5.08	130.84	122.70
3	3	141	ASP	CB-CG-OD2	5.08	122.88	118.30
2	2	18	LEU	CB-CA-C	5.08	119.85	110.20
1	1	274	ASN	CA-C-N	-5.06	106.06	117.20
1	1	17	THR	CA-CB-CG2	-5.06	105.31	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	39	SER	O-C-N	5.06	130.80	122.70
3	3	86	PHE	CB-CA-C	5.05	120.49	110.40
1	1	270	ASN	CB-CA-C	-5.04	100.31	110.40
2	2	170	LEU	CB-CA-C	5.04	119.78	110.20
3	3	172	GLN	CG-CD-NE2	5.04	128.80	116.70
1	1	282	ARG	CB-CA-C	-5.04	100.32	110.40
3	3	187	LEU	N-CA-CB	-5.01	100.39	110.40
1	1	22	SER	CA-C-O	-5.00	109.60	120.10

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	2106	155	0
2	2	1952	0	1926	127	0
3	3	1849	0	1831	146	0
4	4	297	0	294	35	0
5	1	26	0	27	5	0
6	1	6	0	0	1	0
6	2	1	0	0	0	0
All	All	6301	0	6184	382	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 31.

All (382) 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)
4:4:33:LYS:NZ	4:4:33:LYS:CE	1.67	1.57
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.55
1:1:285:ASP:CB	1:1:285:ASP:CA	1.80	1.54
2:2:52:LYS:CE	2:2:52:LYS:NZ	1.68	1.53
1:1:94:ARG:CZ	1:1:101:ASP:OD2	1.95	1.15
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.13
1:1:188:VAL:HG21	5:1:900:W8R:H2C2	1.33	1.09
1:1:285:ASP:CA	1:1:285:ASP:OD2	2.00	1.08
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.07
1:1:151:MET:CE	1:1:170:SER:HB2	1.84	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.07
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.06
1:1:151:MET:HE2	1:1:170:SER:HB2	1.37	1.05
2:2:12:ARG:HG3	2:2:12:ARG:NH1	1.69	1.04
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.00
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	0.99
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.96
3:3:57:ASN:N	3:3:57:ASN:CB	2.28	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
3:3:57:ASN:C	3:3:57:ASN:CB	2.37	0.94
2:2:12:ARG:HH11	2:2:12:ARG:HG3	1.27	0.93
1:1:285:ASP:CG	1:1:285:ASP:CA	2.37	0.93
1:1:58:MET:HE1	3:3:216:ASP:HA	1.48	0.92
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.91
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.90
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.90
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.89
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.88
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.55	0.87
1:1:285:ASP:HA	1:1:285:ASP:OD2	1.73	0.87
1:1:198:ASN:O	1:1:215:ILE:HD11	1.75	0.86
2:2:9:TYR:CD1	2:2:9:TYR:N	2.43	0.85
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
3:3:57:ASN:CG	3:3:57:ASN:CA	2.45	0.84
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.58	0.83
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:9:TYR:N	2:2:9:TYR:HD1	1.77	0.83
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.83
2:2:52:LYS:CD	2:2:52:LYS:NZ	2.43	0.82
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.82
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.81
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.81
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.79
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.79
1:1:188:VAL:HG21	5:1:900:W8R:C2C	2.12	0.79
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.48	0.78
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.78
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.77
1:1:58:MET:HE1	3:3:216:ASP:CA	2.13	0.77
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.77
2:2:12:ARG:CG	2:2:12:ARG:NH1	2.44	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:151:MET:HE3	1:1:170:SER:HB2	1.68	0.76
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.68	0.75
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.20	0.75
2:2:262:GLN:C	2:2:262:GLN:HE21	1.91	0.74
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.74
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.72
1:1:122:VAL:HG13	1:1:124:PHE:HE2	1.53	0.72
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.72
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.71
3:3:57:ASN:OD1	3:3:57:ASN:CA	2.38	0.71
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.70
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.70
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.70
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.69
1:1:152:TYR:O	1:1:173:ASN:ND2	2.26	0.69
1:1:188:VAL:CG2	5:1:900:W8R:H2C2	2.17	0.69
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
1:1:151:MET:HE3	1:1:167:THR:O	1.93	0.69
1:1:201:TYR:HD2	1:1:214:GLY:O	1.76	0.68
3:3:179:ASP:HB3	3:3:182:THR:CG2	2.23	0.68
1:1:104:ILE:HD11	1:1:224:MET:HG3	1.74	0.68
4:4:29:ILE:O	4:4:29:ILE:HG22	1.94	0.68
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.68
1:1:151:MET:CE	1:1:170:SER:CB	2.68	0.67
1:1:151:MET:HE3	1:1:170:SER:CB	2.24	0.67
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.67
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.67
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.76	0.67
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.66
3:3:42:ASN:HD22	3:3:44:LEU:H	1.43	0.66
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.66
1:1:94:ARG:NH1	1:1:101:ASP:OD2	2.28	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.66
1:1:278:VAL:HG12	3:3:62:ASP:OD1	1.95	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.65
3:3:61:LYS:HD3	3:3:63:GLU:OE1	1.95	0.65
1:1:151:MET:CE	1:1:167:THR:O	2.44	0.65
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:94:ARG:CG	1:1:94:ARG:NH1	2.60	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.97	0.63
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.63
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.63
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.63
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.63
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.62
1:1:176:VAL:HG22	5:1:900:W8R:H312	1.81	0.62
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.62
3:3:55:MET:O	3:3:55:MET:HG3	1.99	0.61
1:1:38:GLU:CD	3:3:116:MET:HE1	2.20	0.61
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.61
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
1:1:94:ARG:NH2	1:1:101:ASP:OD2	2.34	0.61
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.61
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
2:2:155:ASP:C	2:2:155:ASP:OD2	2.37	0.60
1:1:187:SER:HB3	3:3:21:SER:CB	2.31	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.60
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59
1:1:100:ASN:HD22	1:1:101:ASP:H	1.49	0.59
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE2	2.38	0.58
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.58
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:58:MET:HE1	3:3:216:ASP:C	2.24	0.58
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.58
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.58
2:2:52:LYS:HD3	2:2:52:LYS:NZ	2.20	0.57
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.57
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.57
1:1:82:ILE:HG22	1:1:100:ASN:HB2	1.86	0.57
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
2:2:64:TYR:CD2	2:2:89:MET:HB3	2.39	0.56
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.56
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.56

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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	0.56
3:3:175:TYR:H	3:3:182:THR:HG21	1.70	0.55
3:3:175:TYR:H	3:3:182:THR:CG2	2.20	0.55
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.55
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.55
1:1:117:GLU:HB3	1:1:200:PHE:HZ	1.70	0.55
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.55
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.55
1:1:216:THR:HG21	3:3:236:GLU:HG2	1.88	0.55
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.55
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.55
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.88	0.55
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.54
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:103:LYS:HA	1:1:223:SER:HB2	1.89	0.54
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.54
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.54
1:1:110:VAL:HG22	3:3:230:GLN:OE1	2.06	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.53
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.53
3:3:57:ASN:C	3:3:57:ASN:HB3	2.27	0.53
3:3:117:TYR:CD2	3:3:155:ILE:HD13	2.44	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.53
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
1:1:214:GLY:O	1:1:217:VAL:CG1	2.57	0.52
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.52
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.52
3:3:18:ASP:OD1	4:4:40:SER:HB2	2.09	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.52
3:3:75:ARG:NH1	3:3:78:GLU:OE1	2.41	0.52
1:1:88:THR:O	1:1:90:ILE:HD13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.52
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.52
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.52
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.52
1:1:194:ALA:HB3	6:1:504:HOH:O	2.10	0.52
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.52
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.52
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.51
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.51
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.51
1:1:117:GLU:HB3	1:1:200:PHE:CZ	2.46	0.50
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.50
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE1	2.44	0.50
1:1:187:SER:HB3	3:3:21:SER:HB2	1.92	0.50
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.49
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.49
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.49
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
1:1:58:MET:CE	3:3:216:ASP:O	2.60	0.49
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.49
1:1:280:LYS:HE3	3:3:89:ASP:OD2	2.13	0.49
3:3:112:ARG:HG2	3:3:112:ARG:NH1	2.27	0.49
1:1:216:THR:CG2	3:3:236:GLU:CG	2.91	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.95	0.48
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.78	0.48
1:1:58:MET:HE1	3:3:216:ASP:O	2.13	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
1:1:152:TYR:O	1:1:154:PRO:HD3	2.13	0.48
2:2:40:GLU:CG	2:2:40:GLU:O	2.61	0.48
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.48
1:1:216:THR:HG21	3:3:236:GLU:CG	2.43	0.48
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.48
1:1:122:VAL:O	1:1:197:TYR:HB2	2.14	0.48
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.48
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.48
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.48
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.47
1:1:201:TYR:CG	1:1:218:LEU:HD22	2.49	0.47
3:3:175:TYR:CD1	3:3:182:THR:HG21	2.49	0.47
1:1:273:LYS:O	1:1:274:ASN:C	2.52	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	2.15	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.47
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.47
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
1:1:43:MET:HE3	1:1:43:MET:HA	1.97	0.46
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.46
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.46
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.62	0.46
2:2:63:PHE:CD2	2:2:245:ALA:HB2	2.50	0.46
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.46
1:1:198:ASN:HB3	1:1:200:PHE:O	2.17	0.45
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
1:1:43:MET:CE	1:1:43:MET:HA	2.46	0.45
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.45
4:4:44:SER:C	4:4:46:SER:N	2.68	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.45
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.99	0.45
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.45
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.82	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
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.45
1:1:207:ASP:HA	2:2:144:TYR:CE1	2.52	0.45
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.44
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.44
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.44
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.44
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.16	0.44
1:1:289:TYR:CE1	3:3:138:GLY:HA3	2.53	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.44
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.44
1:1:289:TYR:CD1	3:3:138:GLY:HA3	2.52	0.44
3:3:57:ASN:H	3:3:57:ASN:CB	2.26	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.43
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.43
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.43
2:2:143:LYS:HG2	2:2:143:LYS:H	1.56	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.48	0.43
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.43
1:1:286:ILE:HG21	1:1:286:ILE:HD13	1.77	0.43
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.42
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.42
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.42
1:1:122:VAL:CG1	1:1:124:PHE:HE2	2.25	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD1	2.55	0.42
1:1:191:VAL:CG2	5:1:900:W8R:H6C1	2.50	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
1:1:136:GLN:HB2	1:1:136:GLN:HE21	1.13	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.20	0.42
1:1:201:TYR:H	2:2:131:GLN:HE21	1.68	0.42
2:2:10:SER:CB	2:2:12:ARG:HB2	2.49	0.42
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.42
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.41
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.41
3:3:44:LEU:HD23	3:3:44:LEU:HA	1.79	0.41
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
1:1:151:MET:HE1	1:1:167:THR:O	2.18	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
1:1:86:ASP:OD2	1:1:88:THR:HB	2.20	0.41
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.41
3:3:113:PHE:CE1	3:3:115:LEU:HD13	2.55	0.41
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.41
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.41
1:1:38:GLU:CD	3:3:116:MET:CE	2.88	0.41
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.41
1:1:187:SER:HB3	3:3:21:SER:HB3	2.01	0.41
2:2:255:ARG:CG	2:2:256:SER:H	1.99	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.03	0.41
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.43	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
1:1:285:ASP:H	1:1:285:ASP:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:38:GLU:N	3:3:116:MET:HE3	2.37	0.40
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.40
1:1:100:ASN:ND2	1:1:101:ASP:H	2.17	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.40
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.40
2:2:53:THR:OG1	2:2:250:GLU:HG2	2.22	0.40
3:3:86:PHE:CG	3:3:178:PRO:HB3	2.57	0.40
1:1:261:LEU:HD11	2:2:171:TYR:CE1	2.57	0.40
2:2:183:ILE:HD12	3:3:49:VAL:HG11	2.03	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%)	249 (92%)	20 (7%)	2 (1%)	26 70
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	24 66
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	21 64
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	7 33
All	All	796/855 (93%)	733 (92%)	56 (7%)	7 (1%)	21 64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
3	3	57	ASN
3	3	77	ASN

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Mol	Chain	Res	Type
1	1	165	ASP
2	2	255	ARG
2	2	257	LYS
4	4	47	MET

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	239/253 (94%)	189 (79%)	50 (21%)	1 7
2	2	223/229 (97%)	179 (80%)	44 (20%)	1 9
3	3	209/209 (100%)	171 (82%)	38 (18%)	2 11
4	4	33/57 (58%)	20 (61%)	13 (39%)	0 0
All	All	704/748 (94%)	559 (79%)	145 (21%)	1 7

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
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	100	ASN
1	1	103	LYS
1	1	105	ASN

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Mol	Chain	Res	Type
1	1	106	LEU
1	1	107	SER
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	161	LYS
1	1	165	ASP
1	1	170	SER
1	1	172	SER
1	1	173	ASN
1	1	175	SER
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	216	THR
1	1	217	VAL
1	1	221	MET
1	1	223	SER
1	1	240	LYS
1	1	256	ARG
1	1	268	ARG
1	1	274	ASN
1	1	278	VAL
1	1	285	ASP
1	1	287	LYS
2	2	11	ASP
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	30	ASN
2	2	49	ASP
2	2	52	LYS
2	2	66	LEU
2	2	69	LYS

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Mol	Chain	Res	Type
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	205	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
2	2	262	GLN
3	3	16	THR
3	3	33	ARG
3	3	46	ILE
3	3	55	MET
3	3	56	ASN
3	3	60	THR
3	3	61	LYS

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Mol	Chain	Res	Type
3	3	65	ASN
3	3	84	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	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
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

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Mol	Chain	Res	Type
4	4	67	LEU
4	4	68	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	92	ASN
1	1	100	ASN
1	1	136	GLN
1	1	173	ASN
1	1	198	ASN
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	131	GLN
2	2	174	ASN
2	2	187	GLN
2	2	190	ASN
2	2	195	ASN
2	2	205	ASN
2	2	216	ASN
2	2	217	ASN
2	2	262	GLN
3	3	20	GLN
3	3	42	ASN
3	3	56	ASN
3	3	84	ASN
3	3	102	GLN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN
4	4	30	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
5	W8R	1	900	-	25,28,28	3.19	5 (20%)	31,36,36	2.91	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	W8R	1	900	-	-	0/14/24/24	0/2/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	900	W8R	C4A-N3A	-6.33	1.36	1.48
5	1	900	W8R	O1A-C2A	-4.11	1.29	1.36
5	1	900	W8R	O1A-C5A	-3.59	1.38	1.45
5	1	900	W8R	C4-C5	-2.00	1.34	1.39
5	1	900	W8R	C2A-N3A	13.20	1.43	1.26

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	900	W8R	O1A-C2A-N3A	-7.56	109.88	118.13
5	1	900	W8R	C5A-C4A-N3A	-3.63	98.52	103.79
5	1	900	W8R	CM1-C4A-C5A	-2.43	104.26	114.06
5	1	900	W8R	C4A-N3A-C2A	4.70	112.90	106.32
5	1	900	W8R	O1A-C5A-C4A	5.26	111.70	105.06
5	1	900	W8R	CM1-C4A-N3A	7.70	135.47	112.00
5	1	900	W8R	O1A-C2A-C4B	8.27	124.28	115.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	900	W8R	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.42	0	100	100	1, 1, 1, 1	0
2	2	255/262 (97%)	-0.53	0	100	100	1, 1, 1, 1	0
3	3	236/236 (100%)	-0.46	0	100	100	1, 1, 1, 1	0
4	4	40/68 (58%)	-0.27	0	100	100	1, 1, 1, 1	0
All	All	804/855 (94%)	-0.46	0	100	100	1, 1, 1, 1	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	W8R	1	900	26/26	0.97	0.14	-0.34	1,1,1,1	0

6.5 Other polymers (i)

There are no such residues in this entry.