Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:22 PM GMT

PDB ID	:	1OPG
Title	:	OPG2 FAB FRAGMENT
Authors	:	Kodandapani, R.; Veerapandian, B.; Ely, K.R.
Deposited on	:	1995-04-28
Resolution	:	2.00 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 ⓘ symbol.

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

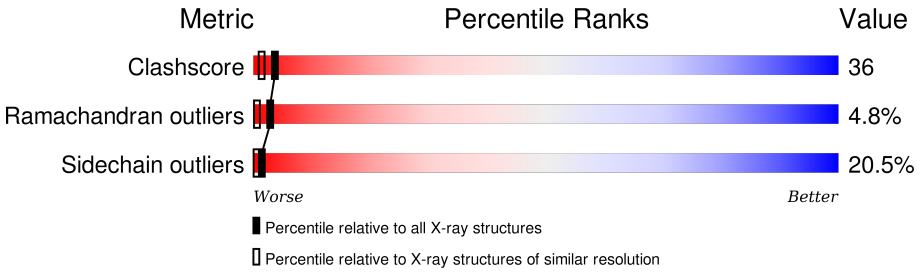
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	27% 45% 21% 7%
2	H	227	29% 43% 19% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3966 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 OPG2 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1654	1023	280	344	7			

- Molecule 2 is a protein called OPG2 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	11	0
			1824	1152	310	353	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	247	Total	O	0	0
			247	247		
3	L	241	Total	O	0	0
			241	241		

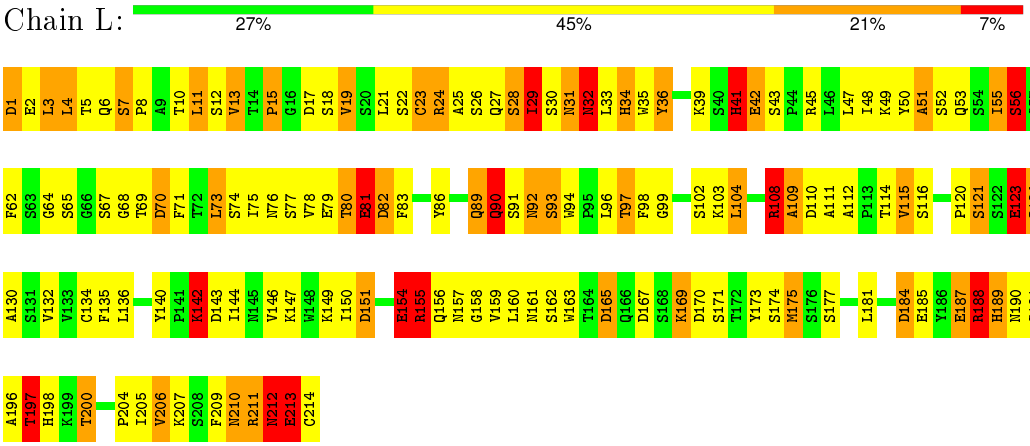
3 Residue-property plots (i)

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

Note EDS was not executed.

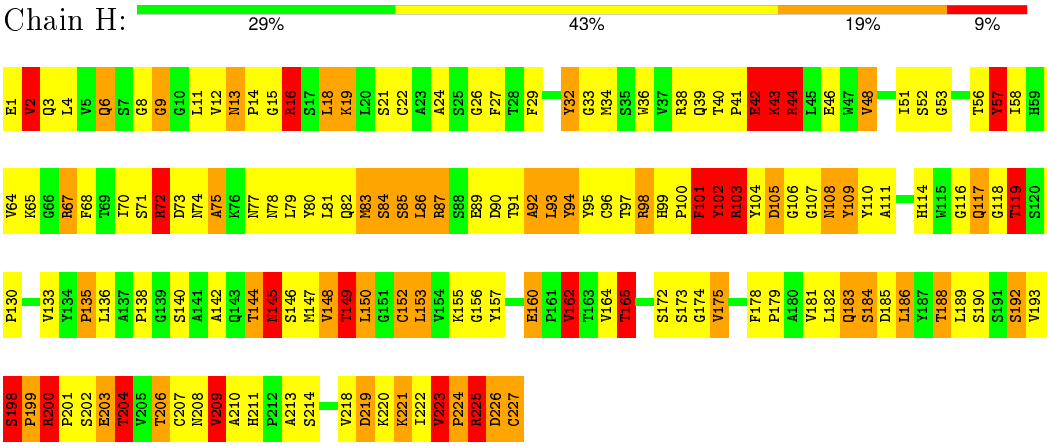
- Molecule 1: OPG2 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: OPG2 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	93.10Å 83.80Å 53.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	L	1.02	0/1691	2.79	131/2293 (5.7%)
2	H	1.01	0/1877	2.69	141/2560 (5.5%)
All	All	1.02	0/3568	2.74	272/4853 (5.6%)

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
2	H	0	1

There are no bond length outliers.

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	24	ARG	CD-NE-CZ	23.96	157.14	123.60
1	L	24	ARG	NE-CZ-NH2	22.55	131.57	120.30
2	H	103[A]	ARG	NE-CZ-NH1	21.76	131.18	120.30
2	H	103[B]	ARG	NE-CZ-NH1	21.76	131.18	120.30
2	H	103[A]	ARG	NE-CZ-NH2	-21.48	109.56	120.30
2	H	103[B]	ARG	NE-CZ-NH2	-21.48	109.56	120.30
1	L	45	ARG	CD-NE-CZ	18.84	149.97	123.60
1	L	155	ARG	NE-CZ-NH1	16.18	128.39	120.30
1	L	211	ARG	NE-CZ-NH2	-16.09	112.26	120.30
1	L	17	ASP	CB-CG-OD2	-15.14	104.68	118.30
1	L	61	ARG	NE-CZ-NH2	15.07	127.83	120.30
1	L	187	GLU	CA-CB-CG	14.61	145.53	113.40
1	L	36	TYR	CB-CG-CD2	-14.05	112.57	121.00
1	L	155	ARG	NE-CZ-NH2	-13.95	113.32	120.30
2	H	98	ARG	NE-CZ-NH1	13.53	127.07	120.30
1	L	61	ARG	NE-CZ-NH1	-13.47	113.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	36	TYR	CB-CG-CD1	13.46	129.07	121.00
2	H	38	ARG	NE-CZ-NH1	12.79	126.70	120.30
1	L	188	ARG	CD-NE-CZ	12.31	140.84	123.60
2	H	38	ARG	CD-NE-CZ	12.28	140.79	123.60
2	H	119	THR	N-CA-CB	11.84	132.79	110.30
2	H	16	ARG	NE-CZ-NH1	11.76	126.18	120.30
2	H	200	ARG	NE-CZ-NH2	11.56	126.08	120.30
1	L	81	GLU	CA-CB-CG	11.48	138.66	113.40
1	L	82	ASP	CB-CG-OD1	11.35	128.52	118.30
2	H	67	ARG	NE-CZ-NH2	-10.84	114.88	120.30
2	H	200	ARG	CD-NE-CZ	10.82	138.74	123.60
1	L	108	ARG	NE-CZ-NH2	10.56	125.58	120.30
2	H	44	ARG	CD-NE-CZ	10.54	138.35	123.60
1	L	211	ARG	NE-CZ-NH1	10.40	125.50	120.30
2	H	223	VAL	CB-CA-C	10.38	131.13	111.40
1	L	206	VAL	CA-CB-CG1	9.94	125.80	110.90
2	H	103[A]	ARG	CD-NE-CZ	9.79	137.30	123.60
2	H	103[B]	ARG	CD-NE-CZ	9.79	137.30	123.60
1	L	165	ASP	CB-CG-OD2	-9.70	109.57	118.30
1	L	151	ASP	CB-CG-OD1	-9.62	109.64	118.30
2	H	200	ARG	NH1-CZ-NH2	-9.41	109.04	119.40
1	L	60	SER	N-CA-CB	-9.40	96.40	110.50
1	L	123	GLU	CA-CB-CG	9.33	133.93	113.40
2	H	44	ARG	NE-CZ-NH1	-9.27	115.67	120.30
2	H	80	TYR	CB-CG-CD1	-9.21	115.48	121.00
1	L	3	LEU	O-C-N	9.16	137.35	122.70
2	H	200	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	L	167	ASP	CB-CG-OD2	9.05	126.44	118.30
2	H	62	ASP	CB-CG-OD1	-9.04	110.16	118.30
1	L	155	ARG	CA-CB-CG	-9.04	93.52	113.40
1	L	154	GLU	CA-CB-CG	8.96	133.12	113.40
1	L	181	LEU	CA-CB-CG	8.95	135.88	115.30
1	L	167	ASP	CB-CG-OD1	-8.87	110.32	118.30
2	H	227	CYS	CA-CB-SG	-8.78	98.20	114.00
1	L	70	ASP	CB-CG-OD2	-8.60	110.56	118.30
2	H	226	ASP	C-N-CA	8.60	143.19	121.70
1	L	151	ASP	CB-CG-OD2	8.59	126.03	118.30
2	H	155	LYS	O-C-N	8.59	137.81	123.20
2	H	219	ASP	CB-CG-OD1	-8.54	110.61	118.30
2	H	226	ASP	CA-C-O	8.54	138.03	120.10
1	L	211	ARG	CD-NE-CZ	8.51	135.51	123.60
2	H	102[A]	TYR	CB-CG-CD2	-8.21	116.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	102[B]	TYR	CB-CG-CD2	-8.21	116.08	121.00
1	L	24	ARG	NH1-CZ-NH2	-8.16	110.43	119.40
2	H	32	TYR	O-C-N	8.12	137.01	123.20
2	H	165	THR	N-CA-CB	-8.11	94.89	110.30
1	L	103	LYS	CA-C-O	-8.10	103.08	120.10
1	L	3	LEU	N-CA-CB	8.06	126.52	110.40
2	H	90	ASP	CB-CG-OD2	-8.06	111.05	118.30
2	H	157	TYR	CB-CG-CD1	-8.03	116.18	121.00
2	H	39	GLN	CB-CG-CD	8.02	132.45	111.60
1	L	1	ASP	CB-CG-OD1	-7.96	111.14	118.30
1	L	56	SER	CB-CA-C	-7.95	94.99	110.10
2	H	39	GLN	CA-C-O	-7.95	103.42	120.10
1	L	17	ASP	OD1-CG-OD2	7.92	138.34	123.30
2	H	84	SER	O-C-N	7.86	135.28	122.70
2	H	200	ARG	CB-CA-C	7.84	126.08	110.40
2	H	80	TYR	CB-CG-CD2	7.73	125.64	121.00
2	H	16	ARG	NH1-CZ-NH2	-7.68	110.95	119.40
1	L	90	GLN	CB-CG-CD	7.68	131.56	111.60
1	L	45	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	H	227	CYS	N-CA-CB	7.66	124.39	110.60
1	L	188	ARG	CA-CB-CG	7.62	130.17	113.40
2	H	185	ASP	CB-CG-OD1	7.57	125.11	118.30
1	L	188	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	L	1	ASP	CB-CG-OD2	-7.52	111.53	118.30
2	H	160	GLU	CG-CD-OE1	7.41	133.12	118.30
1	L	1	ASP	OD1-CG-OD2	7.37	137.31	123.30
1	L	80	THR	CB-CA-C	7.37	131.51	111.60
1	L	192	TYR	CB-CG-CD2	7.36	125.42	121.00
1	L	181	LEU	CB-CG-CD2	-7.29	98.61	111.00
1	L	177	SER	N-CA-CB	7.20	121.30	110.50
2	H	188	THR	CA-CB-OG1	-7.19	93.90	109.00
1	L	175	MET	CA-CB-CG	7.19	125.52	113.30
1	L	79	GLU	OE1-CD-OE2	7.18	131.92	123.30
1	L	103	LYS	O-C-N	7.18	134.19	122.70
1	L	110	ASP	CB-CG-OD1	7.17	124.76	118.30
2	H	4	LEU	CA-C-O	-7.16	105.06	120.10
2	H	149	THR	CA-CB-CG2	7.15	122.42	112.40
1	L	195	GLU	CA-CB-CG	7.11	129.05	113.40
2	H	219	ASP	CB-CG-OD2	7.11	124.70	118.30
2	H	213	ALA	N-CA-CB	-7.00	100.30	110.10
2	H	225	ARG	CA-C-O	7.00	134.81	120.10
1	L	115	VAL	CA-CB-CG2	6.99	121.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	225	ARG	NE-CZ-NH1	-6.98	116.81	120.30
2	H	94	TYR	CB-CG-CD1	-6.98	116.81	121.00
2	H	87	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	H	184	SER	N-CA-CB	-6.96	100.06	110.50
2	H	160	GLU	CG-CD-OE2	-6.86	104.58	118.30
2	H	128	THR	CA-CB-OG1	-6.85	94.61	109.00
2	H	150	LEU	CA-CB-CG	6.79	130.91	115.30
2	H	44	ARG	CB-CA-C	-6.67	97.05	110.40
2	H	14	PRO	CB-CA-C	6.63	128.58	112.00
1	L	111	ALA	CB-CA-C	-6.62	100.17	110.10
1	L	196	ALA	CB-CA-C	-6.62	100.17	110.10
2	H	206	THR	CA-CB-OG1	6.62	122.90	109.00
2	H	44	ARG	CA-CB-CG	6.60	127.92	113.40
2	H	210	ALA	O-C-N	6.59	133.24	122.70
1	L	114	THR	N-CA-C	-6.58	93.22	111.00
2	H	136	LEU	CA-CB-CG	6.58	130.43	115.30
1	L	76	ASN	CB-CA-C	6.55	123.50	110.40
2	H	94	TYR	CB-CG-CD2	6.53	124.92	121.00
1	L	81	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	L	194	CYS	O-C-N	6.52	133.14	122.70
2	H	227	CYS	CA-C-O	-6.49	106.47	120.10
2	H	92	ALA	CB-CA-C	-6.47	100.39	110.10
1	L	58	ILE	CA-CB-CG2	6.44	123.78	110.90
2	H	46	GLU	OE1-CD-OE2	6.44	131.02	123.30
1	L	198	HIS	CB-CA-C	6.40	123.19	110.40
2	H	200	ARG	CA-CB-CG	6.39	127.46	113.40
2	H	9	GLY	CA-C-O	-6.38	109.11	120.60
2	H	16	ARG	CB-CA-C	6.33	123.06	110.40
1	L	200	THR	N-CA-CB	-6.31	98.30	110.30
2	H	67	ARG	CG-CD-NE	-6.31	98.54	111.80
1	L	126	THR	C-N-CA	6.26	137.35	121.70
1	L	124	GLN	N-CA-CB	6.25	121.84	110.60
1	L	109	ALA	N-CA-CB	6.24	118.83	110.10
2	H	72	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	L	211	ARG	CB-CA-C	6.21	122.81	110.40
2	H	192	SER	N-CA-CB	6.20	119.81	110.50
1	L	25	ALA	CB-CA-C	-6.18	100.82	110.10
1	L	213	GLU	C-N-CA	6.17	137.14	121.70
1	L	77	SER	N-CA-CB	6.17	119.75	110.50
2	H	34	MET	N-CA-CB	6.17	121.70	110.60
1	L	4	LEU	O-C-N	6.16	132.55	122.70
1	L	209	PHE	CA-C-O	6.16	133.03	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	153	LEU	CB-CA-C	-6.15	98.51	110.20
2	H	43	LYS	C-N-CA	6.15	137.07	121.70
2	H	93	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	L	175	MET	N-CA-CB	-6.12	99.58	110.60
2	H	152	CYS	CA-CB-SG	-6.11	103.01	114.00
2	H	152	CYS	CA-C-O	-6.10	107.29	120.10
2	H	65	LYS	N-CA-CB	6.10	121.57	110.60
2	H	44	ARG	CG-CD-NE	6.08	124.58	111.80
2	H	153	LEU	CA-CB-CG	6.07	129.25	115.30
1	L	79	GLU	CG-CD-OE2	-6.06	106.17	118.30
2	H	22	CYS	O-C-N	6.06	132.39	122.70
1	L	194	CYS	CB-CA-C	6.04	122.49	110.40
2	H	96	CYS	N-CA-CB	6.04	121.48	110.60
2	H	145	ASN	CA-C-O	6.04	132.78	120.10
1	L	192	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	L	121	SER	N-CA-CB	6.02	119.53	110.50
2	H	42	GLU	CA-CB-CG	5.99	126.58	113.40
1	L	61	ARG	CG-CD-NE	5.97	124.34	111.80
2	H	148	VAL	CB-CA-C	-5.96	100.08	111.40
2	H	185	ASP	CA-C-O	-5.95	107.60	120.10
2	H	4	LEU	CA-C-N	5.95	130.29	117.20
2	H	67	ARG	CD-NE-CZ	5.94	131.91	123.60
2	H	95	TYR	O-C-N	5.93	132.19	122.70
1	L	23	CYS	CA-CB-SG	5.90	124.61	114.00
1	L	42	GLU	CB-CA-C	-5.90	98.61	110.40
2	H	32	TYR	CA-C-N	-5.86	104.48	116.20
1	L	143	ASP	CB-CG-OD2	-5.85	113.04	118.30
2	H	199	PRO	N-CA-C	-5.84	96.91	112.10
1	L	81	GLU	CB-CG-CD	5.83	129.93	114.20
1	L	67	SER	N-CA-CB	5.80	119.20	110.50
1	L	214	CYS	N-CA-C	5.80	126.66	111.00
2	H	97	THR	O-C-N	5.80	131.97	122.70
2	H	72	ARG	N-CA-CB	5.79	121.01	110.60
1	L	36	TYR	CB-CA-C	-5.77	98.85	110.40
2	H	2	VAL	N-CA-C	-5.76	95.46	111.00
1	L	210	ASN	O-C-N	5.75	131.90	122.70
2	H	72	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	H	225	ARG	C-N-CA	5.74	136.04	121.70
2	H	183	GLN	CB-CG-CD	5.73	126.51	111.60
2	H	210	ALA	CB-CA-C	-5.73	101.51	110.10
1	L	184	ASP	CB-CG-OD2	5.71	123.44	118.30
2	H	44	ARG	NE-CZ-NH2	5.70	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	78	ASN	O-C-N	5.70	131.82	122.70
2	H	162	VAL	CG1-CB-CG2	-5.68	101.81	110.90
2	H	145	ASN	N-CA-C	5.67	126.32	111.00
1	L	82	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	H	102[A]	TYR	N-CA-CB	-5.67	100.40	110.60
2	H	102[B]	TYR	N-CA-CB	-5.67	100.40	110.60
1	L	189	HIS	O-C-N	5.66	131.76	122.70
1	L	24	ARG	CB-CA-C	5.66	121.72	110.40
2	H	34	MET	CB-CG-SD	-5.63	95.50	112.40
2	H	67	ARG	O-C-N	5.62	131.70	122.70
2	H	87	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	L	5	THR	N-CA-CB	5.62	120.97	110.30
2	H	150	LEU	CB-CG-CD2	-5.61	101.46	111.00
2	H	144	THR	CA-CB-CG2	5.61	120.25	112.40
1	L	108	ARG	NE-CZ-NH1	-5.59	117.51	120.30
2	H	157	TYR	CB-CG-CD2	5.58	124.35	121.00
2	H	162	VAL	CA-CB-CG2	5.57	119.26	110.90
1	L	196	ALA	N-CA-CB	5.57	117.89	110.10
1	L	165	ASP	OD1-CG-OD2	5.52	133.79	123.30
1	L	51	ALA	N-CA-C	5.50	125.86	111.00
2	H	91	THR	N-CA-CB	5.50	120.75	110.30
1	L	41	HIS	C-N-CA	5.49	135.44	121.70
2	H	162	VAL	CA-CB-CG1	5.49	119.14	110.90
1	L	5	THR	O-C-N	5.47	131.46	122.70
1	L	132	VAL	N-CA-C	-5.46	96.25	111.00
2	H	11	LEU	C-N-CA	5.42	135.24	121.70
2	H	155	LYS	CA-C-O	-5.40	108.76	120.10
2	H	16	ARG	CA-CB-CG	5.39	125.27	113.40
2	H	175	VAL	N-CA-CB	5.35	123.27	111.50
2	H	19	LYS	CB-CG-CD	5.34	125.48	111.60
2	H	204	THR	CA-C-O	5.34	131.31	120.10
1	L	184	ASP	CB-CG-OD1	-5.32	113.51	118.30
2	H	165	THR	CB-CA-C	5.30	125.91	111.60
2	H	119	THR	CB-CA-C	-5.29	97.32	111.60
1	L	3	LEU	CA-C-O	-5.28	109.00	120.10
1	L	34	HIS	C-N-CA	5.27	134.87	121.70
1	L	205	ILE	CA-CB-CG2	5.26	121.42	110.90
1	L	108	ARG	CA-CB-CG	5.26	124.97	113.40
2	H	79	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	L	207	LYS	N-CA-CB	-5.25	101.14	110.60
1	L	77	SER	N-CA-C	-5.25	96.82	111.00
2	H	156	GLY	N-CA-C	5.25	126.23	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	169	LYS	N-CA-CB	5.23	120.02	110.60
2	H	135	PRO	N-CA-CB	5.23	109.58	103.30
1	L	210	ASN	CA-CB-CG	-5.22	101.92	113.40
1	L	92	ASN	OD1-CG-ND2	-5.22	109.90	121.90
1	L	93	SER	CB-CA-C	-5.21	100.19	110.10
1	L	80	THR	CA-C-N	5.21	128.66	117.20
2	H	11	LEU	CB-CA-C	5.21	120.10	110.20
2	H	184	SER	CB-CA-C	5.21	119.99	110.10
1	L	189	HIS	CB-CA-C	5.20	120.80	110.40
2	H	75	ALA	N-CA-CB	-5.20	102.82	110.10
1	L	97	THR	OG1-CB-CG2	-5.19	98.05	110.00
2	H	33	GLY	N-CA-C	-5.18	100.14	113.10
2	H	198	SER	CB-CA-C	5.18	119.95	110.10
1	L	103	LYS	CB-CA-C	-5.17	100.05	110.40
2	H	226	ASP	CA-C-N	-5.17	105.84	117.20
1	L	188	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
2	H	95	TYR	CA-CB-CG	5.16	123.20	113.40
1	L	142	LYS	CB-CG-CD	5.16	125.00	111.60
2	H	86	LEU	CB-CG-CD2	5.15	119.75	111.00
1	L	189	HIS	N-CA-CB	5.14	119.85	110.60
1	L	102	SER	CB-CA-C	5.13	119.85	110.10
2	H	152	CYS	O-C-N	5.13	130.91	122.70
1	L	3	LEU	N-CA-C	-5.13	97.15	111.00
2	H	70	ILE	CA-CB-CG1	-5.12	101.28	111.00
2	H	209	VAL	O-C-N	5.11	130.88	122.70
1	L	89	GLN	CG-CD-NE2	-5.11	104.44	116.70
1	L	15	PRO	N-CA-C	-5.09	98.86	112.10
1	L	29	ILE	C-N-CA	5.09	134.43	121.70
2	H	57	TYR	CB-CA-C	5.09	120.58	110.40
1	L	7	SER	CB-CA-C	-5.08	100.44	110.10
1	L	158	GLY	CA-C-O	-5.08	111.46	120.60
1	L	140	TYR	CA-CB-CG	-5.07	103.78	113.40
2	H	72	ARG	CA-CB-CG	5.05	124.52	113.40
2	H	109[A]	TYR	CA-CB-CG	-5.05	103.81	113.40
2	H	109[B]	TYR	CA-CB-CG	-5.05	103.81	113.40
1	L	173	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	L	197	THR	N-CA-CB	5.04	119.88	110.30
1	L	115	VAL	CB-CA-C	5.04	120.97	111.40
2	H	16	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	L	116	SER	CB-CA-C	5.03	119.66	110.10
2	H	43	LYS	N-CA-C	5.03	124.57	111.00
2	H	145	ASN	C-N-CA	5.03	134.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	212	ASN	CB-CG-ND2	5.01	128.73	116.70
1	L	159	VAL	CA-CB-CG2	5.01	118.41	110.90
1	L	187	GLU	CG-CD-OE2	5.01	128.31	118.30
1	L	114	THR	N-CA-CB	5.00	119.81	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	72	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	L	1654	0	1569	102	4
2	H	1824	0	1753	145	7
3	H	247	0	0	26	1
3	L	241	0	0	28	7
All	All	3966	0	3322	242	10

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 36.

All (242) 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)
2:H:107[B]:GLY:HA2	3:H:404:HOH:O	1.62	0.97
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.50	0.93
2:H:107[B]:GLY:CA	3:H:404:HOH:O	2.14	0.92
2:H:9:GLY:H	2:H:119:THR:HG21	1.38	0.88
1:L:90:GLN:HE22	1:L:93:SER:H	1.16	0.88
1:L:195:GLU:HG2	1:L:206:VAL:HG12	1.54	0.87
2:H:165:THR:HG22	2:H:208:ASN:HB2	1.59	0.84
1:L:136:LEU:HG	3:L:296:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:102[A]:TYR:HB2	2:H:110[A]:TYR:OH	1.80	0.81
2:H:225:ARG:HB3	3:H:257:HOH:O	1.82	0.80
1:L:11:LEU:HD23	1:L:104:LEU:HD21	1.63	0.79
2:H:102[B]:TYR:HB2	2:H:110[B]:TYR:OH	1.83	0.78
1:L:55:ILE:HG13	1:L:56:SER:H	1.47	0.78
2:H:1:GLU:HA	2:H:3:GLN:HE21	1.51	0.76
2:H:200:ARG:HB3	2:H:201:PRO:CD	2.16	0.76
1:L:210:ASN:ND2	3:L:376:HOH:O	2.17	0.76
2:H:94:TYR:O	2:H:118:GLY:HA2	1.87	0.74
2:H:140:SER:OG	2:H:200:ARG:NH1	2.20	0.74
2:H:198:SER:OG	2:H:199:PRO:HD3	1.88	0.74
1:L:146:VAL:HG22	3:L:296:HOH:O	1.88	0.74
2:H:201:PRO:HA	2:H:223:VAL:CG1	2.18	0.73
2:H:72:ARG:NE	2:H:74:ASN:HD21	1.86	0.73
1:L:29:ILE:HG22	1:L:92:ASN:OD1	1.88	0.73
2:H:164:VAL:HG13	3:H:300:HOH:O	1.88	0.73
2:H:82:GLN:HG3	3:H:332:HOH:O	1.88	0.73
1:L:21:LEU:HD11	1:L:104:LEU:HD11	1.71	0.72
2:H:200:ARG:HB3	2:H:201:PRO:HD3	1.73	0.70
2:H:2:VAL:H	2:H:26:GLY:HA3	1.56	0.70
2:H:225:ARG:HG2	2:H:227:CYS:O	1.92	0.70
1:L:135:PHE:CE2	2:H:192:SER:HB3	2.26	0.69
2:H:6:GLN:NE2	2:H:6:GLN:H	1.91	0.69
2:H:6:GLN:HE21	2:H:6:GLN:H	1.39	0.69
1:L:144:ILE:HG22	1:L:163:TRP:CZ3	2.29	0.68
2:H:73:ASP:OD1	2:H:75:ALA:HB3	1.93	0.68
1:L:31:ASN:ND2	3:L:388:HOH:O	2.27	0.68
1:L:4:LEU:HD22	1:L:23:CYS:SG	2.34	0.68
2:H:103[B]:ARG:HA	3:H:462:HOH:O	1.94	0.67
1:L:42:GLU:HG2	1:L:43:SER:N	2.09	0.67
2:H:107[B]:GLY:O	2:H:108[B]:ASN:HB2	1.95	0.67
1:L:169:LYS:HB2	3:L:414:HOH:O	1.94	0.67
1:L:108:ARG:NH1	1:L:109:ALA:O	2.28	0.67
2:H:225:ARG:HD2	2:H:225:ARG:H	1.60	0.67
2:H:184:SER:O	2:H:186:LEU:HD12	1.94	0.66
1:L:90:GLN:NE2	1:L:93:SER:H	1.91	0.66
2:H:18:LEU:O	2:H:83:MET:HG2	1.95	0.66
1:L:55:ILE:HG13	1:L:56:SER:N	2.11	0.65
2:H:223:VAL:O	2:H:225:ARG:N	2.30	0.65
1:L:184:ASP:HB3	3:L:270:HOH:O	1.97	0.64
2:H:200:ARG:HA	2:H:224:PRO:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:28:SER:OG	1:L:29:ILE:N	2.21	0.63
1:L:49:LYS:HB2	1:L:53:GLN:O	1.98	0.63
1:L:211:ARG:O	1:L:212:ASN:HB3	1.98	0.63
2:H:83:MET:CE	2:H:121:VAL:HG11	2.28	0.63
2:H:200:ARG:CD	2:H:201:PRO:HD3	2.28	0.63
2:H:204:THR:HA	2:H:223:VAL:HG22	1.79	0.63
2:H:201:PRO:HA	2:H:223:VAL:HG13	1.80	0.62
1:L:197:THR:HG23	1:L:204:PRO:HB3	1.81	0.62
2:H:172:SER:OG	2:H:173:SER:N	2.32	0.62
2:H:103[A]:ARG:HA	3:H:462:HOH:O	1.98	0.62
1:L:31:ASN:HA	3:L:432:HOH:O	1.99	0.62
1:L:52:SER:HA	1:L:64:GLY:O	1.99	0.61
1:L:39:LYS:HE2	3:L:254:HOH:O	1.98	0.61
2:H:1:GLU:HA	2:H:3:GLN:NE2	2.15	0.61
1:L:13:VAL:HG23	3:L:358:HOH:O	2.00	0.61
1:L:15:PRO:HA	1:L:78:VAL:O	2.00	0.61
2:H:72:ARG:HE	2:H:74:ASN:HD21	1.48	0.60
1:L:142:LYS:NZ	3:L:313:HOH:O	2.34	0.60
2:H:182:LEU:HD21	3:H:328:HOH:O	2.01	0.60
1:L:32:ASN:ND2	1:L:32:ASN:N	2.49	0.60
1:L:80:THR:O	1:L:83:PHE:HD1	1.83	0.60
2:H:101[B]:PHE:CB	2:H:103[B]:ARG:HH11	2.14	0.60
2:H:200:ARG:CB	2:H:201:PRO:HD3	2.31	0.60
2:H:1:GLU:OE1	2:H:3:GLN:NE2	2.33	0.60
2:H:201:PRO:HA	2:H:223:VAL:HG12	1.82	0.60
2:H:147:MET:O	3:H:396:HOH:O	2.16	0.60
2:H:107[A]:GLY:HA2	3:H:459:HOH:O	2.01	0.60
2:H:200:ARG:HD3	2:H:224:PRO:HB2	1.85	0.59
2:H:6:GLN:HE22	2:H:117:GLN:H	1.48	0.59
1:L:108:ARG:HD3	1:L:109:ALA:O	2.02	0.59
2:H:200:ARG:HD2	2:H:201:PRO:HD3	1.84	0.59
2:H:32:TYR:CG	2:H:98:ARG:HD2	2.38	0.59
2:H:174:GLY:HA2	3:H:275:HOH:O	2.01	0.59
1:L:126:THR:HA	3:L:395:HOH:O	2.03	0.58
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.68	0.58
2:H:51:ILE:HG13	2:H:58:ILE:HG22	1.85	0.58
2:H:64:VAL:HG22	2:H:68:PHE:CD2	2.40	0.57
1:L:90:GLN:HB2	3:L:441:HOH:O	2.03	0.57
1:L:91:SER:HB2	2:H:110[A]:TYR:H	1.69	0.57
2:H:196:PRO:O	2:H:199:PRO:HD2	2.04	0.57
2:H:99:HIS:HB3	2:H:110[B]:TYR:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:149:THR:HG23	3:H:242:HOH:O	2.04	0.57
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.34	0.57
2:H:6:GLN:OE1	2:H:116:GLY:HA3	2.05	0.57
2:H:222:ILE:O	2:H:225:ARG:CZ	2.53	0.56
2:H:58:ILE:HD12	2:H:60:TYR:OH	2.05	0.56
2:H:140:SER:CB	2:H:200:ARG:HH12	2.18	0.56
2:H:108[B]:ASN:O	2:H:109[B]:TYR:CD1	2.58	0.56
1:L:32:ASN:HD22	1:L:32:ASN:N	2.03	0.56
2:H:104[B]:TYR:O	2:H:105[B]:ASP:HB2	2.05	0.56
2:H:58:ILE:HG13	2:H:60:TYR:CE2	2.41	0.56
1:L:89:GLN:HB2	1:L:98:PHE:CD2	2.41	0.56
2:H:101[B]:PHE:HB2	2:H:103[B]:ARG:HH11	1.71	0.56
2:H:67:ARG:HD2	2:H:85:SER:HB3	1.88	0.56
1:L:41:HIS:HA	3:L:298:HOH:O	2.06	0.56
2:H:135:PRO:HB3	2:H:222:ILE:HD13	1.88	0.56
2:H:67:ARG:HB3	2:H:84:SER:O	2.07	0.55
1:L:39:LYS:HZ2	1:L:81:GLU:C	2.10	0.55
2:H:133:VAL:HB	2:H:218:VAL:HG11	1.88	0.55
2:H:208:ASN:ND2	3:H:306:HOH:O	2.33	0.55
2:H:16:ARG:HH11	2:H:16:ARG:HB2	1.71	0.55
2:H:208:ASN:ND2	2:H:219:ASP:OD1	2.35	0.55
1:L:144:ILE:HG22	1:L:163:TRP:HZ3	1.72	0.54
2:H:13:ASN:HB2	2:H:16:ARG:HD2	1.88	0.54
2:H:83:MET:HE3	2:H:121:VAL:HG11	1.88	0.54
2:H:43:LYS:HA	2:H:43:LYS:HE3	1.90	0.54
2:H:12:VAL:CG2	2:H:18:LEU:HG	2.30	0.54
2:H:48:VAL:O	2:H:64:VAL:HG11	2.08	0.53
1:L:191:SER:HB3	3:L:329:HOH:O	2.08	0.53
1:L:115:VAL:HB	1:L:136:LEU:HD13	1.89	0.53
1:L:62:PHE:CE1	1:L:75:ILE:HG12	2.43	0.53
2:H:15:GLY:N	2:H:86:LEU:O	2.30	0.53
2:H:108[B]:ASN:ND2	3:H:459:HOH:O	2.41	0.53
2:H:208:ASN:N	3:H:300:HOH:O	2.42	0.53
2:H:221:LYS:H	2:H:221:LYS:HE3	1.74	0.53
2:H:83:MET:HB2	2:H:86:LEU:HD21	1.92	0.52
2:H:93:LEU:HD21	3:H:354:HOH:O	2.09	0.52
1:L:3:LEU:HD12	3:L:404:HOH:O	2.09	0.52
2:H:41:PRO:O	2:H:43:LYS:HD2	2.09	0.52
1:L:11:LEU:HD23	1:L:104:LEU:CD2	2.35	0.52
2:H:48:VAL:HG12	2:H:64:VAL:HG21	1.92	0.52
2:H:99:HIS:HB3	2:H:110[A]:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:HIS:O	1:L:89:GLN:N	2.37	0.51
1:L:28:SER:O	1:L:29:ILE:HG13	2.09	0.51
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.46	0.51
1:L:136:LEU:HD23	1:L:175:MET:SD	2.51	0.51
1:L:28:SER:O	1:L:68:GLY:O	2.28	0.51
1:L:204:PRO:HG2	3:L:300:HOH:O	2.10	0.51
1:L:212:ASN:OD1	1:L:213:GLU:N	2.39	0.50
2:H:221:LYS:CE	2:H:221:LYS:H	2.25	0.50
1:L:154:GLU:HG3	3:L:262:HOH:O	2.09	0.50
2:H:52:SER:O	2:H:72:ARG:NH1	2.45	0.50
1:L:42:GLU:HG2	1:L:43:SER:H	1.75	0.50
1:L:36:TYR:HE2	1:L:89:GLN:HB3	1.77	0.50
2:H:175:VAL:HG22	3:H:274:HOH:O	2.12	0.50
2:H:140:SER:HA	2:H:200:ARG:HH22	1.77	0.50
2:H:87:ARG:HG3	2:H:87:ARG:HH11	1.77	0.49
1:L:155:ARG:NH2	1:L:185:GLU:OE2	2.44	0.49
2:H:9:GLY:N	2:H:119:THR:HG21	2.18	0.49
2:H:101[A]:PHE:HB2	2:H:103[A]:ARG:HH11	1.76	0.49
3:L:393:HOH:O	2:H:149:THR:HG21	2.12	0.49
2:H:43:LYS:N	2:H:43:LYS:HD2	2.28	0.49
2:H:188:THR:O	3:H:248:HOH:O	2.20	0.49
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.11	0.49
1:L:189:HIS:HE1	3:L:336:HOH:O	1.96	0.49
2:H:8:GLY:HA2	3:H:385:HOH:O	2.13	0.49
1:L:6:GLN:HE21	1:L:99:GLY:CA	2.26	0.48
1:L:123:GLU:HA	3:L:319:HOH:O	2.13	0.48
1:L:124:GLN:HG2	1:L:129:GLY:O	2.12	0.48
1:L:121:SER:O	1:L:125:LEU:HG	2.14	0.48
1:L:149:LYS:HB2	1:L:193:THR:HB	1.95	0.48
2:H:200:ARG:CB	2:H:201:PRO:CD	2.86	0.48
1:L:163:TRP:CD1	1:L:163:TRP:N	2.82	0.48
2:H:72:ARG:HE	2:H:74:ASN:ND2	2.11	0.47
2:H:133:VAL:O	2:H:220:LYS:HE3	2.14	0.47
1:L:31:ASN:O	1:L:50:TYR:HA	2.15	0.47
2:H:130:PRO:HB3	2:H:214:SER:OG	2.14	0.47
2:H:42:GLU:N	2:H:42:GLU:OE1	2.47	0.47
1:L:80:THR:O	1:L:83:PHE:CD1	2.67	0.47
2:H:29:PHE:CD2	2:H:77:ASN:HA	2.49	0.47
2:H:149:THR:C	2:H:150:LEU:HD12	2.35	0.47
1:L:155:ARG:HD3	1:L:157:ASN:O	2.14	0.47
1:L:97:THR:HA	3:L:369:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:58:ILE:HG13	2:H:60:TYR:HE2	1.79	0.47
1:L:31:ASN:ND2	3:L:432:HOH:O	2.49	0.46
2:H:53:GLY:HA3	2:H:102[A]:TYR:HE2	1.80	0.46
2:H:103[B]:ARG:C	2:H:105[B]:ASP:H	2.19	0.46
2:H:202:SER:OG	2:H:203:GLU:N	2.49	0.46
1:L:49:LYS:O	1:L:53:GLN:HB2	2.16	0.46
1:L:155:ARG:NH1	3:L:429:HOH:O	2.48	0.46
2:H:130:PRO:HB3	2:H:214:SER:CB	2.46	0.45
1:L:170:ASP:O	1:L:171:SER:HB2	2.16	0.45
2:H:222:ILE:O	2:H:225:ARG:NH1	2.49	0.45
2:H:29:PHE:O	2:H:72:ARG:NH2	2.50	0.45
2:H:73:ASP:C	2:H:73:ASP:OD1	2.54	0.45
2:H:89:GLU:HG3	3:H:353:HOH:O	2.16	0.45
2:H:40:THR:OG1	2:H:44:ARG:HD2	2.16	0.45
1:L:90:GLN:HE21	1:L:92:ASN:HB3	1.81	0.45
2:H:198:SER:H	2:H:199:PRO:CD	2.30	0.45
2:H:53:GLY:HA3	2:H:102[B]:TYR:HE2	1.81	0.44
1:L:21:LEU:HD11	1:L:104:LEU:CD1	2.45	0.44
1:L:211:ARG:O	1:L:212:ASN:CB	2.64	0.44
2:H:182:LEU:HG	2:H:183:GLN:N	2.33	0.44
2:H:178:PHE:O	2:H:189:LEU:HG	2.17	0.44
2:H:6:GLN:HE22	2:H:117:GLN:N	2.13	0.44
1:L:32:ASN:HB2	1:L:92:ASN:HB2	2.00	0.43
1:L:35:TRP:CE3	1:L:73:LEU:HD12	2.53	0.43
2:H:225:ARG:CG	2:H:227:CYS:O	2.64	0.43
1:L:169:LYS:HD2	1:L:169:LYS:HA	1.90	0.43
1:L:32:ASN:ND2	2:H:109[A]:TYR:CD2	2.86	0.43
2:H:102[A]:TYR:HB2	2:H:110[A]:TYR:HH	1.80	0.43
1:L:112:ALA:HB2	1:L:200:THR:HG21	2.01	0.43
2:H:114:HIS:CE1	3:H:468:HOH:O	2.71	0.43
1:L:61:ARG:HH22	1:L:82:ASP:CG	2.19	0.43
2:H:181:VAL:HG22	3:H:248:HOH:O	2.18	0.43
1:L:11:LEU:HD11	3:L:438:HOH:O	2.18	0.43
2:H:6:GLN:HA	2:H:21:SER:O	2.19	0.43
2:H:43:LYS:H	2:H:43:LYS:HD2	1.83	0.43
1:L:26:SER:OG	1:L:27:GLN:OE1	2.15	0.43
2:H:36:TRP:NE1	2:H:81:LEU:HB2	2.34	0.42
1:L:120:PRO:HG3	1:L:130:ALA:HB1	2.01	0.42
1:L:19:VAL:HG13	1:L:75:ILE:HB	2.01	0.42
1:L:18:SER:HA	1:L:75:ILE:O	2.19	0.42
2:H:162:VAL:HG23	2:H:211:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100[A]:PRO:HD3	2:H:111:ALA:O	2.19	0.42
1:L:48:ILE:HG21	1:L:64:GLY:HA3	2.02	0.42
1:L:8:PRO:HB3	3:L:292:HOH:O	2.19	0.42
2:H:1:GLU:CA	2:H:3:GLN:HE21	2.27	0.42
1:L:174:SER:HB3	2:H:178:PHE:HE2	1.84	0.42
1:L:82:ASP:O	1:L:86:TYR:OH	2.25	0.42
2:H:178:PHE:HA	2:H:179:PRO:HD3	1.89	0.42
1:L:197:THR:HG21	3:L:240:HOH:O	2.18	0.42
1:L:197:THR:HG23	1:L:204:PRO:HA	2.02	0.42
2:H:174:GLY:O	2:H:193:VAL:HA	2.20	0.41
1:L:10:THR:HG23	3:L:302:HOH:O	2.20	0.41
2:H:133:VAL:HG21	2:H:209:VAL:HG13	2.01	0.41
2:H:145:ASN:ND2	3:H:457:HOH:O	2.53	0.41
2:H:165:THR:O	3:H:300:HOH:O	2.21	0.41
1:L:155:ARG:HB2	1:L:155:ARG:HH11	1.85	0.41
2:H:6:GLN:NE2	2:H:118:GLY:H	2.19	0.41
2:H:64:VAL:CG2	2:H:68:PHE:CD2	3.03	0.41
1:L:149:LYS:C	1:L:150:ILE:HD12	2.41	0.41
1:L:96:LEU:H	1:L:96:LEU:HG	1.67	0.41
2:H:146:SER:HB3	3:H:273:HOH:O	2.20	0.41
1:L:71:PHE:N	1:L:71:PHE:CD1	2.89	0.41
1:L:61:ARG:HH11	1:L:61:ARG:HD2	1.66	0.41
2:H:100[B]:PRO:HD3	2:H:111:ALA:O	2.21	0.40
2:H:107[B]:GLY:O	2:H:108[B]:ASN:CB	2.67	0.40
1:L:155:ARG:HG2	1:L:156:GLN:N	2.35	0.40
2:H:160:GLU:HB2	3:H:293:HOH:O	2.20	0.40
1:L:91:SER:HB2	2:H:110[B]:TYR:H	1.85	0.40
2:H:64:VAL:HG22	2:H:68:PHE:CE2	2.56	0.40
1:L:188:ARG:CD	3:L:341:HOH:O	2.69	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:333:HOH:O	3:L:333:HOH:O[2_975]	1.54	0.66
2:H:77:ASN:CB	3:H:273:HOH:O[2_985]	1.72	0.48
2:H:87:ARG:CB	3:L:436:HOH:O[4_476]	1.74	0.46
2:H:16:ARG:NH1	3:L:374:HOH:O[4_476]	1.75	0.45
1:L:161:ASN:OD1	2:H:106[A]:GLY:CA[3_845]	1.81	0.39
1:L:190:ASN:OD1	3:L:333:HOH:O[2_975]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:TYR:N	3:L:303:HOH:O[3_855]	2.03	0.17
1:L:190:ASN:ND2	3:L:333:HOH:O[2_975]	2.10	0.10
1:L:161:ASN:OD1	2:H:106[A]:GLY:C[3_845]	2.10	0.10
2:H:87:ARG:CG	3:L:318:HOH:O[4_476]	2.12	0.08

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	L	212/214 (99%)	190 (90%)	12 (6%)	10 (5%)	3 0
2	H	236/227 (104%)	198 (84%)	24 (10%)	14 (6%)	2 0
All	All	448/441 (102%)	388 (87%)	36 (8%)	24 (5%)	3 0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	28	SER
1	L	30	SER
1	L	51	ALA
1	L	56	SER
1	L	212	ASN
2	H	105[A]	ASP
2	H	105[B]	ASP
2	H	108[A]	ASN
2	H	108[B]	ASN
2	H	200	ARG
2	H	223	VAL
1	L	41	HIS
2	H	57	TYR
1	L	213	GLU
2	H	142	ALA
2	H	198	SER

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Mol	Chain	Res	Type
2	H	224	PRO
2	H	92	ALA
2	H	101[A]	PHE
2	H	101[B]	PHE
1	L	11	LEU
2	H	2	VAL
1	L	32	ASN
1	L	29	ILE

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	L	193/193 (100%)	154 (80%)	39 (20%)	1 0
2	H	202/193 (105%)	159 (79%)	43 (21%)	1 0
All	All	395/386 (102%)	313 (79%)	82 (21%)	1 0

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	GLU
1	L	7	SER
1	L	12	SER
1	L	13	VAL
1	L	19	VAL
1	L	22	SER
1	L	24	ARG
1	L	29	ILE
1	L	31	ASN
1	L	32	ASN
1	L	33	LEU
1	L	41	HIS
1	L	47	LEU
1	L	55	ILE

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Mol	Chain	Res	Type
1	L	65	SER
1	L	69	THR
1	L	70	ASP
1	L	73	LEU
1	L	74	SER
1	L	81	GLU
1	L	90	GLN
1	L	94	TRP
1	L	104	LEU
1	L	108	ARG
1	L	123	GLU
1	L	126	THR
1	L	134	CYS
1	L	142	LYS
1	L	147	LYS
1	L	154	GLU
1	L	155	ARG
1	L	160	LEU
1	L	162	SER
1	L	165	ASP
1	L	187	GLU
1	L	188	ARG
1	L	194	CYS
1	L	197	THR
2	H	6	GLN
2	H	13	ASN
2	H	16	ARG
2	H	18	LEU
2	H	19	LYS
2	H	42	GLU
2	H	43	LYS
2	H	44	ARG
2	H	48	VAL
2	H	56	THR
2	H	57	TYR
2	H	71	SER
2	H	83	MET
2	H	85	SER
2	H	101[A]	PHE
2	H	101[B]	PHE
2	H	102[A]	TYR
2	H	102[B]	TYR

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Mol	Chain	Res	Type
2	H	103[A]	ARG
2	H	103[B]	ARG
2	H	117	GLN
2	H	119	THR
2	H	129	THR
2	H	138	PRO
2	H	144	THR
2	H	145	ASN
2	H	148	VAL
2	H	149	THR
2	H	152	CYS
2	H	153	LEU
2	H	162	VAL
2	H	165	THR
2	H	186	LEU
2	H	190	SER
2	H	194	THR
2	H	203	GLU
2	H	204	THR
2	H	206	THR
2	H	207	CYS
2	H	209	VAL
2	H	221	LYS
2	H	225	ARG
2	H	226	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	53	GLN
1	L	90	GLN
1	L	138	ASN
1	L	157	ASN
1	L	161	ASN
2	H	3	GLN
2	H	6	GLN
2	H	74	ASN
2	H	77	ASN
2	H	99	HIS
2	H	145	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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