



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:14 AM UTC

PDB ID : 4IC0 / pdb_00004ic0
Title : Crystal Structure of PAI-1 in Complex with Gallate
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Deposited on : 2012-12-09
Resolution : 2.32 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

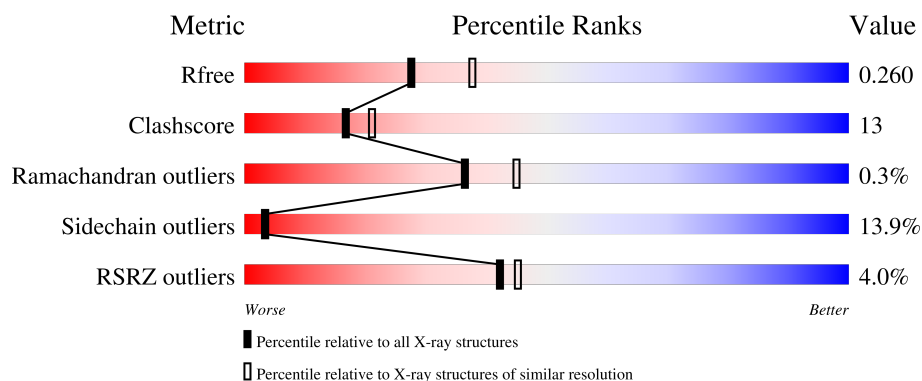
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	379	4% 65% 23% 7% . .
1	B	379	4% 62% 23% 8% . 6%
1	C	379	4% 64% 26% 5% . .
1	D	379	4% 62% 25% 6% . 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GDE	A	401	-	X	X	-
2	GDE	C	401	-	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11613 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.

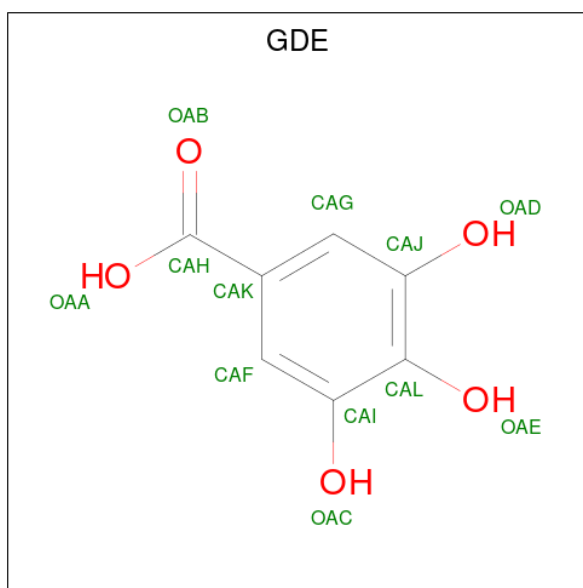
- Molecule 1 is a protein called Plasminogen activator inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2924	1881	499	529	15			
1	B	358	Total	C	N	O	S	0	0	0
			2867	1845	488	520	14			
1	C	366	Total	C	N	O	S	0	0	0
			2924	1881	499	529	15			
1	D	359	Total	C	N	O	S	0	0	0
			2874	1850	489	521	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	HIS	ASN	engineered mutation	UNP P05121
A	154	THR	LYS	engineered mutation	UNP P05121
A	158	GLN	ASP	engineered mutation	UNP P05121
A	319	LEU	GLN	engineered mutation	UNP P05121
A	354	ILE	MET	engineered mutation	UNP P05121
B	150	HIS	ASN	engineered mutation	UNP P05121
B	154	THR	LYS	engineered mutation	UNP P05121
B	158	GLN	ASP	engineered mutation	UNP P05121
B	319	LEU	GLN	engineered mutation	UNP P05121
B	354	ILE	MET	engineered mutation	UNP P05121
C	150	HIS	ASN	engineered mutation	UNP P05121
C	154	THR	LYS	engineered mutation	UNP P05121
C	158	GLN	ASP	engineered mutation	UNP P05121
C	319	LEU	GLN	engineered mutation	UNP P05121
C	354	ILE	MET	engineered mutation	UNP P05121
D	150	HIS	ASN	engineered mutation	UNP P05121
D	154	THR	LYS	engineered mutation	UNP P05121
D	158	GLN	ASP	engineered mutation	UNP P05121
D	319	LEU	GLN	engineered mutation	UNP P05121
D	354	ILE	MET	engineered mutation	UNP P05121

- Molecule 2 is 3,4,5-trihydroxybenzoic acid (CCD ID: GDE) (formula: $C_7H_6O_5$).

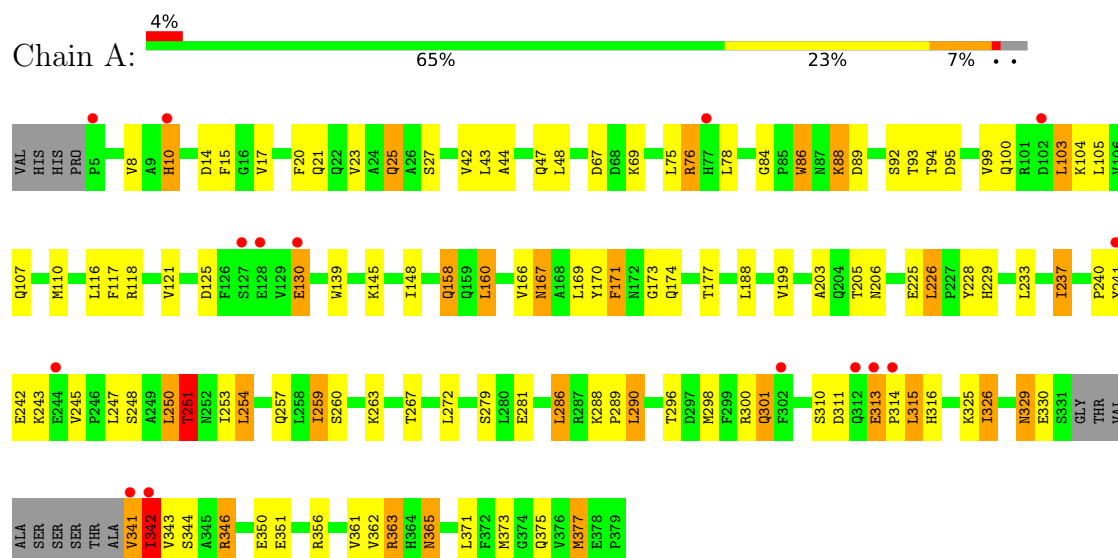


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	7	5		
2	C	1	Total	C	O	0	0
			12	7	5		

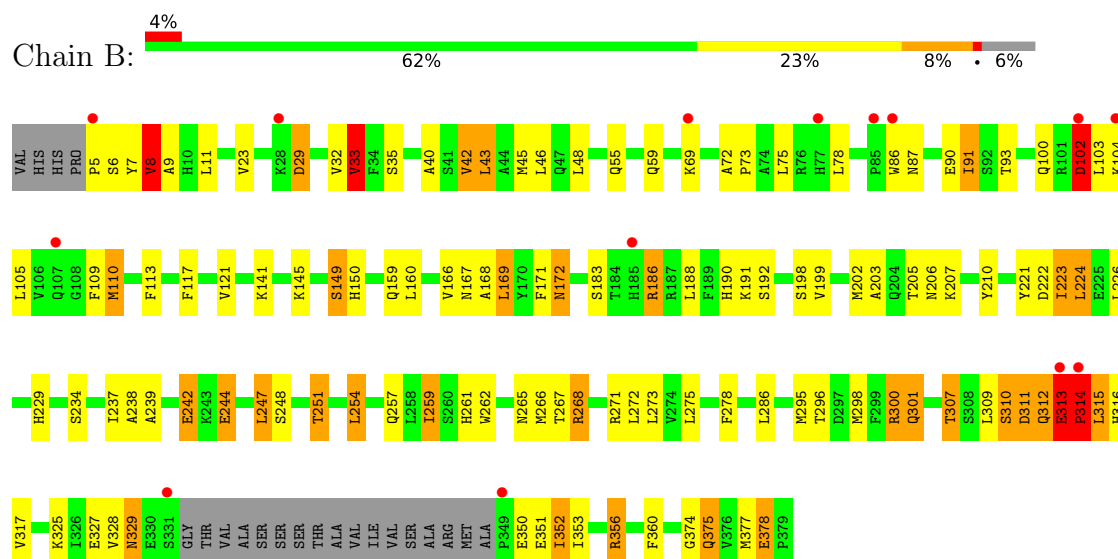
3 Residue-property plots

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.

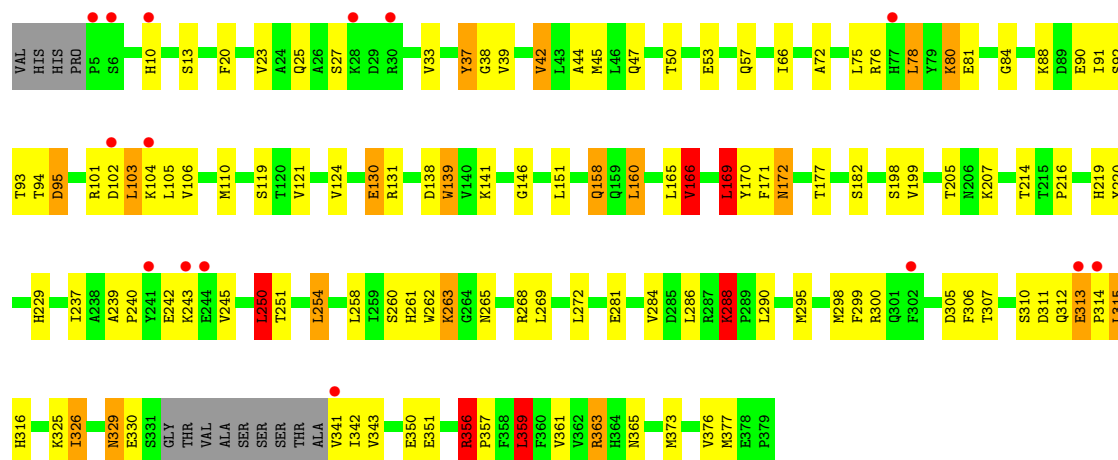
• Molecule 1: Plasminogen activator inhibitor 1



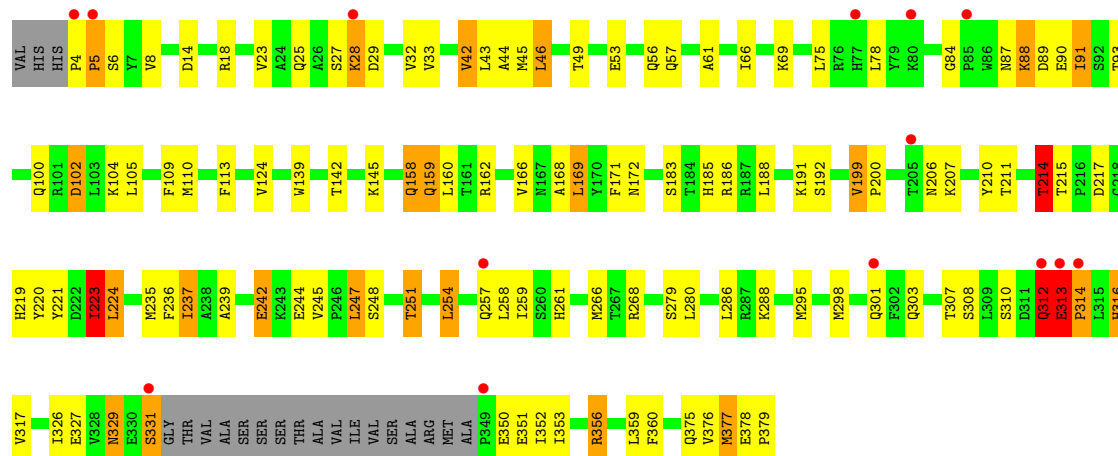
• Molecule 1: Plasminogen activator inhibitor 1



• Molecule 1: Plasminogen activator inhibitor 1



• Molecule 1: Plasminogen activator inhibitor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.28Å 74.99Å 103.87Å 90.91° 93.29° 115.82°	Depositor
Resolution (Å)	38.25 – 2.32 38.25 – 2.32	Depositor EDS
% Data completeness (in resolution range)	94.2 (38.25-2.32) 94.6 (38.25-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.258 0.210 , 0.260	Depositor DCC
R_{free} test set	3860 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11613	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.43	21/2995 (0.7%)	1.34	19/4060 (0.5%)
1	B	1.39	22/2938 (0.7%)	1.20	17/3982 (0.4%)
1	C	1.49	33/2995 (1.1%)	1.25	17/4060 (0.4%)
1	D	1.32	14/2946 (0.5%)	1.26	18/3994 (0.5%)
All	All	1.41	90/11874 (0.8%)	1.26	71/16096 (0.4%)

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	A	0	2
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	6

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	VAL	C-O	-7.58	1.16	1.24
1	B	8	VAL	C-O	-7.56	1.15	1.24
1	C	166	VAL	C-O	-7.46	1.16	1.24
1	B	166	VAL	C-O	-7.43	1.16	1.24
1	D	166	VAL	C-O	-7.32	1.16	1.24
1	B	374	GLY	C-O	-7.19	1.16	1.23
1	A	86	TRP	NE1-CE2	-7.19	1.29	1.37
1	C	39	VAL	C-O	-7.18	1.15	1.24
1	C	219	HIS	CG-ND1	-7.18	1.30	1.38
1	C	170	TYR	C-O	-6.79	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	ALA	C-O	-6.69	1.18	1.24
1	C	229	HIS	CG-ND1	-6.67	1.30	1.38
1	A	316	HIS	CG-ND1	-6.50	1.31	1.38
1	D	316	HIS	CG-ND1	-6.49	1.31	1.38
1	C	356	ARG	C-O	-6.40	1.18	1.24
1	C	316	HIS	CG-ND1	-6.33	1.31	1.38
1	A	279	SER	C-O	-6.28	1.16	1.23
1	A	203	ALA	C-O	-6.21	1.16	1.23
1	D	316	HIS	CD2-NE2	-6.19	1.31	1.37
1	C	38	GLY	C-O	-6.08	1.16	1.23
1	B	307	THR	C-O	-6.06	1.16	1.24
1	B	32	VAL	C-O	-6.05	1.17	1.24
1	A	170	TYR	C-O	-6.04	1.17	1.24
1	A	171	PHE	C-O	-5.99	1.17	1.24
1	C	261	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	239	ALA	C-O	-5.93	1.17	1.24
1	B	43	LEU	C-O	-5.89	1.17	1.24
1	C	42	VAL	C-O	-5.88	1.17	1.24
1	B	316	HIS	CD2-NE2	-5.82	1.31	1.37
1	C	316	HIS	CD2-NE2	-5.80	1.31	1.37
1	D	261	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	342	ILE	CA-C	5.75	1.59	1.52
1	D	377	MET	C-O	-5.74	1.16	1.24
1	C	365	ASN	C-O	-5.72	1.19	1.24
1	B	261	HIS	CD2-NE2	-5.71	1.31	1.37
1	C	219	HIS	CD2-NE2	-5.71	1.31	1.37
1	C	288	LYS	C-O	-5.67	1.17	1.24
1	B	42	VAL	C-O	-5.66	1.17	1.24
1	A	316	HIS	CD2-NE2	-5.62	1.31	1.37
1	C	376	VAL	C-O	-5.62	1.17	1.24
1	B	316	HIS	CG-ND1	-5.62	1.32	1.38
1	D	376	VAL	C-O	-5.60	1.17	1.24
1	C	262	TRP	NE1-CE2	-5.59	1.31	1.37
1	A	251	THR	C-O	-5.59	1.17	1.24
1	A	229	HIS	CD2-NE2	-5.58	1.31	1.37
1	C	261	HIS	CG-ND1	-5.57	1.32	1.38
1	C	357	PRO	C-O	-5.57	1.17	1.23
1	B	9	ALA	C-O	-5.56	1.17	1.24
1	C	81	GLU	C-O	-5.56	1.17	1.24
1	A	10	HIS	CE1-NE2	5.54	1.38	1.32
1	D	261	HIS	CG-ND1	-5.53	1.32	1.38
1	C	361	VAL	C-O	-5.51	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	GLU	C-O	-5.51	1.17	1.24
1	B	190	HIS	CG-ND1	-5.49	1.32	1.38
1	D	219	HIS	CD2-NE2	-5.48	1.31	1.37
1	C	138	ASP	C-O	-5.47	1.17	1.24
1	B	35	SER	C-O	-5.45	1.20	1.25
1	C	76	ARG	C-O	-5.44	1.17	1.24
1	A	362	VAL	C-O	-5.42	1.18	1.24
1	C	377	MET	C-O	-5.40	1.17	1.24
1	A	257	GLN	C-O	-5.37	1.17	1.24
1	C	265	ASN	C-O	-5.36	1.16	1.24
1	C	229	HIS	CD2-NE2	-5.32	1.31	1.37
1	D	220	TYR	C-O	-5.31	1.17	1.23
1	B	375	GLN	C-O	-5.30	1.17	1.24
1	A	229	HIS	CG-ND1	-5.27	1.32	1.38
1	A	286	LEU	C-O	-5.26	1.17	1.24
1	A	167	ASN	C-O	-5.26	1.17	1.23
1	D	214	THR	C-O	-5.26	1.17	1.23
1	B	167	ASN	C-O	-5.25	1.18	1.23
1	C	359	LEU	CA-C	-5.24	1.46	1.52
1	D	219	HIS	CG-ND1	-5.22	1.32	1.38
1	D	317	VAL	C-O	-5.22	1.18	1.23
1	A	228	TYR	C-O	-5.19	1.16	1.23
1	B	190	HIS	CD2-NE2	-5.18	1.32	1.37
1	D	139	TRP	NE1-CE2	-5.13	1.31	1.37
1	B	40	ALA	C-O	-5.13	1.18	1.24
1	C	139	TRP	NE1-CE2	-5.13	1.31	1.37
1	A	361	VAL	C-O	-5.12	1.18	1.24
1	C	80	LYS	C-O	-5.12	1.18	1.24
1	A	344	SER	C-O	-5.11	1.17	1.23
1	B	301	GLN	C-O	-5.09	1.18	1.24
1	B	315	LEU	C-O	-5.08	1.17	1.23
1	C	37	TYR	C-O	-5.06	1.18	1.24
1	D	258	LEU	C-O	-5.05	1.18	1.24
1	A	76	ARG	C-O	-5.04	1.18	1.24
1	B	150	HIS	CG-ND1	-5.03	1.32	1.38
1	C	214	THR	C-O	-5.02	1.18	1.24
1	A	377	MET	C-O	-5.01	1.17	1.24
1	C	216	PRO	C-O	-5.00	1.17	1.24

All (71) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	VAL	N-CA-C	15.17	128.92	108.89
1	A	342	ILE	N-CA-C	11.84	125.45	108.17
1	C	250	LEU	N-CA-C	10.72	123.05	111.36
1	A	343	VAL	CB-CA-C	-10.70	97.24	111.15
1	A	342	ILE	CA-C-N	9.83	135.22	121.66
1	A	342	ILE	C-N-CA	9.83	135.22	121.66
1	A	314	PRO	N-CA-C	-8.82	94.29	112.47
1	A	330	GLU	N-CA-C	7.78	119.76	111.28
1	A	103	LEU	N-CA-C	7.47	121.07	110.23
1	C	177	THR	CA-C-N	7.19	127.24	119.90
1	C	177	THR	C-N-CA	7.19	127.24	119.90
1	D	42	VAL	CB-CA-C	-7.15	100.68	112.26
1	D	288	LYS	CA-C-N	-7.11	111.46	119.28
1	D	288	LYS	C-N-CA	-7.11	111.46	119.28
1	C	42	VAL	CB-CA-C	-7.07	102.47	112.22
1	A	177	THR	CA-C-N	7.03	127.00	119.76
1	A	177	THR	C-N-CA	7.03	127.00	119.76
1	B	91	ILE	N-CA-C	6.88	118.04	107.78
1	A	173	GLY	N-CA-C	6.62	121.63	112.37
1	D	46	LEU	N-CA-C	-6.30	104.41	111.28
1	D	313	GLU	CA-C-N	-6.30	111.96	119.84
1	D	313	GLU	C-N-CA	-6.30	111.96	119.84
1	C	263	LYS	CA-C-N	6.30	126.97	119.98
1	C	263	LYS	C-N-CA	6.30	126.97	119.98
1	D	84	GLY	CA-C-N	6.20	125.69	119.24
1	D	84	GLY	C-N-CA	6.20	125.69	119.24
1	A	290	LEU	N-CA-C	6.17	117.67	111.07
1	A	342	ILE	N-CA-CB	-6.09	101.72	111.58
1	B	8	VAL	N-CA-CB	6.07	119.68	110.58
1	D	32	VAL	CB-CA-C	-6.04	102.50	111.80
1	B	309	LEU	N-CA-C	5.99	117.61	111.14
1	B	314	PRO	CA-N-CD	-5.95	103.67	112.00
1	D	199	VAL	CA-C-N	-5.89	113.46	119.83
1	D	199	VAL	C-N-CA	-5.89	113.46	119.83
1	B	42	VAL	N-CA-C	5.89	116.67	110.72
1	D	142	THR	N-CA-C	5.88	117.77	111.36
1	B	6	SER	N-CA-C	-5.83	105.27	112.38
1	B	29	ASP	N-CA-C	5.83	119.64	111.30
1	A	365	ASN	CA-C-N	-5.81	113.77	119.64
1	A	365	ASN	C-N-CA	-5.81	113.77	119.64
1	D	27	SER	CB-CA-C	-5.81	103.31	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243	LYS	N-CA-C	5.70	119.49	112.54
1	C	103	LEU	N-CA-C	5.69	118.50	109.96
1	D	259	ILE	CB-CA-C	-5.68	104.47	112.14
1	A	241	TYR	N-CA-C	5.53	120.09	113.23
1	B	301	GLN	CA-C-N	-5.51	114.01	122.60
1	B	301	GLN	C-N-CA	-5.51	114.01	122.60
1	B	265	ASN	N-CA-C	5.50	119.98	113.16
1	B	242	GLU	N-CA-C	5.44	118.93	110.17
1	B	307	THR	N-CA-C	5.42	119.16	112.54
1	D	266	MET	N-CA-C	5.42	118.76	110.20
1	D	188	LEU	N-CA-C	5.36	117.95	109.96
1	B	33	VAL	CB-CA-C	-5.31	102.32	110.50
1	A	371	LEU	N-CA-C	-5.28	105.11	112.45
1	C	169	LEU	CA-CB-CG	5.25	134.67	116.30
1	B	312	GLN	N-CA-C	5.25	117.04	109.07
1	C	363	ARG	CG-CD-NE	5.24	123.53	112.00
1	B	42	VAL	CB-CA-C	-5.23	105.01	112.22
1	D	91	ILE	N-CA-C	5.16	115.55	108.12
1	B	317	VAL	CB-CA-C	-5.15	105.67	111.23
1	A	84	GLY	CA-C-N	5.11	124.78	119.56
1	A	84	GLY	C-N-CA	5.11	124.78	119.56
1	C	330	GLU	N-CA-C	5.11	116.66	111.14
1	B	149	SER	N-CA-C	5.09	120.34	113.72
1	C	131	ARG	N-CA-C	5.08	117.72	111.82
1	C	220	TYR	N-CA-C	5.08	118.10	109.76
1	C	95	ASP	N-CA-C	-5.07	101.61	109.72
1	C	101	ARG	N-CA-C	5.06	116.49	111.07
1	D	223	ILE	CB-CA-C	-5.04	102.97	110.33
1	C	42	VAL	N-CA-CB	5.02	118.11	110.58
1	C	284	VAL	N-CA-C	5.01	115.52	108.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	GLU	Peptide
1	A	341	VAL	Peptide
1	B	102	ASP	Peptide
1	C	102	ASP	Peptide
1	C	313	GLU	Peptide
1	D	312	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2924	0	2926	83	0
1	B	2867	0	2862	78	0
1	C	2924	0	2926	68	0
1	D	2874	0	2869	70	0
2	A	12	0	2	5	0
2	C	12	0	2	3	0
All	All	11613	0	11587	298	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 13.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:MET:HB3	1:D:298:MET:HE2	1.15	1.15
1:A:346:ARG:HH11	1:A:346:ARG:CG	1.60	1.14
1:A:247:LEU:HD12	1:A:377:MET:HE1	1.30	1.11
1:C:158:GLN:HE22	1:C:160:LEU:HB2	1.01	1.07
1:A:205:THR:HG22	1:A:272:LEU:HA	1.33	1.07
1:B:295:MET:HB3	1:B:298:MET:HE2	1.14	1.06
1:C:93:THR:HG22	1:C:169:LEU:HD13	1.26	1.06
1:A:93:THR:HG22	1:A:169:LEU:HD23	1.38	1.03
1:C:93:THR:CG2	1:C:169:LEU:HD13	1.91	0.98
1:B:93:THR:HG22	1:B:169:LEU:CD1	1.94	0.98
1:A:341:VAL:O	1:A:342:ILE:HG13	1.63	0.97
1:B:295:MET:HB3	1:B:298:MET:CE	1.94	0.97
1:C:312:GLN:O	1:C:313:GLU:HG2	1.65	0.97
1:A:341:VAL:C	1:A:342:ILE:HG13	1.87	0.96
1:D:206:ASN:HD22	1:D:207:LYS:H	1.13	0.96
1:A:20:PHE:CD2	1:A:373:MET:HE2	2.00	0.95
1:C:312:GLN:C	1:C:313:GLU:CG	2.39	0.95
1:C:158:GLN:NE2	1:C:160:LEU:HB2	1.82	0.94
1:A:346:ARG:HH11	1:A:346:ARG:HG3	1.31	0.94
1:D:295:MET:CB	1:D:298:MET:HE2	1.98	0.93
1:B:221:TYR:CE1	1:B:223:ILE:HD11	2.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:GLN:C	1:C:313:GLU:HG3	1.93	0.93
1:D:295:MET:HB3	1:D:298:MET:CE	1.99	0.92
1:B:93:THR:HG22	1:B:169:LEU:HD13	1.53	0.91
1:B:247:LEU:HD12	1:B:377:MET:HE1	1.52	0.91
1:D:248:SER:HA	1:D:251:THR:OG1	1.69	0.91
1:A:346:ARG:HH11	1:A:346:ARG:HG2	1.38	0.88
1:A:346:ARG:HG3	1:A:346:ARG:NH1	1.84	0.87
1:B:5:PRO:HD2	1:B:7:TYR:HB3	1.57	0.87
1:A:248:SER:HA	1:A:251:THR:CG2	2.04	0.86
1:A:342:ILE:N	1:A:342:ILE:HD12	1.90	0.86
1:B:206:ASN:HD22	1:B:207:LYS:H	1.24	0.86
1:A:247:LEU:CD1	1:A:377:MET:HE1	2.06	0.85
1:B:45:MET:HE3	1:B:113:PHE:HZ	1.41	0.85
1:A:341:VAL:C	1:A:342:ILE:CG1	2.49	0.83
1:B:375:GLN:HB2	1:B:377:MET:HE3	1.57	0.83
1:A:93:THR:CG2	1:A:169:LEU:HD23	2.09	0.83
1:A:341:VAL:O	1:A:342:ILE:CD1	2.29	0.81
1:C:93:THR:HG22	1:C:169:LEU:CD1	2.09	0.81
1:A:341:VAL:O	1:A:342:ILE:CG1	2.29	0.80
1:D:375:GLN:HB2	1:D:377:MET:HE3	1.63	0.80
1:B:248:SER:HA	1:B:251:THR:OG1	1.81	0.80
1:B:5:PRO:N	1:B:8:VAL:HG22	1.98	0.79
1:A:42:VAL:HG11	1:A:167:ASN:HB2	1.65	0.78
1:C:20:PHE:CD2	1:C:373:MET:HE2	2.19	0.78
1:B:93:THR:CG2	1:B:169:LEU:HD13	2.14	0.78
1:D:104:LYS:H	1:D:312:GLN:NE2	1.81	0.78
1:C:312:GLN:O	1:C:313:GLU:CG	2.30	0.77
1:D:301:GLN:HE21	1:D:316:HIS:CD2	2.00	0.77
1:B:93:THR:HG22	1:B:169:LEU:HD12	1.66	0.77
1:A:375:GLN:HB2	1:A:377:MET:HE3	1.67	0.75
1:B:29:ASP:OD1	1:B:192:SER:OG	2.01	0.75
1:D:33:VAL:HG12	1:D:360:PHE:HZ	1.50	0.75
1:A:375:GLN:HB2	1:A:377:MET:CE	2.17	0.75
1:D:251:THR:HA	1:D:254:LEU:HD22	1.68	0.74
1:D:199:VAL:HG11	1:D:379:PRO:HB2	1.69	0.74
1:A:95:ASP:H	2:A:401:GDE:HAF	1.53	0.73
1:A:95:ASP:H	2:A:401:GDE:CAF	2.01	0.73
1:B:251:THR:HA	1:B:254:LEU:CD2	2.19	0.73
1:B:375:GLN:HB2	1:B:377:MET:CE	2.18	0.72
1:B:45:MET:HE3	1:B:113:PHE:CZ	2.25	0.72
1:B:206:ASN:ND2	1:B:207:LYS:H	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ARG:NH1	1:D:313:GLU:OE1	2.23	0.71
1:D:247:LEU:HD12	1:D:377:MET:HE1	1.72	0.71
1:A:313:GLU:HB2	1:A:315:LEU:HB2	1.71	0.71
1:A:342:ILE:N	1:A:342:ILE:CD1	2.47	0.71
1:A:296:THR:HB	1:A:300:ARG:HH21	1.55	0.71
1:B:278:PHE:CZ	1:B:328:VAL:HG21	2.25	0.71
1:B:93:THR:CG2	1:B:169:LEU:CD1	2.68	0.71
1:D:206:ASN:ND2	1:D:207:LYS:H	1.89	0.71
1:A:20:PHE:CE2	1:A:373:MET:HE2	2.25	0.70
1:C:272:LEU:HD23	1:C:351:GLU:HG2	1.73	0.70
1:A:248:SER:HA	1:A:251:THR:HG22	1.72	0.70
1:D:206:ASN:HD22	1:D:207:LYS:N	1.90	0.69
1:D:33:VAL:HG12	1:D:360:PHE:CZ	2.27	0.69
1:A:272:LEU:HD23	1:A:351:GLU:HG2	1.75	0.69
1:B:224:LEU:HD11	1:B:352:ILE:HG21	1.75	0.68
1:A:205:THR:HG22	1:A:272:LEU:CA	2.19	0.68
1:B:221:TYR:HE1	1:B:223:ILE:HD11	1.59	0.68
1:A:313:GLU:O	1:A:313:GLU:HG3	1.91	0.68
1:D:295:MET:CB	1:D:298:MET:CE	2.66	0.68
1:C:313:GLU:HB3	1:C:314:PRO:C	2.17	0.68
1:C:240:PRO:HB3	1:C:245:VAL:HB	1.75	0.68
1:D:313:GLU:O	1:D:314:PRO:C	2.34	0.67
1:B:110:MET:HE1	1:B:121:VAL:H	1.60	0.67
1:D:313:GLU:N	1:D:314:PRO:HD2	2.07	0.67
1:B:295:MET:CB	1:B:298:MET:HE2	2.07	0.66
1:D:221:TYR:CE1	1:D:223:ILE:HD11	2.30	0.66
1:B:141:LYS:HG3	1:B:149:SER:HB3	1.77	0.66
1:A:341:VAL:C	1:A:342:ILE:CD1	2.69	0.66
1:B:312:GLN:C	1:B:314:PRO:N	2.54	0.66
1:D:191:LYS:NZ	1:D:378:GLU:OE1	2.18	0.66
1:C:205:THR:HG22	1:C:272:LEU:HA	1.77	0.65
1:B:313:GLU:N	1:B:314:PRO:CD	2.58	0.65
1:C:45:MET:HE1	1:C:95:ASP:CB	2.26	0.65
1:B:312:GLN:O	1:B:314:PRO:N	2.30	0.65
1:B:93:THR:CB	1:B:169:LEU:HD13	2.27	0.64
1:A:346:ARG:CG	1:A:346:ARG:NH1	2.30	0.64
1:A:240:PRO:HB3	1:A:245:VAL:HB	1.80	0.63
1:B:172:ASN:C	1:B:172:ASN:HD22	2.06	0.63
1:B:313:GLU:O	1:B:314:PRO:HB2	1.98	0.63
1:D:248:SER:HA	1:D:251:THR:HG1	1.61	0.63
1:C:95:ASP:CG	2:C:401:GDE:HAF	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:H	1:A:130:GLU:CD	2.06	0.63
1:B:5:PRO:HG2	1:B:7:TYR:H	1.65	0.62
1:A:363:ARG:HD2	1:A:365:ASN:OD1	1.98	0.62
1:C:240:PRO:HD2	1:C:356:ARG:HD2	1.82	0.62
1:C:45:MET:CE	1:C:95:ASP:HB3	2.29	0.62
1:A:341:VAL:C	1:A:342:ILE:HD12	2.25	0.61
1:D:33:VAL:HG13	1:D:280:LEU:HD12	1.82	0.61
1:C:151:LEU:CD1	1:C:166:VAL:HG21	2.31	0.61
1:C:130:GLU:CD	1:C:130:GLU:H	2.08	0.60
1:C:254:LEU:HD22	1:C:258:LEU:HD23	1.83	0.60
1:D:301:GLN:NE2	1:D:316:HIS:HD2	2.00	0.60
1:C:151:LEU:HD11	1:C:166:VAL:HG21	1.85	0.59
1:D:329:ASN:HD22	1:D:331:SER:H	1.51	0.59
1:C:45:MET:HE1	1:C:95:ASP:HB3	1.85	0.58
1:B:5:PRO:N	1:B:8:VAL:CG2	2.65	0.58
1:D:301:GLN:NE2	1:D:316:HIS:CD2	2.71	0.58
1:B:295:MET:CB	1:B:298:MET:CE	2.75	0.58
1:C:95:ASP:OD2	2:C:401:GDE:HAF	2.02	0.58
1:C:45:MET:HE1	1:C:95:ASP:HB2	1.85	0.57
1:B:206:ASN:HD22	1:B:207:LYS:N	1.99	0.57
1:D:93:THR:HB	1:D:169:LEU:HD13	1.87	0.57
1:A:342:ILE:HD12	1:A:342:ILE:H	1.67	0.56
1:D:221:TYR:CD1	1:D:223:ILE:HD11	2.39	0.56
1:B:5:PRO:CD	1:B:7:TYR:HB3	2.34	0.56
1:B:100:GLN:HG3	1:B:102:ASP:HB2	1.88	0.56
1:C:313:GLU:HB3	1:C:315:LEU:N	2.20	0.56
1:A:42:VAL:CG1	1:A:167:ASN:HB2	2.36	0.55
1:D:44:ALA:HB1	1:D:66:ILE:HD13	1.87	0.55
1:B:221:TYR:CD1	1:B:223:ILE:HD11	2.42	0.55
1:D:172:ASN:HB2	1:D:327:GLU:HB2	1.88	0.55
1:C:45:MET:CE	1:C:95:ASP:CB	2.84	0.54
1:D:350:GLU:HG2	1:D:351:GLU:H	1.70	0.54
1:B:210:TYR:C	1:B:266:MET:HG2	2.33	0.54
1:C:313:GLU:CB	1:C:314:PRO:C	2.80	0.54
1:A:329:ASN:C	1:A:329:ASN:HD22	2.16	0.53
1:B:254:LEU:HD12	1:B:259:ILE:HD11	1.90	0.53
1:A:88:LYS:O	1:A:89:ASP:HB2	2.09	0.53
1:B:313:GLU:O	1:B:314:PRO:CB	2.55	0.53
1:D:307:THR:HA	1:D:310:SER:O	2.09	0.53
1:D:45:MET:HE3	1:D:113:PHE:HZ	1.74	0.52
1:B:109:PHE:C	1:B:109:PHE:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:GLU:OE1	1:C:315:LEU:HB2	2.09	0.52
1:D:158:GLN:HG2	1:D:159:GLN:N	2.24	0.52
1:A:95:ASP:N	2:A:401:GDE:HAF	2.23	0.52
1:B:33:VAL:HG13	1:B:360:PHE:HZ	1.75	0.52
1:B:55:GLN:O	1:B:59:GLN:HG3	2.10	0.51
1:A:281:GLU:CB	1:A:325:LYS:HG2	2.40	0.51
1:C:44:ALA:HB1	1:C:66:ILE:HD13	1.93	0.51
1:C:281:GLU:HB2	1:C:325:LYS:HG2	1.91	0.51
1:A:171:PHE:HD2	1:A:326:ILE:HD12	1.76	0.51
1:B:172:ASN:C	1:B:172:ASN:ND2	2.66	0.51
1:B:313:GLU:N	1:B:314:PRO:HD2	2.25	0.51
1:C:207:LYS:HA	1:C:269:LEU:O	2.09	0.51
1:A:247:LEU:O	1:A:251:THR:HG22	2.11	0.51
1:B:90:GLU:O	1:B:171:PHE:HA	2.11	0.51
1:D:100:GLN:HG3	1:D:102:ASP:HB2	1.93	0.50
1:D:104:LYS:H	1:D:312:GLN:HE22	1.55	0.50
1:A:243:LYS:HD3	1:A:356:ARG:NH1	2.25	0.50
1:C:310:SER:O	1:C:313:GLU:OE2	2.29	0.50
1:D:329:ASN:HD22	1:D:329:ASN:C	2.19	0.50
1:A:310:SER:O	1:A:313:GLU:CD	2.55	0.50
1:A:301:GLN:O	1:A:301:GLN:HG2	2.12	0.49
1:C:298:MET:HE2	1:C:299:PHE:CE2	2.48	0.49
1:D:29:ASP:OD1	1:D:192:SER:OG	2.28	0.49
1:D:33:VAL:HG11	1:D:326:ILE:CG2	2.42	0.49
1:C:329:ASN:C	1:C:329:ASN:HD22	2.19	0.49
1:A:225:GLU:C	1:A:226:LEU:HD12	2.37	0.49
1:B:307:THR:HA	1:B:310:SER:O	2.12	0.49
1:D:224:LEU:HD11	1:D:352:ILE:HG21	1.95	0.49
1:C:37:TYR:CE1	1:C:78:LEU:HD13	2.47	0.49
1:C:90:GLU:O	1:C:171:PHE:HA	2.12	0.49
1:A:248:SER:HA	1:A:251:THR:HG23	1.92	0.49
1:A:310:SER:O	1:A:313:GLU:OE1	2.29	0.49
1:A:243:LYS:HD3	1:A:356:ARG:HH11	1.78	0.49
1:C:44:ALA:O	1:C:47:GLN:HB2	2.13	0.49
1:D:236:PHE:O	1:D:360:PHE:HA	2.13	0.49
1:D:93:THR:CB	1:D:169:LEU:HD13	2.43	0.48
1:C:172:ASN:C	1:C:172:ASN:HD22	2.20	0.48
1:D:33:VAL:CG1	1:D:280:LEU:HD12	2.43	0.48
1:A:92:SER:O	1:A:169:LEU:HA	2.13	0.48
1:B:202:MET:CE	1:B:275:LEU:HD23	2.44	0.48
1:C:254:LEU:HD22	1:C:258:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:H	2:A:401:GDE:CAI	2.27	0.48
1:A:250:LEU:O	1:A:250:LEU:HD23	2.14	0.48
1:C:251:THR:CG2	1:C:359:LEU:HD22	2.43	0.48
1:D:53:GLU:O	1:D:57:GLN:HG3	2.14	0.48
1:A:89:ASP:OD2	1:A:145:LYS:HE2	2.14	0.47
1:C:110:MET:HE1	1:C:121:VAL:O	2.14	0.47
1:C:313:GLU:CB	1:C:314:PRO:CA	2.92	0.47
1:A:86:TRP:HH2	1:A:233:LEU:HD11	1.79	0.47
1:A:290:LEU:HD13	1:A:298:MET:HE1	1.96	0.47
1:A:99:VAL:HG22	1:A:100:GLN:N	2.29	0.47
1:C:94:THR:HA	2:C:401:GDE:CAI	2.23	0.47
1:D:5:PRO:HA	1:D:8:VAL:HG22	1.96	0.47
1:B:168:ALA:C	1:B:169:LEU:HD22	2.39	0.47
1:C:53:GLU:O	1:C:57:GLN:HG3	2.14	0.47
1:C:151:LEU:CD1	1:C:166:VAL:CG2	2.92	0.47
1:D:4:PRO:O	1:D:8:VAL:HG13	2.15	0.47
1:B:242:GLU:HB2	1:B:244:GLU:OE2	2.14	0.47
1:C:313:GLU:HB3	1:C:315:LEU:HB2	1.96	0.47
1:C:182:SER:HB2	1:C:343:VAL:HG22	1.96	0.47
1:D:168:ALA:C	1:D:169:LEU:HD22	2.39	0.47
1:A:94:THR:HA	2:A:401:GDE:CAI	2.38	0.47
1:B:272:LEU:HD23	1:B:351:GLU:HG2	1.96	0.47
1:B:311:ASP:OD1	1:B:311:ASP:N	2.47	0.46
1:D:235:MET:HG2	1:D:237:ILE:HD12	1.96	0.46
1:A:158:GLN:OE1	1:A:160:LEU:HB2	2.15	0.46
1:C:141:LYS:HG3	1:C:146:GLY:HA2	1.97	0.46
1:D:28:LYS:HB2	1:D:28:LYS:HE3	1.48	0.46
1:B:296:THR:O	1:B:300:ARG:HD2	2.16	0.46
1:B:248:SER:HA	1:B:251:THR:HG1	1.79	0.46
1:C:106:VAL:HG22	1:C:311:ASP:OD1	2.16	0.46
1:D:313:GLU:O	1:D:313:GLU:OE2	2.34	0.46
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.84	0.46
1:A:226:LEU:HD22	1:A:237:ILE:HD13	1.98	0.45
1:B:186:ARG:HG2	1:B:198:SER:OG	2.16	0.45
1:B:191:LYS:HD2	1:B:378:GLU:CD	2.40	0.45
1:B:259:ILE:HD12	1:B:262:TRP:CZ3	2.50	0.45
1:D:247:LEU:HD12	1:D:377:MET:CE	2.45	0.45
1:C:165:LEU:HD12	1:C:165:LEU:C	2.41	0.45
1:D:214:THR:HG22	1:D:215:THR:O	2.16	0.45
1:D:239:ALA:HB1	1:D:356:ARG:HD2	1.98	0.45
1:B:93:THR:HB	1:B:169:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:GLU:HG3	1:D:245:VAL:HG23	1.99	0.45
1:A:103:LEU:N	1:A:103:LEU:HD12	2.31	0.44
1:D:46:LEU:HD12	1:D:46:LEU:HA	1.78	0.44
1:B:7:TYR:CZ	1:B:11:LEU:HD11	2.53	0.44
1:D:375:GLN:HB2	1:D:377:MET:CE	2.42	0.44
1:C:33:VAL:HG11	1:C:326:ILE:CG2	2.48	0.44
1:A:375:GLN:CB	1:A:377:MET:HE3	2.40	0.44
1:C:207:LYS:O	1:C:268:ARG:NH1	2.51	0.44
1:B:239:ALA:HB1	1:B:356:ARG:HD2	2.00	0.44
1:C:20:PHE:CE2	1:C:373:MET:HE2	2.53	0.44
1:D:88:LYS:O	1:D:89:ASP:C	2.61	0.44
1:A:259:ILE:H	1:A:259:ILE:HG12	1.62	0.43
1:A:281:GLU:HB2	1:A:325:LYS:HG2	2.00	0.43
1:A:17:VAL:HG11	1:A:254:LEU:O	2.18	0.43
1:B:86:TRP:O	1:B:229:HIS:HE1	2.01	0.43
1:D:49:THR:HG22	1:D:109:PHE:CZ	2.54	0.43
1:D:295:MET:HB2	1:D:298:MET:CE	2.48	0.43
1:A:226:LEU:N	1:A:226:LEU:CD1	2.82	0.43
1:D:199:VAL:HG13	1:D:200:PRO:HD2	2.01	0.43
1:D:210:TYR:CD2	1:D:211:THR:N	2.86	0.43
1:B:251:THR:HA	1:B:254:LEU:HD23	1.97	0.43
1:D:33:VAL:HG13	1:D:280:LEU:CD1	2.49	0.43
1:B:72:ALA:HB3	1:B:73:PRO:HD3	2.01	0.43
1:D:90:GLU:O	1:D:171:PHE:HA	2.19	0.43
1:D:221:TYR:CD1	1:D:223:ILE:CD1	3.01	0.43
1:A:341:VAL:HG12	1:A:342:ILE:HG23	1.99	0.43
1:B:45:MET:HA	1:B:117:PHE:CZ	2.54	0.43
1:C:250:LEU:HD13	1:C:359:LEU:HD21	2.00	0.43
1:C:251:THR:HG22	1:C:359:LEU:HD22	2.01	0.43
1:B:350:GLU:HG2	1:B:351:GLU:H	1.84	0.43
1:A:125:ASP:C	1:A:125:ASP:OD1	2.61	0.42
1:B:86:TRP:O	1:B:229:HIS:CE1	2.72	0.42
1:C:104:LYS:HD3	1:C:104:LYS:HA	1.90	0.42
1:C:139:TRP:CD1	1:C:139:TRP:C	2.96	0.42
1:C:50:THR:HG22	1:C:306:PHE:CE1	2.55	0.42
1:C:307:THR:HA	1:C:310:SER:O	2.19	0.42
1:D:18:ARG:NH2	1:D:61:ALA:O	2.52	0.42
1:B:329:ASN:C	1:B:329:ASN:HD22	2.26	0.42
1:C:288:LYS:HD3	1:D:185:HIS:CE1	2.55	0.42
1:C:172:ASN:C	1:C:172:ASN:ND2	2.78	0.42
1:A:311:ASP:N	1:A:311:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:O	1:A:206:ASN:HB3	2.20	0.42
1:C:313:GLU:HB2	1:C:314:PRO:HA	2.02	0.42
1:C:92:SER:O	1:C:169:LEU:HB3	2.20	0.41
1:A:48:LEU:HD22	1:A:117:PHE:CE1	2.55	0.41
1:B:87:ASN:CG	1:B:91:ILE:HG22	2.45	0.41
1:A:14:ASP:O	1:A:15:PHE:C	2.61	0.41
1:A:110:MET:HE1	1:A:121:VAL:O	2.20	0.41
1:B:205:THR:HA	1:B:271:ARG:O	2.20	0.41
1:C:290:LEU:HD22	1:C:295:MET:CE	2.50	0.41
1:D:109:PHE:CD2	1:D:109:PHE:C	2.99	0.41
1:C:250:LEU:CD1	1:C:359:LEU:HD21	2.51	0.41
1:A:44:ALA:O	1:A:47:GLN:HB2	2.21	0.41
1:B:100:GLN:HE21	1:B:102:ASP:HB2	1.86	0.41
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.80	0.41
1:C:295:MET:HE3	1:C:295:MET:HB2	1.88	0.41
1:A:104:LYS:HE2	1:A:104:LYS:HA	2.02	0.41
1:A:288:LYS:HB2	1:A:289:PRO:HD3	2.03	0.41
1:A:296:THR:HB	1:A:300:ARG:NH2	2.29	0.41
1:B:188:LEU:HA	1:B:188:LEU:HD23	1.79	0.41
1:B:222:ASP:O	1:B:238:ALA:HA	2.20	0.41
1:C:305:ASP:OD1	1:C:305:ASP:C	2.64	0.41
1:D:168:ALA:C	1:D:169:LEU:CD2	2.94	0.41
1:A:76:ARG:HD3	1:A:118:ARG:HG2	2.03	0.41
1:A:21:GLN:O	1:A:25:GLN:NE2	2.54	0.40
1:A:100:GLN:HB3	1:A:103:LEU:HD13	2.03	0.40
1:B:203:ALA:HA	1:B:273:LEU:O	2.22	0.40
1:D:87:ASN:ND2	1:D:91:ILE:HG23	2.37	0.40
1:A:139:TRP:CD1	1:A:139:TRP:C	2.99	0.40
1:B:268:ARG:H	1:B:268:ARG:HG3	1.75	0.40
1:B:5:PRO:N	1:B:8:VAL:H	2.20	0.40
1:D:169:LEU:CD2	1:D:169:LEU:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/379 (96%)	355 (98%)	7 (2%)	0	100	100
1	B	354/379 (93%)	347 (98%)	5 (1%)	2 (1%)	21	25
1	C	362/379 (96%)	350 (97%)	11 (3%)	1 (0%)	36	45
1	D	355/379 (94%)	348 (98%)	5 (1%)	2 (1%)	21	25
All	All	1433/1516 (94%)	1400 (98%)	28 (2%)	5 (0%)	36	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	313	GLU
1	B	314	PRO
1	D	314	PRO
1	D	5	PRO
1	C	84	GLY

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	A	323/333 (97%)	281 (87%)	42 (13%)	4	4
1	B	317/333 (95%)	268 (84%)	49 (16%)	2	2
1	C	323/333 (97%)	282 (87%)	41 (13%)	4	4
1	D	318/333 (96%)	272 (86%)	46 (14%)	3	3
All	All	1281/1332 (96%)	1103 (86%)	178 (14%)	3	3

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	10	HIS
1	A	23	VAL

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Mol	Chain	Res	Type
1	A	25	GLN
1	A	27	SER
1	A	43	LEU
1	A	67	ASP
1	A	69	LYS
1	A	75	LEU
1	A	78	LEU
1	A	88	LYS
1	A	105	LEU
1	A	107	GLN
1	A	116	LEU
1	A	130	GLU
1	A	148	ILE
1	A	158	GLN
1	A	160	LEU
1	A	166	VAL
1	A	174	GLN
1	A	188	LEU
1	A	199	VAL
1	A	226	LEU
1	A	237	ILE
1	A	242	GLU
1	A	250	LEU
1	A	251	THR
1	A	253	ILE
1	A	254	LEU
1	A	259	ILE
1	A	260	SER
1	A	263	LYS
1	A	267	THR
1	A	286	LEU
1	A	301	GLN
1	A	315	LEU
1	A	326	ILE
1	A	329	ASN
1	A	342	ILE
1	A	346	ARG
1	A	350	GLU
1	A	363	ARG
1	B	8	VAL
1	B	23	VAL
1	B	33	VAL

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Mol	Chain	Res	Type
1	B	42	VAL
1	B	43	LEU
1	B	48	LEU
1	B	69	LYS
1	B	75	LEU
1	B	78	LEU
1	B	102	ASP
1	B	103	LEU
1	B	104	LYS
1	B	105	LEU
1	B	110	MET
1	B	145	LYS
1	B	159	GLN
1	B	160	LEU
1	B	169	LEU
1	B	172	ASN
1	B	183	SER
1	B	186	ARG
1	B	199	VAL
1	B	223	ILE
1	B	224	LEU
1	B	226	LEU
1	B	234	SER
1	B	237	ILE
1	B	244	GLU
1	B	247	LEU
1	B	251	THR
1	B	254	LEU
1	B	257	GLN
1	B	259	ILE
1	B	267	THR
1	B	268	ARG
1	B	286	LEU
1	B	300	ARG
1	B	301	GLN
1	B	310	SER
1	B	311	ASP
1	B	313	GLU
1	B	314	PRO
1	B	315	LEU
1	B	325	LYS
1	B	327	GLU

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Mol	Chain	Res	Type
1	B	329	ASN
1	B	352	ILE
1	B	353	ILE
1	B	356	ARG
1	C	10	HIS
1	C	13	SER
1	C	23	VAL
1	C	25	GLN
1	C	27	SER
1	C	42	VAL
1	C	75	LEU
1	C	78	LEU
1	C	80	LYS
1	C	88	LYS
1	C	91	ILE
1	C	103	LEU
1	C	105	LEU
1	C	119	SER
1	C	124	VAL
1	C	130	GLU
1	C	158	GLN
1	C	160	LEU
1	C	166	VAL
1	C	169	LEU
1	C	172	ASN
1	C	198	SER
1	C	199	VAL
1	C	237	ILE
1	C	242	GLU
1	C	250	LEU
1	C	254	LEU
1	C	260	SER
1	C	263	LYS
1	C	286	LEU
1	C	288	LYS
1	C	300	ARG
1	C	315	LEU
1	C	326	ILE
1	C	329	ASN
1	C	341	VAL
1	C	342	ILE
1	C	350	GLU

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Mol	Chain	Res	Type
1	C	356	ARG
1	C	359	LEU
1	C	363	ARG
1	D	6	SER
1	D	14	ASP
1	D	23	VAL
1	D	25	GLN
1	D	28	LYS
1	D	42	VAL
1	D	43	LEU
1	D	56	GLN
1	D	69	LYS
1	D	75	LEU
1	D	78	LEU
1	D	88	LYS
1	D	102	ASP
1	D	105	LEU
1	D	110	MET
1	D	124	VAL
1	D	145	LYS
1	D	158	GLN
1	D	159	GLN
1	D	160	LEU
1	D	169	LEU
1	D	183	SER
1	D	186	ARG
1	D	214	THR
1	D	217	ASP
1	D	223	ILE
1	D	224	LEU
1	D	237	ILE
1	D	242	GLU
1	D	244	GLU
1	D	247	LEU
1	D	251	THR
1	D	254	LEU
1	D	257	GLN
1	D	268	ARG
1	D	279	SER
1	D	286	LEU
1	D	303	GLN
1	D	308	SER

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Mol	Chain	Res	Type
1	D	312	GLN
1	D	313	GLU
1	D	329	ASN
1	D	331	SER
1	D	353	ILE
1	D	356	ARG
1	D	359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	172	ASN
1	A	174	GLN
1	A	204	GLN
1	A	265	ASN
1	A	292	ASN
1	A	301	GLN
1	A	329	ASN
1	A	375	GLN
1	B	172	ASN
1	B	174	GLN
1	B	185	HIS
1	B	206	ASN
1	B	265	ASN
1	B	292	ASN
1	B	301	GLN
1	B	329	ASN
1	B	375	GLN
1	C	150	HIS
1	C	158	GLN
1	C	172	ASN
1	C	265	ASN
1	C	292	ASN
1	C	329	ASN
1	D	21	GLN
1	D	150	HIS
1	D	159	GLN
1	D	172	ASN
1	D	185	HIS
1	D	206	ASN
1	D	261	HIS

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Mol	Chain	Res	Type
1	D	265	ASN
1	D	292	ASN
1	D	312	GLN
1	D	316	HIS
1	D	329	ASN
1	D	375	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GDE	A	401	-	12,12,12	2.87	8 (66%)	17,17,17	3.44	9 (52%)
2	GDE	C	401	-	12,12,12	1.83	3 (25%)	17,17,17	3.02	9 (52%)

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
2	GDE	A	401	-	-	4/4/4/4	0/1/1/1
2	GDE	C	401	-	-	4/4/4/4	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDE	CAI-CAL	-5.27	1.33	1.40
2	A	401	GDE	CAJ-CAL	-5.22	1.33	1.40
2	C	401	GDE	CAJ-CAL	-4.38	1.34	1.40
2	A	401	GDE	OAB-CAH	3.00	1.31	1.22
2	A	401	GDE	OAA-CAH	-2.65	1.22	1.30
2	A	401	GDE	OAE-CAL	-2.60	1.30	1.36
2	A	401	GDE	OAC-CAI	2.47	1.41	1.36
2	C	401	GDE	OAC-CAI	2.42	1.41	1.36
2	C	401	GDE	CAG-CAK	-2.35	1.36	1.39
2	A	401	GDE	CAG-CAJ	-2.28	1.35	1.38
2	A	401	GDE	CAG-CAK	-2.17	1.36	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	GDE	CAF-CAI-CAL	-6.94	115.64	120.45
2	A	401	GDE	CAF-CAK-CAH	6.31	131.26	119.96
2	C	401	GDE	CAG-CAJ-CAL	6.28	124.81	120.45
2	A	401	GDE	CAF-CAI-CAL	-5.70	116.50	120.45
2	A	401	GDE	OAA-CAH-CAK	5.67	129.40	114.84
2	A	401	GDE	CAJ-CAL-CAI	5.41	122.88	119.53
2	A	401	GDE	OAA-CAH-OAB	-4.70	113.25	123.35
2	A	401	GDE	CAG-CAK-CAH	-4.47	111.95	119.96
2	C	401	GDE	CAK-CAF-CAI	4.01	123.59	120.09
2	C	401	GDE	OAC-CAI-CAL	3.17	126.06	117.90
2	C	401	GDE	OAE-CAL-CAI	3.08	127.59	119.46
2	A	401	GDE	OAC-CAI-CAF	2.92	127.34	119.45
2	C	401	GDE	CAK-CAG-CAJ	-2.76	117.68	120.09
2	C	401	GDE	OAE-CAL-CAJ	-2.52	112.81	119.46
2	A	401	GDE	CAG-CAK-CAF	-2.48	116.75	119.65
2	C	401	GDE	OAA-CAH-OAB	-2.46	118.06	123.35
2	C	401	GDE	CAF-CAK-CAH	2.27	124.03	119.96
2	A	401	GDE	CAK-CAF-CAI	2.11	121.93	120.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	GDE	OAA-CAH-CAK-CAG
2	C	401	GDE	OAB-CAH-CAK-CAF
2	A	401	GDE	OAA-CAH-CAK-CAG
2	C	401	GDE	OAA-CAH-CAK-CAF
2	A	401	GDE	OAB-CAH-CAK-CAF
2	A	401	GDE	OAB-CAH-CAK-CAG
2	C	401	GDE	OAB-CAH-CAK-CAG
2	A	401	GDE	OAA-CAH-CAK-CAF

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GDE	5	0
2	C	401	GDE	3	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, 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	A	366/379 (96%)	0.24	15 (4%) 41 44	17, 30, 54, 85	0
1	B	358/379 (94%)	0.26	14 (3%) 43 46	17, 33, 57, 88	0
1	C	366/379 (96%)	0.19	15 (4%) 41 44	16, 29, 54, 91	0
1	D	359/379 (94%)	0.24	14 (3%) 43 46	16, 33, 55, 94	0
All	All	1449/1516 (95%)	0.23	58 (4%) 42 45	16, 31, 55, 94	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	PRO	6.3
1	A	5	PRO	5.2
1	D	349	PRO	5.1
1	D	5	PRO	4.9
1	A	314	PRO	4.7
1	A	342	ILE	4.7
1	D	28	LYS	4.6
1	B	28	LYS	4.0
1	B	5	PRO	4.0
1	A	313	GLU	3.8
1	C	241	TYR	3.7
1	A	341	VAL	3.7
1	B	349	PRO	3.7
1	D	4	PRO	3.7
1	C	314	PRO	3.6
1	B	314	PRO	3.4
1	C	30	ARG	3.4
1	B	313	GLU	3.4
1	D	85	PRO	3.1
1	C	6	SER	3.0
1	B	331	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	313	GLU	3.0
1	D	301	GLN	3.0
1	D	77	HIS	2.9
1	A	127	SER	2.9
1	A	102	ASP	2.9
1	C	313	GLU	2.7
1	D	314	PRO	2.7
1	C	77	HIS	2.6
1	B	102	ASP	2.6
1	B	185	HIS	2.5
1	C	28	LYS	2.5
1	B	85	PRO	2.5
1	A	302	PHE	2.5
1	C	341	VAL	2.5
1	C	10	HIS	2.5
1	D	80	LYS	2.4
1	C	102	ASP	2.4
1	A	312	GLN	2.4
1	A	130	GLU	2.4
1	B	107	GLN	2.4
1	D	331	SER	2.4
1	C	243	LYS	2.3
1	D	312	GLN	2.3
1	B	104	LYS	2.3
1	C	104	LYS	2.2
1	D	205	THR	2.2
1	C	244	GLU	2.2
1	A	10	HIS	2.2
1	A	241	TYR	2.1
1	B	86	TRP	2.1
1	C	302	PHE	2.1
1	D	257	GLN	2.1
1	B	77	HIS	2.1
1	A	77	HIS	2.1
1	A	128	GLU	2.0
1	A	244	GLU	2.0
1	B	69	LYS	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GDE	A	401	12/12	0.59	0.27	20,20,20,20	0
2	GDE	C	401	12/12	0.66	0.23	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.