



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:50 AM UTC

PDB ID : 1WYG / pdb_00001wyg
Title : Crystal Structure of a Rat Xanthine Dehydrogenase Triple Mutant (C535A, C992R and C1324S)
Authors : Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Hori, H.; Matsumura, T.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on : 2005-02-14
Resolution : 2.60 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

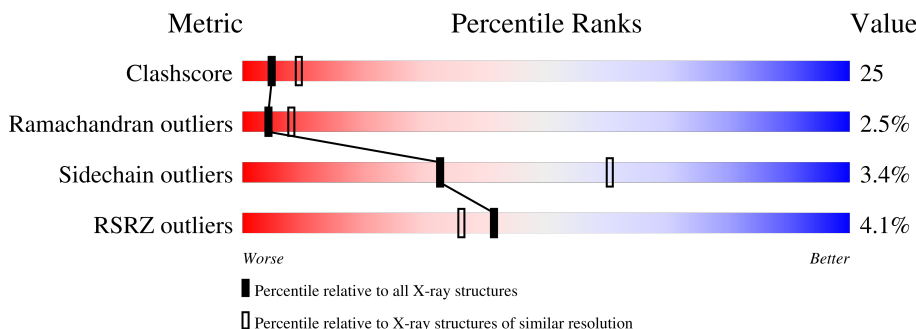
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	1331	

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
4	FES	A	4002	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10330 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.

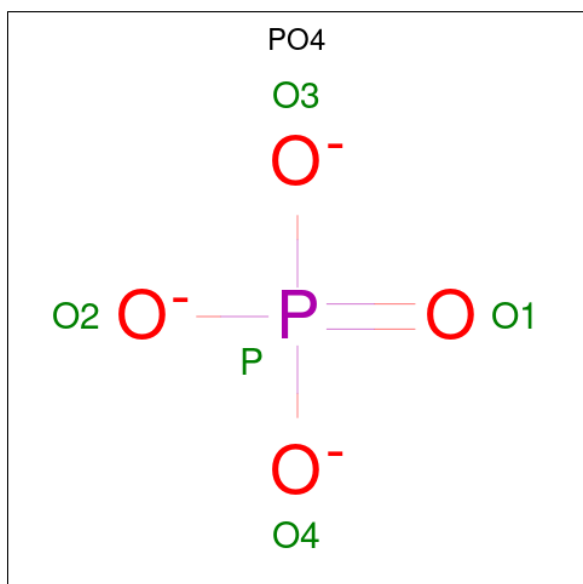
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1297	Total	C	N	O	S	0	0	0
			10033	6359	1730	1882	62			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P22985
A	535	ALA	CYS	engineered mutation	UNP P22985
A	992	ARG	CYS	engineered mutation	UNP P22985
A	1324	SER	CYS	engineered mutation	UNP P22985

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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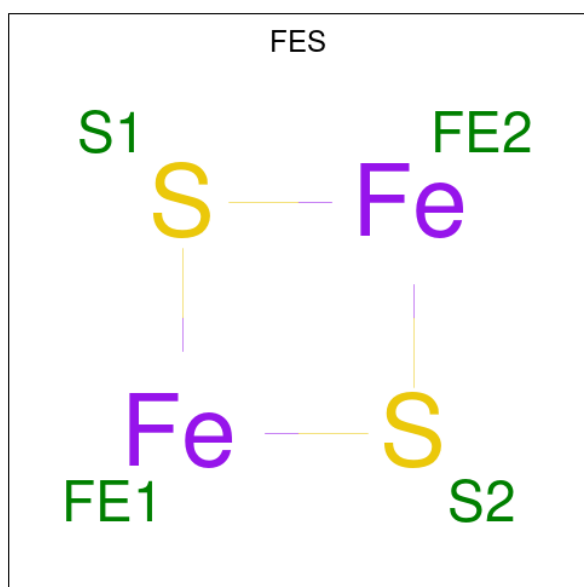
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

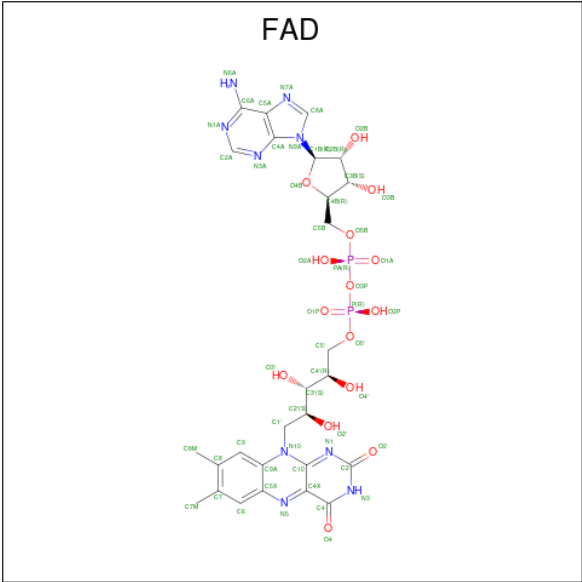
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



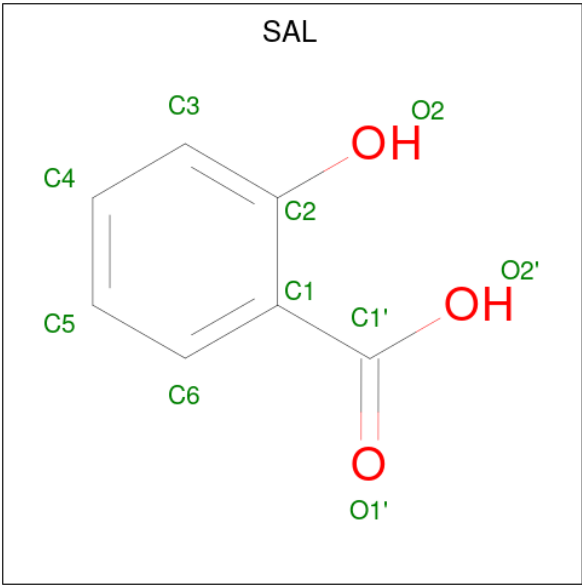
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



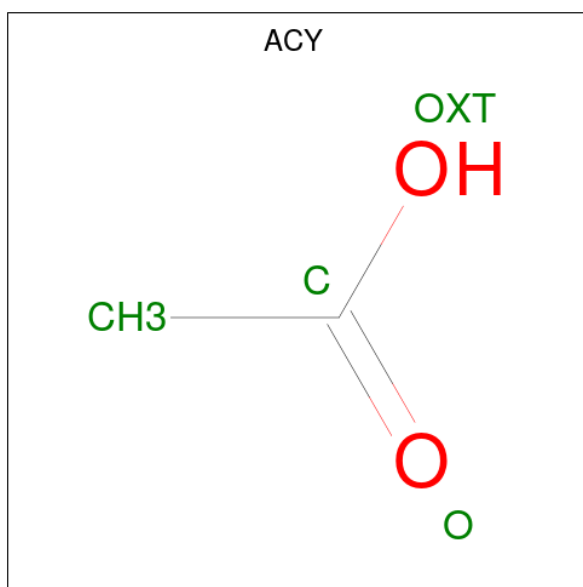
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: C₇H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

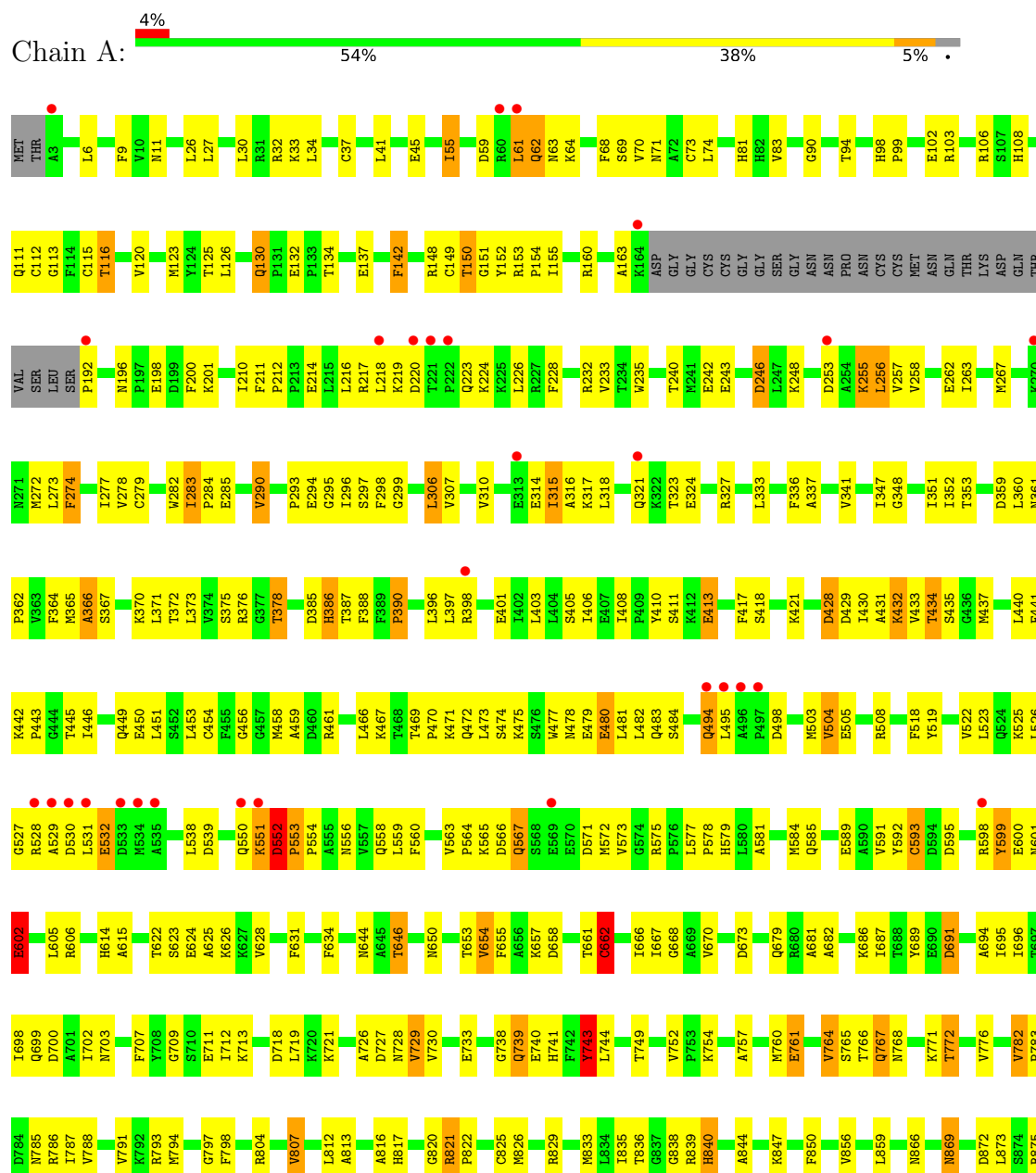
- Molecule 8 is water.

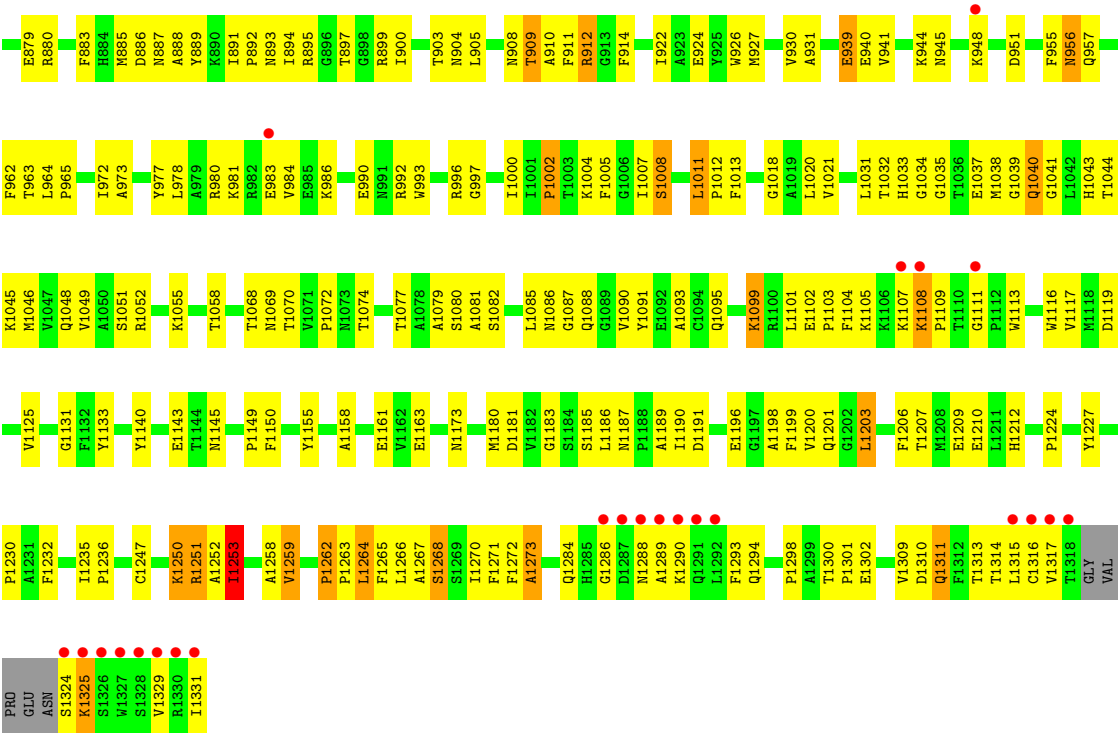
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	206	Total	O	0	0
			206	206		

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: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.25Å 134.25Å 523.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 25.00 – 2.63	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.60) 91.7 (25.00-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.04 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.248 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PO4, FES, SAL, ACY, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/10244	1.00	56/13859 (0.4%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	ILE	N-CA-C	9.83	119.66	110.42
1	A	163	ALA	N-CA-C	9.69	123.72	110.35
1	A	835	ILE	N-CA-C	9.26	119.80	110.82
1	A	743	TYR	N-CA-C	-7.97	98.48	110.28
1	A	1273	ALA	N-CA-C	-7.50	102.79	112.23
1	A	116	THR	CA-C-N	-7.46	111.22	118.97
1	A	116	THR	C-N-CA	-7.46	111.22	118.97
1	A	889	TYR	N-CA-C	7.42	121.50	109.40
1	A	150	THR	N-CA-C	7.39	120.39	111.82
1	A	654	VAL	N-CA-C	-7.37	102.97	111.00
1	A	836	THR	N-CA-C	7.19	121.64	113.01
1	A	691	ASP	N-CA-C	6.84	119.13	110.24
1	A	600	GLU	N-CA-C	-6.80	104.08	112.38
1	A	869	ASN	N-CA-C	6.66	119.37	111.71
1	A	956	ASN	N-CA-C	6.35	120.37	112.24
1	A	599	TYR	N-CA-C	-6.24	101.70	110.50
1	A	767	GLN	N-CA-C	-6.23	104.16	112.94
1	A	1108	LYS	CA-C-N	6.21	127.61	119.84
1	A	1108	LYS	C-N-CA	6.21	127.61	119.84
1	A	930	VAL	N-CA-C	-6.17	104.84	110.82
1	A	432	LYS	N-CA-C	-6.14	104.13	111.69
1	A	112	CYS	N-CA-C	-5.96	104.90	111.82
1	A	1186	LEU	N-CA-C	-5.91	104.92	111.36
1	A	442	LYS	N-CA-C	-5.87	102.18	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1011	LEU	CA-C-N	5.85	127.16	119.84
1	A	1011	LEU	C-N-CA	5.85	127.16	119.84
1	A	840	HIS	N-CA-C	5.81	118.02	109.42
1	A	1099	LYS	N-CA-C	-5.78	104.67	110.97
1	A	151	GLY	N-CA-C	-5.74	106.25	115.08
1	A	37	CYS	N-CA-C	5.73	119.25	112.72
1	A	337	ALA	CB-CA-C	-5.73	109.99	116.63
1	A	764	VAL	N-CA-C	5.71	118.16	108.86
1	A	408	ILE	CA-C-N	5.69	125.64	119.78
1	A	408	ILE	C-N-CA	5.69	125.64	119.78
1	A	130	GLN	CA-C-N	5.67	125.78	119.32
1	A	130	GLN	C-N-CA	5.67	125.78	119.32
1	A	552	ASP	CA-C-N	5.61	126.16	120.38
1	A	552	ASP	C-N-CA	5.61	126.16	120.38
1	A	290	VAL	N-CA-C	5.48	115.99	107.99
1	A	1101	LEU	N-CA-C	5.48	119.81	113.18
1	A	787	ILE	N-CA-C	5.47	115.83	108.17
1	A	283	ILE	CA-C-N	5.44	124.62	118.97
1	A	283	ILE	C-N-CA	5.44	124.62	118.97
1	A	274	PHE	CA-C-N	5.32	125.03	119.82
1	A	274	PHE	C-N-CA	5.32	125.03	119.82
1	A	553	PRO	CA-C-N	5.30	125.59	119.92
1	A	553	PRO	C-N-CA	5.30	125.59	119.92
1	A	435	SER	N-CA-C	5.25	117.23	108.99
1	A	727	ASP	N-CA-C	-5.23	105.47	111.07
1	A	602	GLU	N-CA-C	5.22	121.93	110.80
1	A	1262	PRO	N-CA-C	5.18	117.02	110.70
1	A	1264	LEU	N-CA-C	5.16	116.99	111.36
1	A	504	VAL	N-CA-C	5.07	115.50	110.23
1	A	142	PHE	N-CA-C	5.04	118.58	112.93
1	A	820	GLY	N-CA-C	-5.02	109.05	115.42
1	A	772	THR	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

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	10033	0	10046	514	0
2	A	15	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	0	3	0
5	A	53	0	31	3	0
6	A	10	0	5	0	0
7	A	4	0	3	0	0
8	A	206	0	0	5	0
All	All	10330	0	10085	515	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 25.

All (515) 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:A:766:THR:HG22	1:A:768:ASN:H	0.99	1.08
1:A:1038:MET:H	1:A:1040:GLN:NE2	1.56	1.02
1:A:398:ARG:HH11	1:A:398:ARG:HB3	1.27	0.99
1:A:196:ASN:OD1	1:A:198:GLU:HB3	1.63	0.97
1:A:602:GLU:HG2	1:A:822:PRO:HB2	1.45	0.97
1:A:494:GLN:HA	1:A:508:ARG:HH12	1.32	0.95
1:A:766:THR:HG22	1:A:768:ASN:N	1.82	0.94
1:A:1004:LYS:HG3	1:A:1155:TYR:HE2	1.32	0.92
1:A:1311:GLN:H	1:A:1311:GLN:HE21	0.97	0.91
1:A:298:PHE:HE2	1:A:310:VAL:HG11	1.36	0.91
1:A:371:LEU:HD22	1:A:406:ILE:HD12	1.51	0.91
1:A:1033:HIS:HB2	1:A:1086:ASN:HD22	1.34	0.90
1:A:432:LYS:HE3	1:A:503:MET:SD	2.12	0.89
1:A:398:ARG:HB3	1:A:398:ARG:NH1	1.88	0.89
1:A:711:GLU:HB3	1:A:899:ARG:HH11	1.35	0.88
1:A:403:LEU:HD21	1:A:406:ILE:HD11	1.56	0.88
1:A:55:ILE:HD13	1:A:55:ILE:C	2.00	0.86
1:A:1173:ASN:ND2	1:A:1270:ILE:HD13	1.91	0.85
1:A:494:GLN:HA	1:A:508:ARG:NH1	1.92	0.84
1:A:718:ASP:H	1:A:893:ASN:ND2	1.77	0.83
1:A:740:GLU:HG2	1:A:833:MET:HE3	1.60	0.83
1:A:749:THR:HB	1:A:812:LEU:HD12	1.62	0.81
1:A:963:THR:HG22	1:A:1155:TYR:HD1	1.43	0.80
1:A:821:ARG:HH11	1:A:821:ARG:HB3	1.46	0.79
1:A:1038:MET:H	1:A:1040:GLN:HE22	1.30	0.79
1:A:605:LEU:HD13	1:A:812:LEU:HD23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:GLN:H	1:A:1311:GLN:NE2	1.78	0.77
1:A:614:HIS:HB2	1:A:904:ASN:ND2	2.01	0.77
1:A:32:ARG:HD2	1:A:598:ARG:CZ	2.15	0.76
1:A:812:LEU:HD21	1:A:825:CYS:HB2	1.66	0.76
1:A:718:ASP:HB3	1:A:721:LYS:HE2	1.67	0.76
1:A:11:ASN:OD1	1:A:90:GLY:HA3	1.84	0.76
1:A:45:GLU:OE1	1:A:1224:PRO:HD2	1.87	0.75
1:A:375:SER:HB3	1:A:378:THR:OG1	1.86	0.75
1:A:55:ILE:HD12	1:A:68:PHE:CZ	2.22	0.75
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.12	0.75
1:A:821:ARG:HH11	1:A:821:ARG:CB	2.00	0.75
1:A:1311:GLN:HE21	1:A:1311:GLN:N	1.80	0.74
1:A:103:ARG:HG2	1:A:200:PHE:CD1	2.23	0.73
1:A:1046:MET:HA	1:A:1046:MET:HE2	1.69	0.73
1:A:508:ARG:HH11	1:A:508:ARG:HG2	1.53	0.73
1:A:1032:THR:HG21	1:A:1070:THR:HB	1.69	0.73
1:A:963:THR:HG22	1:A:1155:TYR:CD1	2.23	0.73
1:A:1108:LYS:HG2	1:A:1111:GLY:HA3	1.70	0.73
1:A:385:ASP:OD1	1:A:387:THR:HG22	1.89	0.72
1:A:388:PHE:HA	1:A:396:LEU:HG	1.70	0.72
1:A:192:PRO:HB2	1:A:560:PHE:CZ	2.25	0.72
1:A:646:THR:O	1:A:650:ASN:HA	1.90	0.71
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.26	0.71
1:A:216:LEU:O	1:A:219:LYS:HG3	1.91	0.71
1:A:794:MET:HE3	1:A:1038:MET:HB3	1.72	0.71
1:A:1048:GLN:HE22	1:A:1187:ASN:HD22	1.37	0.70
1:A:530:ASP:C	1:A:532:GLU:H	1.99	0.70
1:A:298:PHE:CE2	1:A:310:VAL:HG11	2.25	0.70
1:A:306:LEU:O	1:A:310:VAL:HG12	1.91	0.70
1:A:872:ASP:OD1	1:A:909:THR:HG22	1.91	0.70
1:A:718:ASP:H	1:A:893:ASN:HD22	1.38	0.70
1:A:760:MET:HE2	1:A:816:ALA:HB3	1.74	0.70
1:A:766:THR:HG22	1:A:767:GLN:N	2.06	0.69
1:A:957:GLN:OE1	1:A:1149:PRO:HD2	1.93	0.69
1:A:1250:LYS:HD3	1:A:1251:ARG:H	1.57	0.69
1:A:467:LYS:O	1:A:470:PRO:HD2	1.93	0.69
1:A:875:ARG:O	1:A:879:GLU:HG3	1.92	0.69
1:A:565:LYS:H	1:A:565:LYS:HD3	1.57	0.69
1:A:622:THR:HG22	1:A:626:LYS:HG3	1.75	0.69
1:A:102:GLU:OE1	1:A:201:LYS:HG2	1.93	0.69
1:A:290:VAL:HG23	1:A:297:SER:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:TRP:O	1:A:1117:VAL:HG23	1.92	0.69
1:A:347:ILE:HG13	1:A:348:GLY:H	1.58	0.68
1:A:622:THR:HG23	1:A:625:ALA:HB3	1.75	0.68
1:A:324:GLU:HB2	1:A:411:SER:CB	2.24	0.68
1:A:458:MET:HE1	1:A:495:LEU:HD11	1.76	0.68
1:A:662:CYS:HB3	1:A:869:ASN:ND2	2.09	0.68
1:A:1289:ALA:O	1:A:1290:LYS:HB3	1.92	0.68
1:A:498:ASP:HB2	1:A:1325:LYS:HG3	1.75	0.68
1:A:1004:LYS:HG3	1:A:1155:TYR:CE2	2.23	0.67
1:A:1203:LEU:C	1:A:1203:LEU:HD12	2.18	0.67
1:A:844:ALA:HB2	1:A:922:ILE:HD13	1.77	0.67
1:A:1173:ASN:HD22	1:A:1270:ILE:HD13	1.58	0.67
1:A:606:ARG:HD3	1:A:679:GLN:HA	1.77	0.67
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.75	0.67
1:A:1044:THR:O	1:A:1048:GLN:HG3	1.95	0.67
1:A:372:THR:O	1:A:373:LEU:HD23	1.95	0.67
1:A:317:LYS:HG3	1:A:318:LEU:HD12	1.77	0.66
1:A:572:MET:HA	1:A:575:ARG:HD2	1.78	0.66
1:A:766:THR:CG2	1:A:768:ASN:H	1.92	0.66
1:A:599:TYR:H	1:A:602:GLU:HG3	1.60	0.66
1:A:1099:LYS:O	1:A:1102:GLU:HG2	1.96	0.66
1:A:451:LEU:HD23	1:A:469:THR:HG22	1.78	0.65
1:A:315:ILE:HG12	1:A:315:ILE:O	1.96	0.65
1:A:421:LYS:HE3	1:A:431:ALA:HB2	1.79	0.65
1:A:115:CYS:HB3	1:A:744:LEU:CD1	2.27	0.65
1:A:26:LEU:O	1:A:30:LEU:HG	1.96	0.64
1:A:272:MET:HA	1:A:272:MET:HE2	1.78	0.64
1:A:1035:GLY:H	1:A:1086:ASN:ND2	1.94	0.64
1:A:160:ARG:HH22	1:A:556:ASN:HD21	1.45	0.64
1:A:55:ILE:HG12	1:A:83:VAL:CG1	2.28	0.64
1:A:192:PRO:HB2	1:A:560:PHE:CE1	2.32	0.64
1:A:405:SER:O	1:A:406:ILE:HD13	1.96	0.64
1:A:504:VAL:O	1:A:508:ARG:HG3	1.97	0.64
1:A:872:ASP:OD1	1:A:873:LEU:N	2.31	0.64
1:A:1180:MET:HE3	1:A:1263:PRO:HG3	1.80	0.64
1:A:472:GLN:HE21	1:A:481:LEU:HG	1.63	0.64
1:A:214:GLU:O	1:A:218:LEU:HG	1.97	0.63
1:A:880:ARG:NH2	1:A:1150:PHE:HE2	1.96	0.63
1:A:1158:ALA:HB2	1:A:1266:LEU:HB3	1.79	0.63
1:A:359:ASP:CG	1:A:434:THR:HG21	2.23	0.63
1:A:62:GLN:OE1	1:A:64:LYS:HE2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HH11	1:A:398:ARG:CB	2.08	0.63
1:A:749:THR:CB	1:A:812:LEU:HD12	2.28	0.63
1:A:360:LEU:HB3	1:A:364:PHE:CE2	2.34	0.62
1:A:1313:THR:O	1:A:1317:VAL:HG13	2.00	0.62
1:A:615:ALA:HB1	1:A:689:TYR:HB3	1.81	0.62
1:A:142:PHE:HB3	1:A:1232:PHE:CE1	2.35	0.62
1:A:1259:VAL:O	1:A:1259:VAL:HG22	1.99	0.62
4:A:4003:FES:FE1	4:A:4003:FES:S2	1.91	0.62
1:A:115:CYS:HB3	1:A:744:LEU:HD12	1.81	0.61
1:A:565:LYS:HD3	1:A:565:LYS:N	2.15	0.61
1:A:926:TRP:CZ3	1:A:927:MET:HE2	2.36	0.61
1:A:911:PHE:O	1:A:912:ARG:C	2.43	0.61
1:A:367:SER:HB3	1:A:417:PHE:HE1	1.65	0.61
1:A:718:ASP:N	1:A:893:ASN:HD22	1.99	0.61
1:A:277:ILE:HG22	1:A:278:VAL:N	2.15	0.61
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.30	0.61
1:A:694:ALA:C	1:A:695:ILE:HD13	2.25	0.61
1:A:295:GLY:HA2	1:A:410:TYR:CE1	2.36	0.61
1:A:324:GLU:HB2	1:A:411:SER:HB3	1.82	0.61
1:A:606:ARG:CD	1:A:679:GLN:HA	2.31	0.61
1:A:224:LYS:H	1:A:224:LYS:HD2	1.65	0.60
1:A:566:ASP:O	1:A:567:GLN:C	2.43	0.60
1:A:584:MET:HG3	8:A:4039:HOH:O	2.01	0.60
1:A:1048:GLN:NE2	1:A:1187:ASN:HD22	2.00	0.60
1:A:347:ILE:HG13	1:A:348:GLY:N	2.16	0.60
1:A:754:LYS:HE2	1:A:761:GLU:HB2	1.83	0.60
1:A:153:ARG:NE	1:A:1196:GLU:OE1	2.29	0.60
1:A:470:PRO:C	1:A:472:GLN:H	2.10	0.59
1:A:741:HIS:HA	1:A:911:PHE:CZ	2.37	0.59
1:A:518:PHE:O	1:A:522:VAL:HG23	2.03	0.59
1:A:956:ASN:ND2	1:A:1145:ASN:ND2	2.50	0.59
1:A:1105:LYS:HG3	1:A:1116:TRP:CZ2	2.37	0.59
1:A:764:VAL:O	1:A:791:VAL:HG22	2.02	0.59
1:A:718:ASP:O	1:A:893:ASN:ND2	2.36	0.59
1:A:98:HIS:ND1	1:A:99:PRO:HD2	2.17	0.59
1:A:955:PHE:HA	1:A:1145:ASN:OD1	2.03	0.59
1:A:232:ARG:NH1	1:A:273:LEU:HD13	2.18	0.58
1:A:712:ILE:HD13	1:A:879:GLU:HG2	1.84	0.58
1:A:153:ARG:HE	1:A:1196:GLU:CD	2.10	0.58
1:A:255:LYS:HG3	1:A:274:PHE:CD2	2.38	0.58
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:ARG:NH1	1:A:1284:GLN:HB2	2.18	0.58
1:A:666:ILE:HD12	1:A:807:VAL:HG22	1.85	0.58
1:A:844:ALA:HB2	1:A:922:ILE:CD1	2.33	0.58
1:A:479:GLU:O	1:A:483:GLN:HG2	2.03	0.58
1:A:573:VAL:HG21	1:A:1052:ARG:HD3	1.86	0.58
1:A:508:ARG:NH1	1:A:508:ARG:HG2	2.18	0.58
1:A:323:THR:OG1	1:A:327:ARG:NH1	2.37	0.58
1:A:385:ASP:CG	1:A:387:THR:HG22	2.28	0.58
1:A:366:ALA:HB2	1:A:454:CYS:SG	2.44	0.57
1:A:32:ARG:HD2	1:A:598:ARG:NH1	2.19	0.57
1:A:601:ASN:O	1:A:821:ARG:NH1	2.24	0.57
1:A:655:PHE:CD2	1:A:668:GLY:HA2	2.38	0.57
1:A:785:ASN:HB3	1:A:786:ARG:HH11	1.69	0.57
1:A:1013:PHE:C	1:A:1013:PHE:CD1	2.83	0.57
1:A:1038:MET:H	1:A:1040:GLN:HE21	1.48	0.56
1:A:739:GLN:HG3	1:A:1209:GLU:OE2	2.04	0.56
1:A:388:PHE:O	1:A:390:PRO:HD3	2.04	0.56
1:A:571:ASP:OD1	1:A:1052:ARG:HD2	2.06	0.56
1:A:718:ASP:CB	1:A:721:LYS:HE2	2.36	0.56
1:A:599:TYR:C	1:A:601:ASN:N	2.63	0.56
1:A:718:ASP:C	1:A:893:ASN:HD22	2.14	0.56
1:A:153:ARG:HG2	1:A:153:ARG:HH11	1.71	0.56
1:A:299:GLY:O	1:A:347:ILE:HD11	2.06	0.56
1:A:529:ALA:O	1:A:530:ASP:HB2	2.06	0.56
1:A:482:LEU:C	1:A:482:LEU:HD23	2.31	0.56
1:A:986:LYS:O	1:A:990:GLU:HG3	2.06	0.55
1:A:1209:GLU:HB3	1:A:1227:TYR:CZ	2.40	0.55
1:A:1140:TYR:HB2	1:A:1149:PRO:HB3	1.89	0.55
1:A:94:THR:HG23	1:A:589:GLU:OE2	2.05	0.55
1:A:295:GLY:HA2	1:A:410:TYR:CD1	2.41	0.55
1:A:709:GLY:HA3	1:A:875:ARG:NH2	2.22	0.55
1:A:602:GLU:HA	1:A:822:PRO:O	2.07	0.54
1:A:397:LEU:HD12	1:A:397:LEU:H	1.72	0.54
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.89	0.54
1:A:285:GLU:H	1:A:285:GLU:CD	2.15	0.54
1:A:622:THR:HG22	1:A:622:THR:O	2.07	0.54
1:A:866:ASN:ND2	1:A:1331:ILE:HG23	2.21	0.54
1:A:472:GLN:HE22	1:A:484:SER:CB	2.21	0.54
1:A:880:ARG:HH22	1:A:1150:PHE:HE2	1.55	0.54
1:A:525:LYS:HA	1:A:528:ARG:NH1	2.22	0.54
1:A:821:ARG:HH11	1:A:821:ARG:CG	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:SER:HB3	1:A:417:PHE:CE1	2.42	0.54
1:A:601:ASN:ND2	1:A:822:PRO:HD3	2.22	0.54
1:A:218:LEU:C	1:A:220:ASP:H	2.15	0.54
1:A:565:LYS:H	1:A:565:LYS:CD	2.20	0.54
1:A:1293:PHE:H	1:A:1293:PHE:HD2	1.54	0.54
1:A:371:LEU:CD2	1:A:406:ILE:HG23	2.37	0.54
1:A:872:ASP:CG	1:A:909:THR:HG22	2.32	0.53
1:A:504:VAL:HG23	1:A:505:GLU:H	1.74	0.53
1:A:1105:LYS:HA	1:A:1116:TRP:NE1	2.23	0.53
1:A:103:ARG:HG2	1:A:200:PHE:CE1	2.43	0.53
1:A:879:GLU:O	1:A:883:PHE:CD2	2.62	0.53
1:A:1035:GLY:H	1:A:1086:ASN:HD21	1.54	0.53
1:A:530:ASP:C	1:A:532:GLU:N	2.67	0.53
1:A:160:ARG:HH22	1:A:556:ASN:ND2	2.05	0.53
1:A:478:ASN:HD21	1:A:480:GLU:HB3	1.73	0.53
1:A:838:GLY:O	1:A:908:ASN:HB3	2.08	0.53
1:A:760:MET:HE1	1:A:813:ALA:O	2.09	0.52
1:A:670:VAL:HG21	1:A:682:ALA:HA	1.91	0.52
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.91	0.52
1:A:446:ILE:O	1:A:446:ILE:HG13	2.09	0.52
1:A:1108:LYS:HG2	1:A:1111:GLY:CA	2.38	0.52
1:A:130:GLN:HE21	1:A:132:GLU:H	1.58	0.52
1:A:599:TYR:C	1:A:601:ASN:H	2.18	0.52
1:A:766:THR:CG2	1:A:767:GLN:N	2.72	0.52
1:A:924:GLU:HB3	1:A:1272:PHE:CE2	2.45	0.52
1:A:698:ILE:HG13	1:A:1331:ILE:OXT	2.10	0.52
1:A:1035:GLY:N	1:A:1086:ASN:HD21	2.08	0.52
1:A:698:ILE:O	1:A:702:ILE:HG13	2.10	0.52
1:A:711:GLU:N	1:A:899:ARG:NH1	2.58	0.51
1:A:33:LYS:HG3	1:A:33:LYS:O	2.10	0.51
1:A:421:LYS:HG3	1:A:434:THR:HG23	1.91	0.51
1:A:859:LEU:HD22	1:A:926:TRP:CZ2	2.46	0.51
1:A:964:LEU:HB3	1:A:965:PRO:HD3	1.93	0.51
1:A:405:SER:C	1:A:406:ILE:HD13	2.36	0.51
1:A:469:THR:OG1	1:A:470:PRO:HD3	2.10	0.51
1:A:235:TRP:CD1	1:A:235:TRP:C	2.88	0.51
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.92	0.51
1:A:856:VAL:HG12	1:A:945:ASN:OD1	2.10	0.51
1:A:752:VAL:HG13	1:A:752:VAL:O	2.10	0.51
1:A:1265:PHE:O	1:A:1268:SER:HB2	2.10	0.51
1:A:375:SER:HB2	1:A:401:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASP:OD1	1:A:430:ILE:N	2.42	0.51
1:A:223:GLN:NE2	1:A:282:TRP:HB3	2.26	0.50
1:A:277:ILE:HG22	1:A:278:VAL:H	1.76	0.50
1:A:1091:TYR:O	1:A:1095:GLN:HG2	2.09	0.50
1:A:1158:ALA:CB	1:A:1266:LEU:HB3	2.41	0.50
1:A:503:MET:HG2	1:A:1302:GLU:OE2	2.11	0.50
1:A:599:TYR:HB2	1:A:602:GLU:HG3	1.94	0.50
1:A:240:THR:OG1	1:A:243:GLU:HG3	2.10	0.50
1:A:606:ARG:NE	1:A:679:GLN:HG3	2.25	0.50
1:A:1045:LYS:HE3	1:A:1190:ILE:HG21	1.94	0.50
1:A:262:GLU:HB3	5:A:4004:FAD:O2A	2.11	0.50
1:A:527:GLY:HA2	1:A:532:GLU:HA	1.93	0.50
1:A:673:ASP:OD1	1:A:673:ASP:N	2.42	0.50
1:A:972:ILE:HG13	1:A:973:ALA:N	2.27	0.50
1:A:428:ASP:OD1	5:A:4004:FAD:H6	2.12	0.50
1:A:615:ALA:HA	1:A:691:ASP:HA	1.93	0.50
1:A:1021:VAL:HG23	1:A:1093:ALA:HB1	1.93	0.50
1:A:498:ASP:HB2	1:A:1325:LYS:O	2.12	0.50
1:A:503:MET:HE2	1:A:1302:GLU:HB2	1.93	0.50
1:A:605:LEU:HD23	1:A:605:LEU:C	2.37	0.50
1:A:98:HIS:CE1	1:A:99:PRO:HD2	2.47	0.50
1:A:1140:TYR:CB	1:A:1149:PRO:HB3	2.42	0.50
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.12	0.50
1:A:1262:PRO:HB2	1:A:1263:PRO:HD3	1.92	0.50
1:A:661:THR:O	1:A:662:CYS:HB3	2.12	0.50
1:A:667:ILE:HD13	1:A:687:ILE:HD13	1.92	0.50
1:A:741:HIS:CE1	1:A:838:GLY:HA2	2.47	0.50
1:A:481:LEU:C	1:A:481:LEU:HD23	2.37	0.49
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.60	0.49
1:A:1200:VAL:O	1:A:1230:PRO:HG2	2.12	0.49
1:A:601:ASN:HD22	1:A:822:PRO:HD3	1.76	0.49
1:A:760:MET:HE2	1:A:816:ALA:CB	2.40	0.49
1:A:478:ASN:ND2	1:A:480:GLU:H	2.10	0.49
1:A:592:TYR:O	1:A:593:CYS:C	2.56	0.49
1:A:1032:THR:HG21	1:A:1070:THR:CB	2.42	0.49
1:A:55:ILE:HG12	1:A:83:VAL:HG13	1.93	0.49
1:A:657:LYS:O	1:A:658:ASP:HB2	2.13	0.49
1:A:766:THR:HG22	1:A:767:GLN:H	1.74	0.49
1:A:459:ALA:C	1:A:461:ARG:H	2.20	0.49
1:A:525:LYS:HA	1:A:528:ARG:HH12	1.76	0.49
1:A:558:GLN:O	1:A:559:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:GLY:CA	1:A:1074:THR:HG21	2.42	0.49
1:A:772:THR:O	1:A:776:VAL:HG23	2.12	0.49
1:A:887:ASN:OD1	1:A:888:ALA:N	2.45	0.49
1:A:1034:GLY:HA3	1:A:1074:THR:HG21	1.95	0.49
1:A:472:GLN:NE2	1:A:481:LEU:HG	2.27	0.49
1:A:606:ARG:CZ	1:A:679:GLN:HG3	2.43	0.49
1:A:812:LEU:HD21	1:A:825:CYS:CB	2.40	0.49
1:A:437:MET:HG2	1:A:453:LEU:HD22	1.94	0.48
1:A:475:LYS:HD3	1:A:480:GLU:OE2	2.13	0.48
1:A:577:LEU:HD12	1:A:578:PRO:HD2	1.94	0.48
1:A:59:ASP:OD1	1:A:61:LEU:HB3	2.13	0.48
1:A:315:ILE:HD13	1:A:315:ILE:C	2.38	0.48
1:A:628:VAL:HG21	1:A:681:ALA:HA	1.94	0.48
1:A:255:LYS:HE3	5:A:4004:FAD:O3B	2.14	0.48
1:A:579:HIS:CE1	1:A:581:ALA:HB3	2.48	0.48
1:A:55:ILE:HD13	1:A:55:ILE:O	2.12	0.48
1:A:749:THR:CG2	1:A:812:LEU:HD12	2.44	0.48
1:A:314:GLU:C	1:A:316:ALA:H	2.22	0.48
1:A:634:PHE:CZ	1:A:668:GLY:HA3	2.48	0.48
1:A:210:ILE:HG12	1:A:211:PHE:N	2.29	0.47
1:A:341:VAL:HG23	8:A:4023:HOH:O	2.14	0.47
1:A:1033:HIS:CE1	1:A:1043:HIS:ND1	2.82	0.47
1:A:1037:GLU:HA	1:A:1040:GLN:HE22	1.78	0.47
1:A:1324:SER:O	1:A:1325:LYS:HB2	2.14	0.47
1:A:323:THR:O	1:A:327:ARG:HG3	2.14	0.47
1:A:817:HIS:O	1:A:817:HIS:CG	2.67	0.47
1:A:148:ARG:O	1:A:148:ARG:HG3	2.15	0.47
1:A:386:HIS:CG	1:A:466:LEU:HD11	2.50	0.47
1:A:6:LEU:HB2	1:A:228:PHE:CE2	2.49	0.47
1:A:804:ARG:HG2	8:A:4106:HOH:O	2.13	0.47
1:A:579:HIS:HD2	1:A:1041:GLY:HA2	1.79	0.47
1:A:997:GLY:HA3	1:A:1273:ALA:O	2.15	0.47
1:A:760:MET:CE	1:A:816:ALA:HB3	2.42	0.47
1:A:1038:MET:N	1:A:1040:GLN:HE22	2.07	0.47
1:A:553:PRO:HA	1:A:554:PRO:HD3	1.73	0.47
1:A:909:THR:HB	1:A:910:ALA:H	1.36	0.47
1:A:1005:PHE:HB3	1:A:1262:PRO:HG3	1.96	0.46
1:A:579:HIS:CD2	1:A:1041:GLY:HA2	2.51	0.46
1:A:744:LEU:HD12	4:A:4002:FES:S2	2.55	0.46
1:A:992:ARG:HG3	1:A:993:TRP:CE2	2.49	0.46
1:A:1102:GLU:HG3	1:A:1103:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG22	1:A:71:ASN:N	2.30	0.46
1:A:440:LEU:HB3	1:A:450:GLU:HB2	1.98	0.46
1:A:886:ASP:O	1:A:887:ASN:C	2.58	0.46
1:A:481:LEU:HD23	1:A:481:LEU:O	2.15	0.46
1:A:667:ILE:CD1	1:A:687:ILE:HD13	2.45	0.46
1:A:749:THR:O	1:A:812:LEU:HD13	2.15	0.46
1:A:45:GLU:OE1	1:A:1224:PRO:CD	2.60	0.46
1:A:440:LEU:HD23	1:A:450:GLU:OE1	2.16	0.46
1:A:551:LYS:O	1:A:552:ASP:CB	2.64	0.46
1:A:1203:LEU:C	1:A:1203:LEU:CD1	2.87	0.46
1:A:441:PHE:CE1	1:A:526:LEU:HD21	2.51	0.46
1:A:866:ASN:HD22	1:A:1331:ILE:HG23	1.80	0.46
1:A:108:HIS:CE1	1:A:1189:ALA:HB1	2.51	0.46
1:A:153:ARG:N	1:A:154:PRO:HD2	2.30	0.46
1:A:1253:ILE:O	1:A:1253:ILE:CG2	2.64	0.46
1:A:148:ARG:NE	1:A:1201:GLN:HE21	2.14	0.46
1:A:315:ILE:HA	1:A:323:THR:HG21	1.98	0.46
1:A:503:MET:HE2	1:A:1302:GLU:CB	2.46	0.46
1:A:149:CYS:HB2	4:A:4002:FES:S1	2.55	0.46
1:A:567:GLN:HE21	1:A:567:GLN:HB3	1.57	0.46
1:A:768:ASN:HD21	1:A:771:LYS:CG	2.29	0.46
1:A:1309:VAL:HA	1:A:1313:THR:HG21	1.96	0.46
1:A:55:ILE:C	1:A:55:ILE:CD1	2.74	0.45
1:A:390:PRO:O	1:A:461:ARG:NH1	2.49	0.45
1:A:470:PRO:C	1:A:472:GLN:N	2.75	0.45
1:A:713:LYS:HG3	1:A:897:THR:HG22	1.98	0.45
1:A:458:MET:HE3	1:A:495:LEU:HD21	1.99	0.45
1:A:470:PRO:O	1:A:473:LEU:HG	2.16	0.45
1:A:1149:PRO:HG2	1:A:1150:PHE:CD1	2.51	0.45
1:A:709:GLY:HA3	1:A:875:ARG:HH21	1.82	0.45
1:A:113:GLY:HA3	1:A:585:GLN:HG2	1.97	0.45
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.80	0.45
1:A:948:LYS:HB2	1:A:951:ASP:OD2	2.16	0.45
1:A:996:ARG:HG2	1:A:1163:GLU:HB2	1.98	0.45
1:A:592:TYR:O	1:A:595:ASP:N	2.32	0.45
1:A:654:VAL:HG12	1:A:655:PHE:CD1	2.52	0.45
1:A:1031:LEU:HD11	1:A:1090:VAL:HG22	1.99	0.45
1:A:1259:VAL:O	1:A:1259:VAL:CG2	2.63	0.45
1:A:297:SER:HA	1:A:406:ILE:O	2.16	0.45
1:A:738:GLY:O	1:A:739:GLN:HB2	2.16	0.45
1:A:1038:MET:HG2	1:A:1040:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:LYS:HB3	1:A:1055:LYS:HE2	1.81	0.45
1:A:1235:ILE:O	1:A:1236:PRO:C	2.59	0.45
1:A:440:LEU:O	1:A:449:GLN:HB3	2.16	0.45
1:A:622:THR:O	1:A:623:SER:C	2.59	0.45
1:A:757:ALA:O	1:A:786:ARG:HD2	2.17	0.45
1:A:219:LYS:HD2	1:A:219:LYS:C	2.42	0.45
1:A:1051:SER:CB	1:A:1058:THR:HG22	2.46	0.45
1:A:1080:SER:HB3	1:A:1258:ALA:HB1	1.99	0.45
1:A:1264:LEU:C	1:A:1264:LEU:HD23	2.42	0.45
1:A:550:GLN:OE1	1:A:550:GLN:HA	2.17	0.44
1:A:581:ALA:CB	1:A:584:MET:HE2	2.47	0.44
1:A:33:LYS:O	1:A:34:LEU:HD23	2.17	0.44
1:A:153:ARG:HD2	1:A:558:GLN:NE2	2.32	0.44
1:A:1199:PHE:CE1	1:A:1267:ALA:HA	2.52	0.44
1:A:153:ARG:HG2	1:A:153:ARG:NH1	2.32	0.44
1:A:686:LYS:HB3	1:A:686:LYS:HE3	1.82	0.44
1:A:1107:LYS:C	1:A:1109:PRO:HD3	2.43	0.44
1:A:353:THR:HB	8:A:4120:HOH:O	2.17	0.44
1:A:905:LEU:HD11	1:A:1331:ILE:HG13	1.99	0.44
1:A:939:GLU:HG3	1:A:940:GLU:N	2.32	0.44
1:A:1021:VAL:HG22	1:A:1031:LEU:HD13	1.99	0.44
1:A:373:LEU:HD13	1:A:397:LEU:HG	1.99	0.44
1:A:1209:GLU:HB3	1:A:1227:TYR:OH	2.17	0.44
1:A:1314:THR:HG22	1:A:1315:LEU:HD12	2.00	0.44
1:A:70:VAL:HG22	1:A:71:ASN:H	1.83	0.44
1:A:1185:SER:OG	1:A:1191:ASP:OD2	2.34	0.44
1:A:232:ARG:HH12	1:A:273:LEU:HD13	1.80	0.44
1:A:1038:MET:N	1:A:1040:GLN:NE2	2.41	0.44
1:A:27:LEU:HD21	1:A:41:LEU:HB2	2.00	0.44
1:A:111:GLN:HG3	1:A:150:THR:CG2	2.48	0.44
1:A:263:ILE:HG22	1:A:267:MET:HE2	1.98	0.44
1:A:743:TYR:O	1:A:829:ARG:NH2	2.35	0.44
1:A:931:ALA:HA	1:A:941:VAL:HG21	2.00	0.44
1:A:1268:SER:O	1:A:1271:PHE:N	2.51	0.44
1:A:351:ILE:HD11	1:A:364:PHE:CE2	2.53	0.44
1:A:592:TYR:CE2	1:A:793:ARG:HD2	2.53	0.44
1:A:1046:MET:HE2	1:A:1046:MET:CA	2.44	0.44
1:A:218:LEU:C	1:A:220:ASP:N	2.73	0.43
1:A:644:ASN:O	1:A:653:THR:HA	2.18	0.43
1:A:55:ILE:HD12	1:A:68:PHE:CE1	2.52	0.43
1:A:293:PRO:HG2	1:A:294:GLU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ILE:HD13	1:A:695:ILE:N	2.33	0.43
1:A:768:ASN:HD21	1:A:771:LYS:HG3	1.83	0.43
1:A:783:PRO:HB2	1:A:785:ASN:HB2	2.01	0.43
1:A:980:ARG:NH1	1:A:1161:GLU:OE1	2.51	0.43
1:A:81:HIS:CD2	1:A:226:LEU:HD11	2.52	0.43
1:A:348:GLY:O	1:A:352:ILE:HG12	2.19	0.43
1:A:1310:ASP:OD2	1:A:1313:THR:HG23	2.18	0.43
1:A:403:LEU:HD11	1:A:406:ILE:CD1	2.49	0.43
1:A:472:GLN:HE22	1:A:484:SER:HB3	1.82	0.43
1:A:134:THR:OG1	1:A:137:GLU:HG3	2.18	0.43
1:A:530:ASP:O	1:A:532:GLU:N	2.52	0.43
1:A:666:ILE:CD1	1:A:807:VAL:HG22	2.48	0.43
1:A:741:HIS:HE1	1:A:838:GLY:HA2	1.83	0.43
1:A:1046:MET:HA	1:A:1046:MET:CE	2.45	0.43
1:A:1088:GLN:HG2	1:A:1133:TYR:CG	2.54	0.43
1:A:388:PHE:C	1:A:390:PRO:HD3	2.43	0.43
1:A:433:VAL:HA	1:A:456:GLY:O	2.18	0.43
1:A:699:GLN:O	1:A:700:ASP:C	2.61	0.43
1:A:963:THR:HG21	1:A:1181:ASP:OD2	2.18	0.43
1:A:333:LEU:HA	1:A:336:PHE:HB2	2.00	0.43
1:A:1000:ILE:HG23	1:A:1000:ILE:O	2.18	0.43
1:A:1018:GLY:HA2	1:A:1131:GLY:O	2.19	0.43
1:A:1104:PHE:CD2	1:A:1119:ASP:HB3	2.53	0.43
1:A:63:ASN:O	1:A:63:ASN:CG	2.61	0.43
1:A:766:THR:CG2	1:A:767:GLN:H	2.32	0.43
1:A:782:VAL:HG23	1:A:783:PRO:O	2.19	0.43
1:A:839:ARG:HB2	1:A:911:PHE:CD1	2.53	0.43
1:A:1039:GLY:N	1:A:1040:GLN:HE21	2.17	0.43
1:A:443:PRO:O	1:A:445:THR:HG23	2.19	0.43
1:A:477:TRP:HD1	1:A:523:LEU:HD23	1.84	0.43
1:A:103:ARG:HE	1:A:200:PHE:HB3	1.84	0.42
1:A:473:LEU:O	1:A:474:SER:HB2	2.18	0.42
1:A:785:ASN:CB	1:A:786:ARG:HH11	2.32	0.42
1:A:9:PHE:N	1:A:9:PHE:CD1	2.87	0.42
1:A:123:MET:CE	1:A:126:LEU:HD23	2.49	0.42
1:A:154:PRO:O	1:A:155:ILE:C	2.60	0.42
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.49	0.42
1:A:361:ASN:HB2	1:A:362:PRO:HD3	2.01	0.42
1:A:417:PHE:CD2	1:A:418:SER:N	2.87	0.42
1:A:1300:THR:HB	1:A:1301:PRO:CD	2.48	0.42
1:A:707:PHE:CD1	1:A:899:ARG:NE	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ILE:O	1:A:1008:SER:CB	2.67	0.42
1:A:1104:PHE:HZ	1:A:1125:VAL:HG21	1.84	0.42
1:A:482:LEU:HD23	1:A:482:LEU:O	2.19	0.42
1:A:695:ILE:O	1:A:903:THR:HB	2.19	0.42
1:A:699:GLN:HE21	1:A:703:ASN:ND2	2.18	0.42
1:A:726:ALA:HB1	1:A:728:ASN:O	2.19	0.42
1:A:794:MET:HE3	1:A:794:MET:HB2	1.81	0.42
1:A:872:ASP:CG	1:A:909:THR:CG2	2.92	0.42
1:A:978:LEU:O	1:A:981:LYS:HB2	2.19	0.42
1:A:563:VAL:O	1:A:564:PRO:C	2.62	0.42
1:A:622:THR:O	1:A:622:THR:CG2	2.68	0.42
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.89	0.42
1:A:1252:ALA:O	1:A:1253:ILE:C	2.63	0.42
1:A:359:ASP:OD2	1:A:359:ASP:N	2.52	0.42
1:A:581:ALA:HB1	1:A:584:MET:HE2	2.01	0.42
1:A:730:VAL:O	1:A:847:LYS:HA	2.19	0.42
1:A:752:VAL:O	1:A:752:VAL:CG1	2.67	0.42
1:A:1079:ALA:C	1:A:1081:ALA:H	2.27	0.42
1:A:1104:PHE:CZ	1:A:1125:VAL:HG21	2.54	0.42
1:A:233:VAL:HG22	1:A:273:LEU:HD11	2.00	0.42
1:A:324:GLU:OE2	1:A:327:ARG:NH2	2.53	0.42
1:A:1210:GLU:HG2	1:A:1212:HIS:NE2	2.35	0.42
1:A:98:HIS:ND1	1:A:99:PRO:CD	2.83	0.42
1:A:116:THR:O	1:A:120:VAL:HG23	2.20	0.42
1:A:372:THR:C	1:A:373:LEU:HD23	2.45	0.42
1:A:1077:THR:HG23	1:A:1082:SER:OG	2.20	0.42
1:A:214:GLU:HG2	1:A:217:ARG:HH21	1.85	0.42
1:A:307:VAL:HG21	1:A:347:ILE:CG2	2.49	0.42
1:A:482:LEU:HD12	1:A:519:TYR:CD2	2.54	0.42
1:A:591:VAL:HG13	1:A:595:ASP:HB2	2.02	0.42
1:A:728:ASN:O	1:A:729:VAL:HG23	2.20	0.42
1:A:102:GLU:OE2	1:A:106:ARG:NH2	2.53	0.41
1:A:730:VAL:HG23	1:A:850:PHE:HE2	1.83	0.41
1:A:940:GLU:O	1:A:944:LYS:HG3	2.20	0.41
1:A:1046:MET:SD	1:A:1087:GLY:HA2	2.60	0.41
1:A:365:MET:C	1:A:367:SER:H	2.28	0.41
1:A:626:LYS:HA	1:A:631:PHE:CD2	2.55	0.41
1:A:1045:LYS:O	1:A:1049:VAL:HG23	2.21	0.41
1:A:242:GLU:O	1:A:246:ASP:HB2	2.20	0.41
1:A:397:LEU:HD12	1:A:397:LEU:N	2.35	0.41
1:A:733:GLU:O	1:A:1294:GLN:NE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:ILE:HA	1:A:892:PRO:HD2	1.86	0.41
1:A:283:ILE:HA	1:A:284:PRO:HD3	1.87	0.41
1:A:504:VAL:HG23	1:A:505:GLU:N	2.34	0.41
1:A:850:PHE:N	1:A:850:PHE:CD2	2.88	0.41
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.55	0.41
1:A:1068:THR:HG22	8:A:4080:HOH:O	2.21	0.41
1:A:765:SER:OG	1:A:794:MET:HG2	2.20	0.41
1:A:883:PHE:HZ	1:A:1140:TYR:CD2	2.39	0.41
1:A:964:LEU:N	1:A:965:PRO:CD	2.82	0.41
1:A:1173:ASN:HD22	1:A:1270:ILE:CD1	2.32	0.41
1:A:980:ARG:O	1:A:984:VAL:HG23	2.20	0.41
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.02	0.41
1:A:248:LYS:HD3	1:A:256:LEU:HD21	2.02	0.41
1:A:257:VAL:O	1:A:279:CYS:HA	2.21	0.41
1:A:538:LEU:HD12	1:A:539:ASP:H	1.86	0.41
1:A:614:HIS:CB	1:A:904:ASN:ND2	2.80	0.41
1:A:768:ASN:ND2	1:A:771:LYS:HB2	2.35	0.41
1:A:365:MET:HE2	1:A:385:ASP:C	2.45	0.41
1:A:421:LYS:HG3	1:A:434:THR:CG2	2.51	0.41
1:A:739:GLN:HE21	1:A:1209:GLU:CD	2.29	0.41
1:A:900:ILE:HD12	1:A:900:ILE:N	2.36	0.41
1:A:1020:LEU:HB3	1:A:1032:THR:HG22	2.03	0.41
1:A:1298:PRO:HG2	1:A:1300:THR:HG23	2.02	0.41
1:A:1033:HIS:HD2	1:A:1035:GLY:N	2.19	0.41
1:A:123:MET:HE1	1:A:126:LEU:HD23	2.04	0.40
1:A:296:ILE:HD11	1:A:314:GLU:HG3	2.03	0.40
1:A:972:ILE:CG1	1:A:973:ALA:N	2.84	0.40
1:A:1011:LEU:HD12	1:A:1012:PRO:HD2	2.03	0.40
1:A:69:SER:N	1:A:125:THR:HG21	2.36	0.40
1:A:431:ALA:CB	1:A:434:THR:HG23	2.51	0.40
1:A:1250:LYS:H	1:A:1250:LYS:HG3	1.68	0.40
1:A:73:CYS:SG	1:A:74:LEU:HG	2.61	0.40
1:A:398:ARG:HG3	1:A:401:GLU:CD	2.47	0.40
1:A:699:GLN:HE21	1:A:703:ASN:CG	2.30	0.40
1:A:924:GLU:HA	1:A:924:GLU:OE1	2.20	0.40
1:A:788:VAL:HG21	1:A:1069:ASN:OD1	2.22	0.40
1:A:839:ARG:HG2	1:A:840:HIS:N	2.36	0.40
1:A:1206:PHE:C	1:A:1207:THR:CG2	2.94	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	1291/1331 (97%)	1142 (88%)	117 (9%)	32 (2%)	4 8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	602	GLU
1	A	1008	SER
1	A	1325	LYS
1	A	152	TYR
1	A	212	PRO
1	A	428	ASP
1	A	551	LYS
1	A	567	GLN
1	A	1253	ILE
1	A	1316	CYS
1	A	62	GLN
1	A	390	PRO
1	A	471	LYS
1	A	531	LEU
1	A	739	GLN
1	A	797	GLY
1	A	912	ARG
1	A	1288	ASN
1	A	552	ASP
1	A	1251	ARG
1	A	662	CYS
1	A	977	TYR
1	A	366	ALA
1	A	386	HIS
1	A	593	CYS
1	A	1002	PRO
1	A	1259	VAL

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Mol	Chain	Res	Type
1	A	258	VAL
1	A	1286	GLY
1	A	729	VAL
1	A	1329	VAL

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	1095/1123 (98%)	1058 (97%)	37 (3%)	32 60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	246	ASP
1	A	253	ASP
1	A	255	LYS
1	A	256	LEU
1	A	306	LEU
1	A	315	ILE
1	A	370	LYS
1	A	378	THR
1	A	413	GLU
1	A	434	THR
1	A	480	GLU
1	A	494	GLN
1	A	532	GLU
1	A	624	GLU
1	A	646	THR
1	A	662	CYS
1	A	743	TYR
1	A	761	GLU
1	A	782	VAL
1	A	798	PHE
1	A	807	VAL

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Mol	Chain	Res	Type
1	A	821	ARG
1	A	826	MET
1	A	909	THR
1	A	939	GLU
1	A	983	GLU
1	A	1002	PRO
1	A	1040	GLN
1	A	1072	PRO
1	A	1085	LEU
1	A	1143	GLU
1	A	1203	LEU
1	A	1250	LYS
1	A	1253	ILE
1	A	1268	SER
1	A	1311	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	130	GLN
1	A	223	GLN
1	A	250	GLN
1	A	260	ASN
1	A	332	GLN
1	A	472	GLN
1	A	478	ASN
1	A	483	GLN
1	A	556	ASN
1	A	567	GLN
1	A	585	GLN
1	A	614	HIS
1	A	642	ASN
1	A	699	GLN
1	A	705	ASN
1	A	768	ASN
1	A	893	ASN
1	A	904	ASN
1	A	908	ASN
1	A	956	ASN
1	A	1033	HIS
1	A	1040	GLN

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Mol	Chain	Res	Type
1	A	1048	GLN
1	A	1086	ASN
1	A	1173	ASN
1	A	1220	HIS
1	A	1288	ASN
1	A	1311	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	PO4	A	2003	-	4,4,4	1.80	2 (50%)	6,6,6	0.45	0
6	SAL	A	4005	-	10,10,10	2.10	5 (50%)	13,13,13	2.13	4 (30%)
7	ACY	A	3001	-	3,3,3	0.62	0	3,3,3	0.84	0
4	FES	A	4002	1	0,4,4	-	-	-	-	-
2	PO4	A	2001	-	4,4,4	1.73	1 (25%)	6,6,6	0.47	0
2	PO4	A	2002	-	4,4,4	1.71	1 (25%)	6,6,6	0.48	0
4	FES	A	4003	1	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	A	4004	-	58,58,58	2.29	19 (32%)	85,89,89	2.08	23 (27%)

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	FAD	A	4004	-	-	6/34/50/50	0/6/6/6
6	SAL	A	4005	-	-	0/4/4/4	0/1/1/1
4	FES	A	4003	1	-	-	0/1/1/1
4	FES	A	4002	1	-	-	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4004	FAD	C9A-C5X	5.63	1.50	1.41
5	A	4004	FAD	C9A-N10	5.34	1.50	1.41
5	A	4004	FAD	C9-C9A	4.68	1.47	1.39
5	A	4004	FAD	C4A-N3A	4.45	1.42	1.34
5	A	4004	FAD	C6-C5X	4.12	1.46	1.40
5	A	4004	FAD	C5A-C4A	4.12	1.46	1.39
5	A	4004	FAD	C2A-N1A	4.09	1.41	1.33
5	A	4004	FAD	O4B-C1B	4.05	1.51	1.42
5	A	4004	FAD	C8-C7	3.92	1.50	1.40
6	A	4005	SAL	C5-C6	3.72	1.45	1.38
5	A	4004	FAD	C4X-N5	3.61	1.38	1.30
5	A	4004	FAD	C10-N1	3.56	1.40	1.33
5	A	4004	FAD	C2-N3	3.49	1.46	1.39
5	A	4004	FAD	C2A-N3A	3.13	1.39	1.33
5	A	4004	FAD	C5A-C6A	3.08	1.49	1.41
5	A	4004	FAD	O4B-C4B	3.06	1.51	1.45
6	A	4005	SAL	C6-C1	2.90	1.44	1.39
6	A	4005	SAL	C3-C2	2.45	1.43	1.39
5	A	4004	FAD	C4X-C10	2.44	1.51	1.44
6	A	4005	SAL	C1-C1'	-2.38	1.44	1.49
5	A	4004	FAD	C6A-N1A	2.20	1.41	1.35
5	A	4004	FAD	C6-C7	2.17	1.42	1.39
5	A	4004	FAD	C4-N3	2.14	1.42	1.38
2	A	2003	PO4	P-O3	-2.09	1.48	1.54
6	A	4005	SAL	O2'-C1'	-2.06	1.24	1.30
2	A	2003	PO4	P-O2	-2.03	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	PO4	P-O2	-2.02	1.48	1.54
2	A	2001	PO4	P-O4	-2.00	1.48	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4004	FAD	C9-C9A-N10	6.82	131.02	121.85
5	A	4004	FAD	C5X-C9A-N10	-6.75	111.87	117.97
5	A	4004	FAD	C4-C4X-N5	5.22	125.42	118.21
5	A	4004	FAD	N3A-C2A-N1A	-4.84	121.25	128.58
5	A	4004	FAD	O4B-C1B-N9A	-4.62	99.22	108.09
6	A	4005	SAL	O2'-C1'-O1'	-4.19	114.35	123.35
5	A	4004	FAD	C10-N1-C2	3.81	125.11	116.85
5	A	4004	FAD	C8M-C8-C7	3.65	128.21	120.76
6	A	4005	SAL	C2-C1-C1'	3.41	123.50	120.00
5	A	4004	FAD	C8M-C8-C9	-3.36	113.65	119.57
5	A	4004	FAD	C9A-N10-C10	3.32	125.81	120.75
6	A	4005	SAL	C3-C2-C1	3.06	123.08	119.89
5	A	4004	FAD	C4'-C3'-C2'	-2.86	108.81	113.57
5	A	4004	FAD	O3B-C3B-C4B	-2.71	103.30	111.08
5	A	4004	FAD	C2A-N3A-C4A	2.70	118.41	111.83
5	A	4004	FAD	C10-C4X-N5	-2.51	119.68	124.81
6	A	4005	SAL	O2'-C1'-C1	2.51	122.42	115.28
5	A	4004	FAD	O4-C4-C4X	-2.48	119.99	126.53
5	A	4004	FAD	O3'-C3'-C4'	2.41	114.40	108.93
5	A	4004	FAD	O4B-C4B-C5B	-2.34	101.85	109.33
5	A	4004	FAD	C5X-N5-C4X	2.29	121.80	118.09
5	A	4004	FAD	C2'-C1'-N10	2.27	120.94	110.20
5	A	4004	FAD	C1'-N10-C9A	-2.15	116.46	120.63
5	A	4004	FAD	N3A-C4A-N9A	2.14	130.81	127.17
5	A	4004	FAD	O2'-C2'-C3'	2.13	114.23	109.25
5	A	4004	FAD	C6A-C5A-C4A	-2.06	114.37	117.18
5	A	4004	FAD	C2A-N1A-C6A	2.01	122.04	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4004	FAD	N10-C1'-C2'-O2'
5	A	4004	FAD	N10-C1'-C2'-C3'
5	A	4004	FAD	C2'-C3'-C4'-C5'
5	A	4004	FAD	C2'-C3'-C4'-O4'

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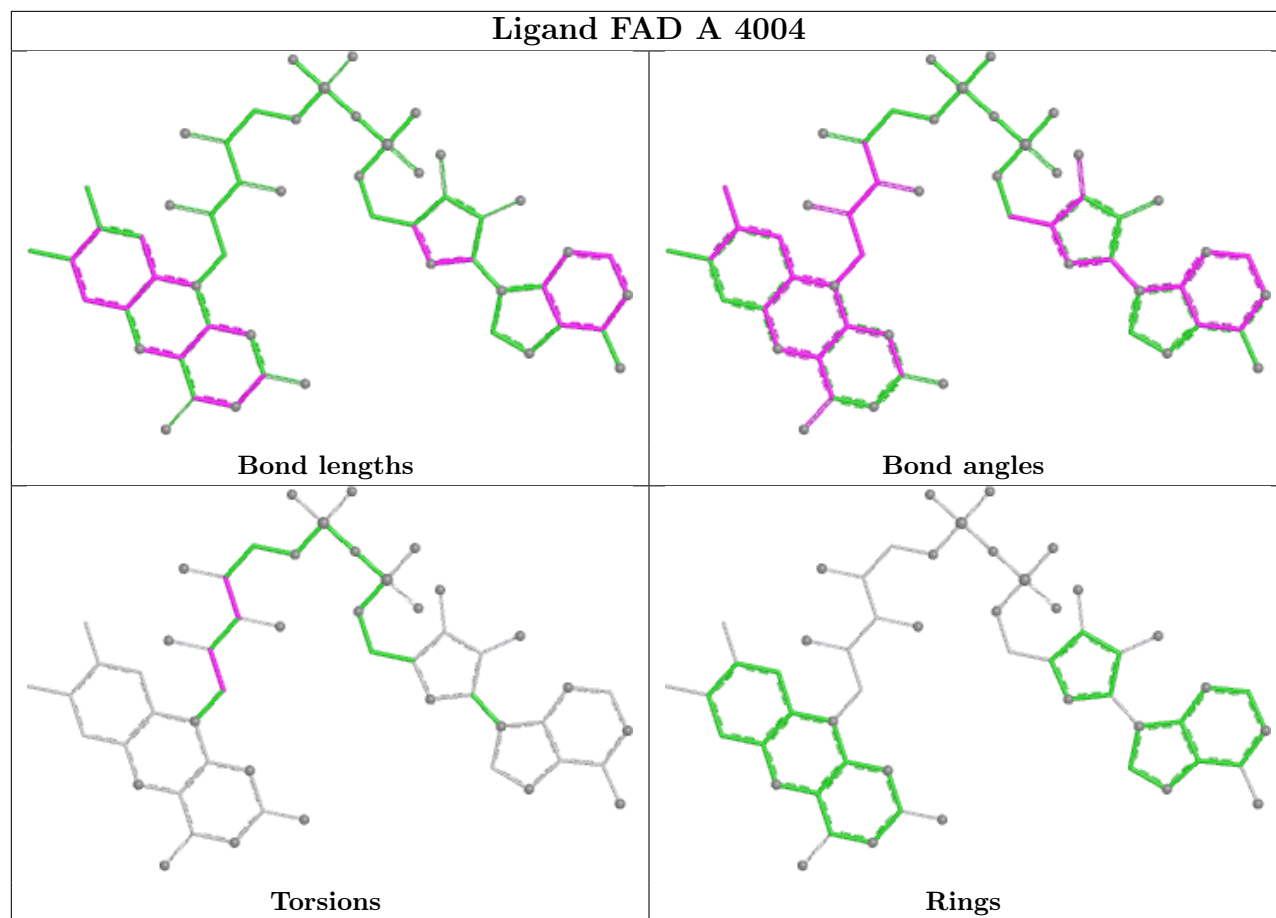
Mol	Chain	Res	Type	Atoms
5	A	4004	FAD	O3'-C3'-C4'-O4'
5	A	4004	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4002	FES	2	0
4	A	4003	FES	1	0
5	A	4004	FAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1297/1331 (97%)	0.29	53 (4%) 41 36	9, 35, 61, 88	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1317	VAL	6.6
1	A	1289	ALA	6.3
1	A	1318	THR	6.2
1	A	1315	LEU	6.0
1	A	3	ALA	5.5
1	A	1331	ILE	5.3
1	A	1324	SER	4.9
1	A	1326	SER	4.2
1	A	1291	GLN	4.0
1	A	1316	CYS	4.0
1	A	1286	GLY	3.9
1	A	1325	LYS	3.9
1	A	221	THR	3.7
1	A	1288	ASN	3.7
1	A	398	ARG	3.7
1	A	192	PRO	3.4
1	A	61	LEU	3.4
1	A	1329	VAL	3.3
1	A	321	GLN	3.2
1	A	1328	SER	3.2
1	A	164	LYS	3.2
1	A	1330	ARG	3.1
1	A	1290	LYS	3.0
1	A	534	MET	3.0
1	A	60	ARG	2.8
1	A	531	LEU	2.8
1	A	220	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	497	PRO	2.7
1	A	1287	ASP	2.7
1	A	1108	LYS	2.6
1	A	529	ALA	2.6
1	A	533	ASP	2.5
1	A	530	ASP	2.4
1	A	535	ALA	2.4
1	A	1327	TRP	2.4
1	A	551	LYS	2.4
1	A	494	GLN	2.4
1	A	1292	LEU	2.3
1	A	253	ASP	2.2
1	A	1111	GLY	2.2
1	A	550	GLN	2.2
1	A	1107	LYS	2.2
1	A	983	GLU	2.1
1	A	270	LYS	2.1
1	A	313	GLU	2.1
1	A	222	PRO	2.1
1	A	496	ALA	2.1
1	A	495	LEU	2.1
1	A	569	GLU	2.1
1	A	528	ARG	2.0
1	A	598	ARG	2.0
1	A	948	LYS	2.0
1	A	218	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

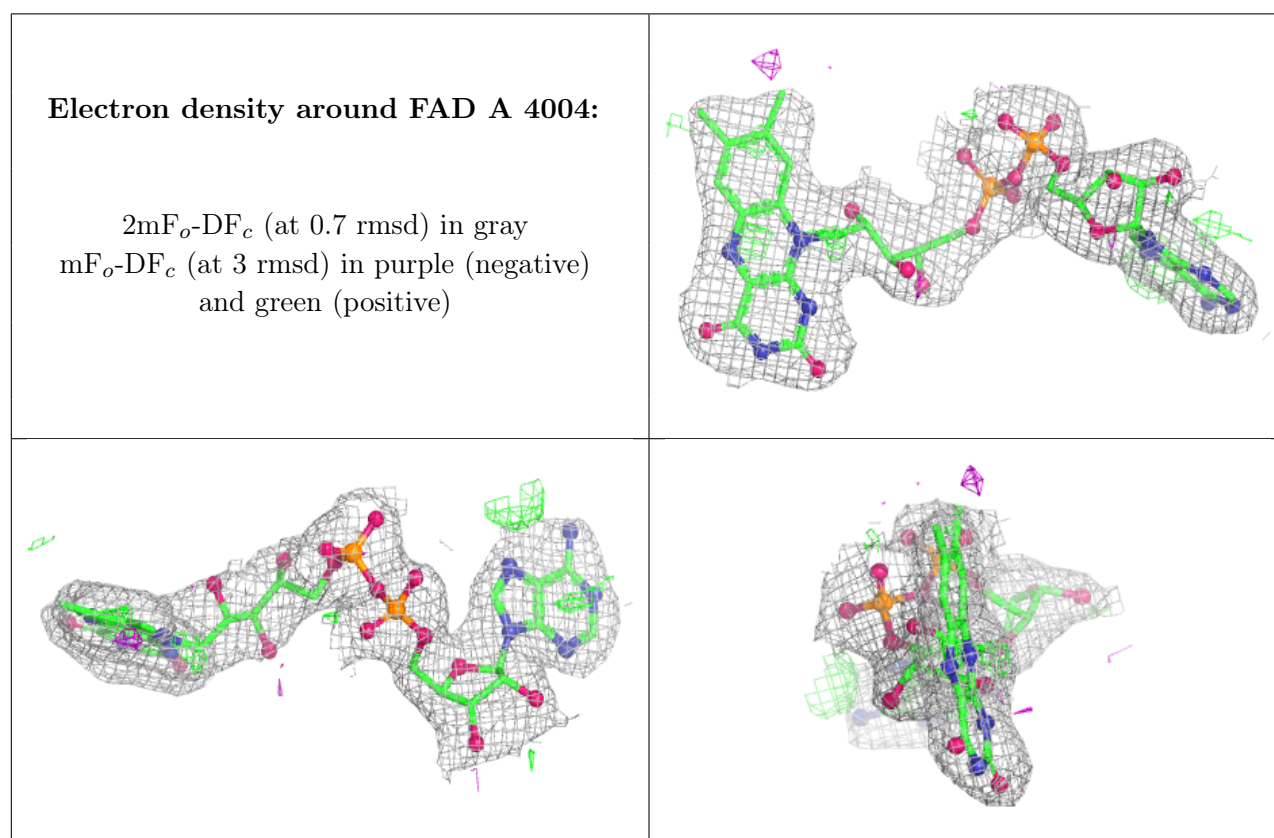
There are no oligosaccharides in this entry.

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
7	ACY	A	3001	4/4	0.77	0.25	55,55,56,56	0
6	SAL	A	4005	10/10	0.81	0.16	31,33,42,42	0
2	PO4	A	2002	5/5	0.87	0.12	68,68,69,70	0
2	PO4	A	2003	5/5	0.92	0.12	70,70,71,72	0
3	CA	A	4001	1/1	0.94	0.05	28,28,28,28	0
5	FAD	A	4004	53/53	0.94	0.11	25,36,44,45	0
2	PO4	A	2001	5/5	0.98	0.08	41,42,44,45	0
4	FES	A	4002	4/4	0.98	0.07	31,31,34,36	0
4	FES	A	4003	4/4	0.98	0.04	22,23,23,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.