Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:31 PM GMT

PDB ID	:	1FZ5
Title	:	METHANE MONOOXYGENASE HYDROXYLASE, FORM II CRYSTALLIZED ANAEROBICALLY FROM REDUCED ENZYME
Authors	:	Whittington, D.A.; Lippard, S.J.
Deposited on	:	2000-10-03
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

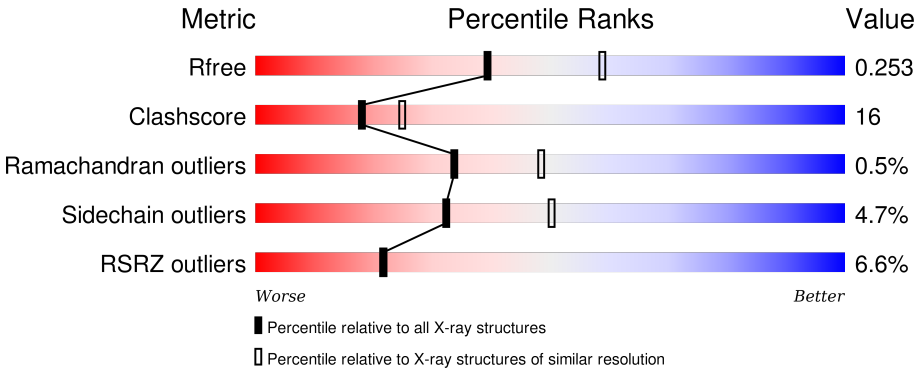
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	6% 65% 29%
1	B	527	7% 65% 29%
2	C	389	74% 23%
2	D	389	10% 72% 25%
3	E	170	% 61% 32%

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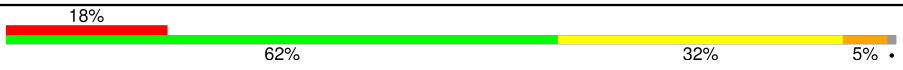
Mol	Chain	Length	Quality of chain
3	F	170	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18004 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 METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4181	2675	721	767	18			
1	B	510	Total	C	N	O	S	0	0	0
			4177	2673	719	767	18			

- Molecule 2 is a protein called METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3193	2054	551	580	8			
2	D	386	Total	C	N	O	S	0	0	0
			3175	2042	548	577	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	370	ARG	ALA	CONFLICT	UNP P18798
D	370	ARG	ALA	CONFLICT	UNP P18798

- Molecule 3 is a protein called METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			
3	F	168	Total	C	N	O	S	0	0	0
			1382	875	249	253	5			

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0

- Molecule 6 is water.

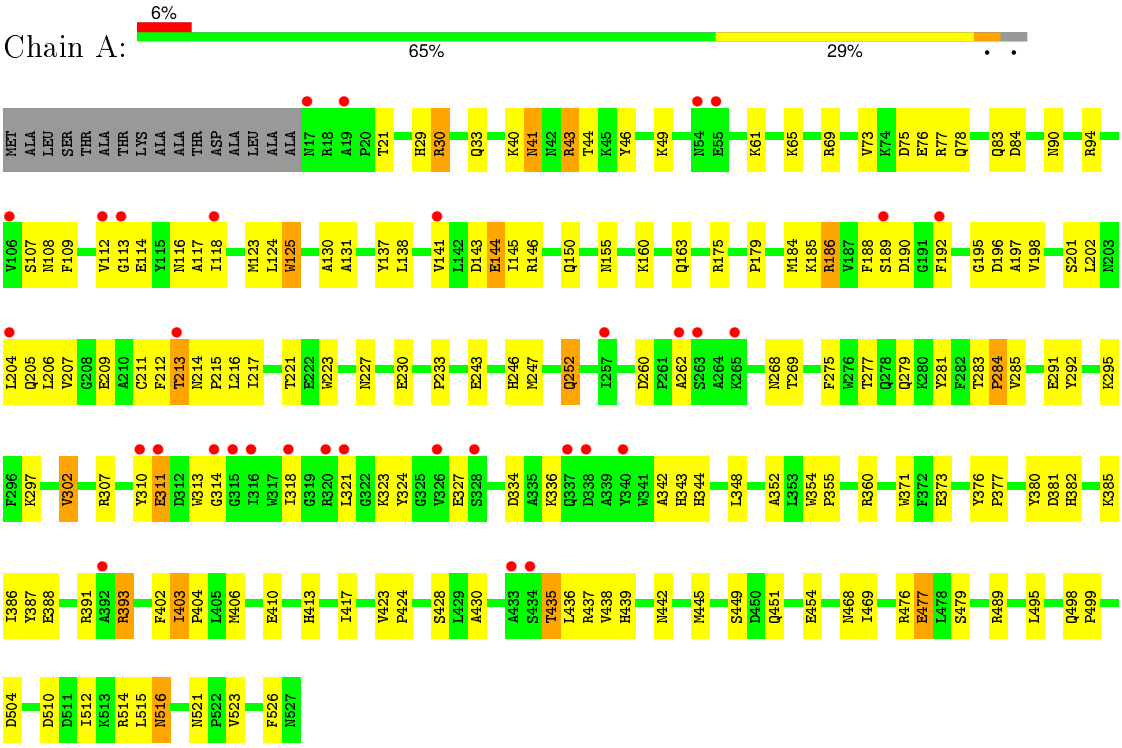
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	133	Total O 133 133	0	0
6	B	89	Total O 89 89	0	0
6	C	178	Total O 178 178	0	0
6	D	42	Total O 42 42	0	0
6	E	70	Total O 70 70	0	0
6	F	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

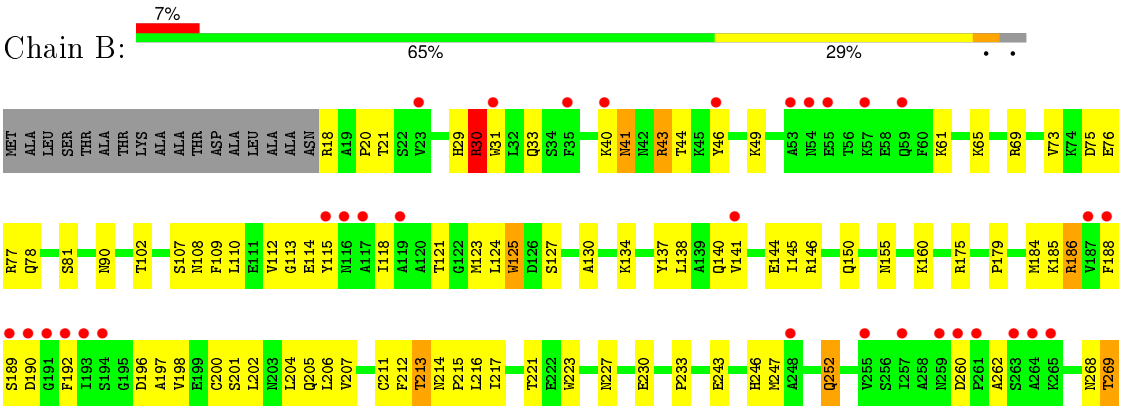
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

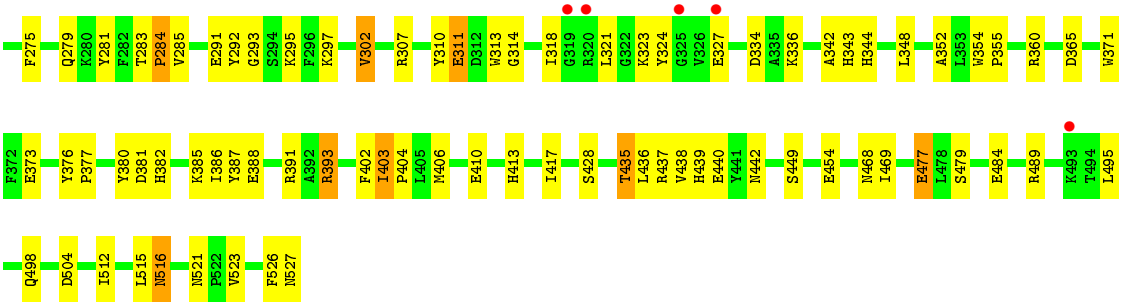
Chain A:

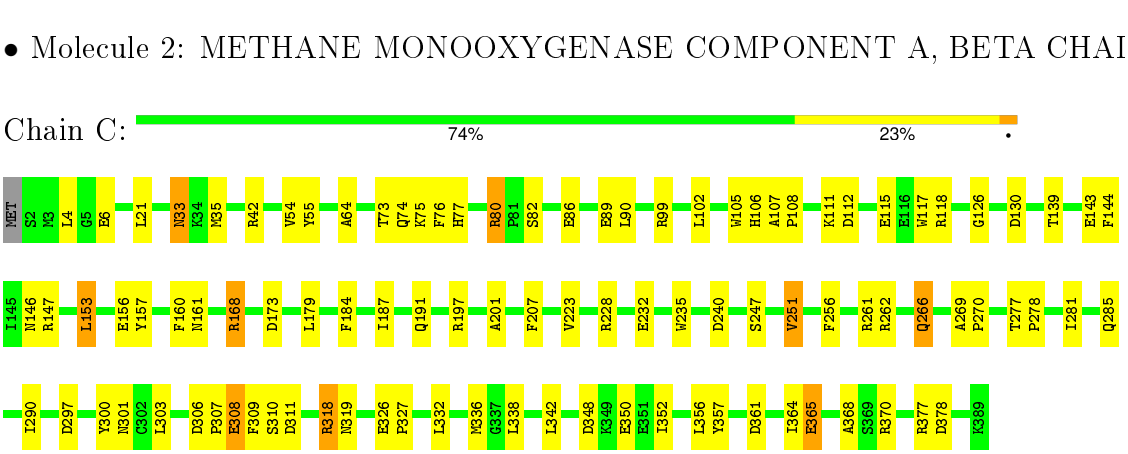


• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

Chain B:





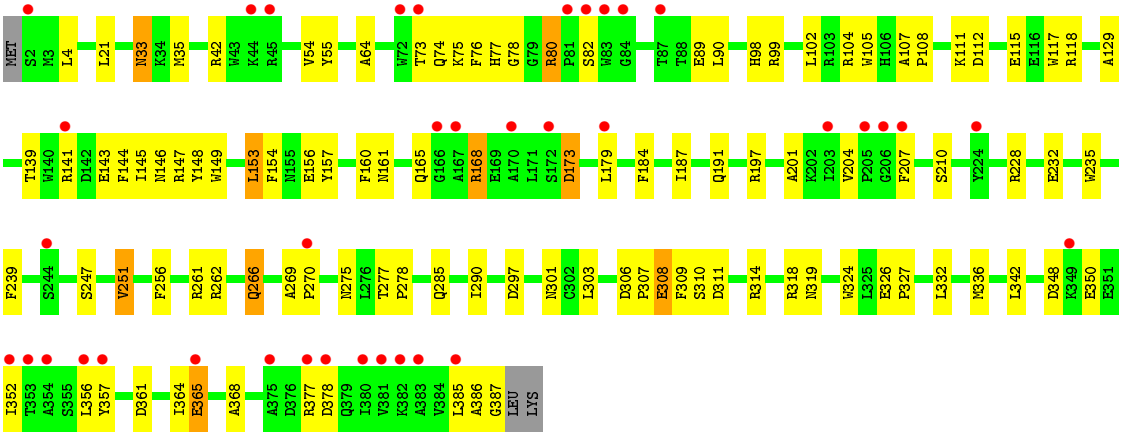


• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:

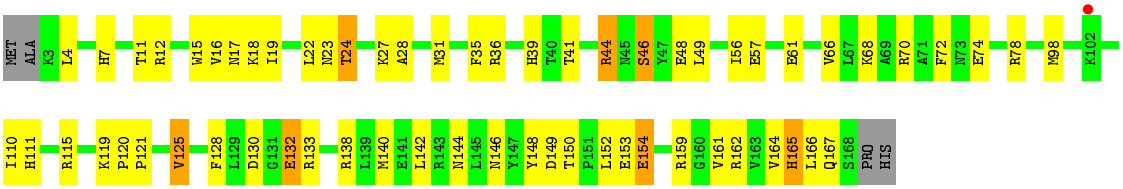
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:



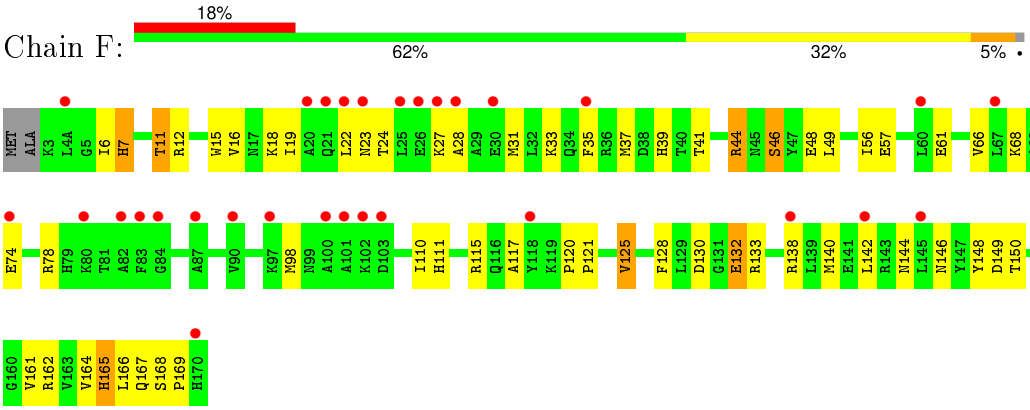
• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E:



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:


18%
62%
32%
5%
MET ALA K3 L4A G5 I6 H7 T11 R12 W15 V16 N17 K18 I19 A20 Q21 L22 N23 T24 L25 E26 K27 A28 A29 E30 M31 L32 K33 Q34 F35 R36 M37 D38 H39 T40 T41 R44 N45 S46 Y47 E48 L49 I56 E57 L60 E61 V66 L67 K68 A69 R70 A71 F72 N73
E74 R78 H79 K80 T81 A82 F83 G84 A87 V90 K97 M98 N99 A100 A101 K102 D103 I110 H111 R115 Q116 A117 Y118 K119 P120 P121 V125 F128 L129 D130 G131 E132 R133 R138 L139 M140 E141 L142 R143 N144 L145 N146 Y147 Y148 D149 T150 E153 E154 R159
G160 V161 R162 V163 V164 H165 L166 Q167 S168 P169 H170

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.24Å 171.57Å 220.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.40 – 2.40 49.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.2 (46.40-2.40) 89.3 (49.08-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.253 0.219 , 0.253	Depositor DCC
R_{free} test set	3359 reflections (3.53%)	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 104302 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18004	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE2

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	0.38	0/4306	0.70	9/5848 (0.2%)
1	B	0.39	0/4302	0.71	9/5842 (0.2%)
2	C	0.40	0/3289	0.65	3/4464 (0.1%)
2	D	0.36	0/3271	0.65	4/4442 (0.1%)
3	E	0.42	0/1396	0.61	0/1880
3	F	0.35	0/1412	0.58	0/1903
All	All	0.38	0/17976	0.67	25/24379 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	318	ARG	NE-CZ-NH1	13.78	127.19	120.30
2	C	318	ARG	NE-CZ-NH1	-13.70	113.45	120.30
2	D	318	ARG	NE-CZ-NH2	-13.58	113.51	120.30
1	B	77	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	A	77	ARG	NE-CZ-NH1	-12.11	114.25	120.30
1	A	391	ARG	NE-CZ-NH1	-12.11	114.25	120.30
1	B	391	ARG	NE-CZ-NH2	-12.02	114.29	120.30
2	C	318	ARG	NE-CZ-NH2	12.00	126.30	120.30
1	B	30	ARG	NE-CZ-NH2	-11.97	114.32	120.30
1	A	30	ARG	NE-CZ-NH2	11.90	126.25	120.30
1	A	30	ARG	NE-CZ-NH1	-11.80	114.40	120.30
1	A	77	ARG	NE-CZ-NH2	11.65	126.13	120.30
1	B	77	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	B	391	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	391	ARG	NE-CZ-NH2	11.40	126.00	120.30
1	B	30	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	A	30	ARG	CD-NE-CZ	6.18	132.25	123.60
2	C	318	ARG	CD-NE-CZ	5.86	131.80	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	ARG	CD-NE-CZ	5.84	131.78	123.60
2	D	104	ARG	NE-CZ-NH2	5.75	123.17	120.30
2	D	318	ARG	CD-NE-CZ	5.72	131.61	123.60
1	B	30	ARG	CD-NE-CZ	5.72	131.61	123.60
1	B	391	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	77	ARG	CD-NE-CZ	5.59	131.43	123.60
1	B	77	ARG	CD-NE-CZ	5.05	130.66	123.60

There are no chirality outliers.

There are no planarity outliers.

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	A	4181	0	3977	153	0
1	B	4177	0	3975	156	0
2	C	3193	0	3042	87	0
2	D	3175	0	3018	92	0
3	E	1368	0	1363	59	0
3	F	1382	0	1366	62	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	133	0	0	3	0
6	B	89	0	0	2	0
6	C	178	0	0	8	0
6	D	42	0	0	0	0
6	E	70	0	0	1	0
6	F	12	0	0	0	0
All	All	18004	0	16741	538	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 16.

All (538) 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:352:ALA:HA	1:A:404:PRO:HB2	1.36	1.06
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.38	1.02
1:A:355:PRO:HG2	1:A:403:ILE:HD11	1.43	0.99
1:B:355:PRO:HG2	1:B:403:ILE:HD11	1.42	0.99
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.45	0.98
2:D:146:ASN:HD21	2:D:197:ARG:HH21	1.12	0.98
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.12	0.95
2:C:319:ASN:HA	3:E:74:GLU:OE1	1.68	0.94
3:F:15:TRP:O	3:F:19:ILE:HG13	1.69	0.92
1:A:252:GLN:HA	1:A:252:GLN:NE2	1.85	0.92
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.17	0.91
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.03	0.90
3:F:132:GLU:OE2	3:F:132:GLU:HA	1.67	0.90
3:E:132:GLU:OE2	3:E:132:GLU:HA	1.71	0.89
1:A:78:GLN:HE22	1:A:150:GLN:HE21	0.92	0.89
3:E:15:TRP:O	3:E:19:ILE:HG13	1.73	0.89
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.16	0.88
1:B:252:GLN:NE2	1:B:252:GLN:HA	1.88	0.85
1:A:252:GLN:HE21	1:A:252:GLN:HA	1.39	0.85
2:D:319:ASN:HA	3:F:74:GLU:OE1	1.77	0.84
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.75	0.83
1:A:44:THR:HG22	1:A:46:TYR:H	1.44	0.82
1:B:44:THR:HG22	1:B:46:TYR:H	1.43	0.80
1:B:227:ASN:HD21	1:B:295:LYS:H	1.28	0.80
1:B:269:THR:HG22	3:F:148:TYR:CE1	2.18	0.79
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.76	0.78
1:B:252:GLN:HE21	1:B:252:GLN:HA	1.48	0.77
1:B:41:ASN:HD22	1:B:41:ASN:N	1.84	0.76
1:A:118:ILE:HG12	1:A:144:GLU:HB3	1.68	0.75
1:A:41:ASN:HD22	1:A:41:ASN:N	1.83	0.75
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.68	0.75
3:E:138:ARG:HH21	3:E:142:LEU:HD21	1.51	0.74
2:D:146:ASN:ND2	2:D:197:ARG:HH21	1.83	0.74
1:A:355:PRO:HG2	1:A:403:ILE:CD1	2.18	0.74
1:B:381:ASP:HA	1:B:385:LYS:HE2	1.70	0.74
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.83	0.74
3:F:12:ARG:O	3:F:16:VAL:HG23	1.88	0.73
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.37	0.73
1:B:307:ARG:HA	1:B:311:GLU:HG3	1.71	0.73
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.71	0.72
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.73	0.72
1:A:355:PRO:CG	1:A:403:ILE:HD11	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:HA	1:A:311:GLU:HG3	1.72	0.72
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.20	0.72
3:F:138:ARG:HH21	3:F:142:LEU:HD21	1.53	0.72
2:C:365:GLU:OE1	2:C:365:GLU:HA	1.90	0.72
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.72	0.71
1:A:117:ALA:HB3	1:A:144:GLU:CG	2.20	0.71
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.71	0.71
1:A:117:ALA:HB3	1:A:144:GLU:HG2	1.72	0.71
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.38	0.71
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.89	0.71
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.89	0.70
1:B:213:THR:O	1:B:217:ILE:HG12	1.91	0.70
3:E:24:THR:HG22	3:E:27:LYS:H	1.55	0.70
2:C:223:VAL:HG13	6:C:5175:HOH:O	1.92	0.70
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.85	0.70
2:C:361:ASP:O	2:C:365:GLU:HB2	1.92	0.70
1:B:436:LEU:HB3	3:F:167:GLN:HE21	1.57	0.70
1:A:213:THR:O	1:A:217:ILE:HG12	1.91	0.69
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.73	0.69
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.40	0.69
3:E:12:ARG:O	3:E:16:VAL:HG23	1.92	0.69
1:B:160:LYS:HA	2:D:33:ASN:HB2	1.74	0.69
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.21	0.69
1:B:355:PRO:HG2	1:B:403:ILE:CD1	2.19	0.68
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.57	0.68
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.74	0.68
1:B:355:PRO:CG	1:B:403:ILE:HD11	2.20	0.68
1:B:206:LEU:HB2	6:B:5079:HOH:O	1.93	0.67
2:C:111:LYS:O	2:C:115:GLU:HG3	1.94	0.67
1:A:107:SER:HB3	1:A:155:ASN:HD21	1.59	0.67
2:D:111:LYS:O	2:D:115:GLU:HG3	1.94	0.67
2:D:385:LEU:C	2:D:387:GLY:H	1.98	0.67
1:A:269:THR:HG22	3:E:148:TYR:CE1	2.30	0.67
2:D:228:ARG:O	2:D:232:GLU:HG3	1.94	0.66
3:E:17:ASN:HB3	6:E:214:HOH:O	1.94	0.66
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.76	0.66
1:A:124:LEU:HD21	1:A:201:SER:HB2	1.77	0.66
1:A:76:GLU:HG2	1:B:76:GLU:HG2	1.78	0.66
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.30	0.66
1:B:78:GLN:HE22	1:B:150:GLN:NE2	1.87	0.66
1:B:526:PHE:O	1:B:527:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.77	0.66
2:D:365:GLU:OE1	2:D:365:GLU:HA	1.95	0.66
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.77	0.65
1:A:117:ALA:CB	1:A:144:GLU:HG2	2.26	0.65
3:F:41:THR:O	3:F:44:ARG:HD2	1.97	0.65
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.79	0.65
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.32	0.65
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.80	0.64
3:E:150:THR:HG23	3:E:154:GLU:HG2	1.79	0.64
2:D:146:ASN:HD21	2:D:197:ARG:NH2	1.90	0.64
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.79	0.64
1:A:438:VAL:HB	3:E:164:VAL:HG23	1.77	0.64
1:A:227:ASN:HD21	1:A:295:LYS:H	1.45	0.64
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.44	0.64
2:C:228:ARG:O	2:C:232:GLU:HG3	1.98	0.64
1:B:526:PHE:HE2	3:F:165:HIS:HD2	1.46	0.64
1:B:184:MET:CE	1:B:188:PHE:HB2	2.27	0.64
3:F:24:THR:HG22	3:F:27:LYS:H	1.61	0.64
2:C:146:ASN:HD21	2:C:197:ARG:NH2	1.91	0.63
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.80	0.63
2:D:385:LEU:O	2:D:387:GLY:N	2.31	0.63
2:C:308:GLU:HG2	2:C:309:PHE:CE1	2.34	0.63
1:A:184:MET:CE	1:A:188:PHE:HB2	2.28	0.63
2:D:361:ASP:O	2:D:365:GLU:HB2	1.99	0.63
3:F:150:THR:HG23	3:F:154:GLU:HG2	1.81	0.62
2:D:336:MET:CE	2:D:356:LEU:HD11	2.29	0.62
3:E:41:THR:O	3:E:44:ARG:HD2	1.98	0.62
2:C:348:ASP:O	2:C:352:ILE:HG13	1.99	0.62
3:E:98:MET:HE1	3:E:110:ILE:HB	1.81	0.62
3:E:39:HIS:CD2	3:E:49:LEU:HD12	2.34	0.62
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.65	0.61
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.61
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.61
1:A:190:ASP:HB3	2:C:74:GLN:O	2.00	0.61
2:D:348:ASP:O	2:D:352:ILE:HG13	2.00	0.61
1:B:314:GLY:HA2	1:B:318:ILE:HD12	1.83	0.61
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.35	0.61
2:C:336:MET:HE1	2:C:356:LEU:HD11	1.83	0.60
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.66	0.60
1:B:107:SER:HB3	1:B:155:ASN:HD21	1.65	0.60
1:B:269:THR:HG22	3:F:148:TYR:HE1	1.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:LEU:HB2	6:C:5175:HOH:O	2.00	0.60
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.82	0.60
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.84	0.60
2:D:308:GLU:HG2	2:D:309:PHE:CE1	2.37	0.60
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.84	0.60
2:C:336:MET:CE	2:C:356:LEU:HD11	2.32	0.60
2:D:357:TYR:CD2	2:D:377:ARG:NH1	2.70	0.59
3:F:98:MET:HE1	3:F:110:ILE:HB	1.84	0.59
3:F:57:GLU:O	3:F:61:GLU:HG3	2.01	0.59
1:A:314:GLY:HA2	1:A:318:ILE:HD12	1.84	0.59
2:C:105:TRP:O	2:C:108:PRO:HD2	2.02	0.59
3:F:111:HIS:HE1	3:F:132:GLU:OE2	1.86	0.59
3:F:22:LEU:HD11	3:F:31:MET:SD	2.43	0.58
1:A:243:GLU:O	1:A:247:MET:HG2	2.03	0.58
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.38	0.58
2:C:139:THR:O	2:C:143:GLU:HB3	2.03	0.58
2:D:153:LEU:C	2:D:153:LEU:HD12	2.24	0.58
1:A:207:VAL:HG22	1:A:313:TRP:CZ2	2.39	0.58
3:E:111:HIS:HE1	3:E:132:GLU:OE2	1.87	0.58
1:A:65:LYS:HD2	2:C:117:TRP:HB2	1.86	0.57
2:D:139:THR:O	2:D:143:GLU:HB3	2.04	0.57
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.85	0.57
2:C:6:GLU:HG3	6:C:5095:HOH:O	2.04	0.57
3:F:165:HIS:ND1	3:F:166:LEU:N	2.53	0.57
2:D:105:TRP:O	2:D:108:PRO:HD2	2.05	0.57
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.40	0.57
1:A:185:LYS:O	1:A:189:SER:HB2	2.05	0.57
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.87	0.57
1:B:30:ARG:O	1:B:30:ARG:HD3	2.05	0.57
2:D:33:ASN:HD22	2:D:33:ASN:C	2.07	0.56
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.40	0.56
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.85	0.56
1:B:184:MET:HE3	1:B:188:PHE:HB2	1.87	0.56
2:C:357:TYR:CD2	2:C:377:ARG:NH1	2.73	0.56
1:A:323:LYS:HE2	1:A:324:TYR:CE1	2.40	0.56
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.26	0.56
2:D:187:ILE:O	2:D:191:GLN:HG3	2.04	0.56
1:B:403:ILE:HG22	1:B:406:MET:HG3	1.88	0.56
2:D:385:LEU:C	2:D:387:GLY:N	2.59	0.56
1:A:436:LEU:HB3	3:E:167:GLN:HE21	1.71	0.56
1:A:393:ARG:HH11	1:A:393:ARG:CG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASN:ND2	1:B:295:LYS:H	1.99	0.56
2:C:89:GLU:CD	3:E:125:VAL:HG13	2.26	0.56
2:C:187:ILE:O	2:C:191:GLN:HG3	2.06	0.56
3:E:111:HIS:CE1	3:E:132:GLU:OE2	2.59	0.56
1:A:41:ASN:N	1:A:41:ASN:ND2	2.53	0.56
3:F:98:MET:CE	3:F:110:ILE:HB	2.36	0.56
1:B:190:ASP:HB3	2:D:74:GLN:O	2.06	0.56
1:A:438:VAL:HG12	3:E:164:VAL:HG21	1.86	0.55
2:C:86:GLU:HG2	6:C:5132:HOH:O	2.06	0.55
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.87	0.55
1:B:243:GLU:O	1:B:247:MET:HG2	2.05	0.55
1:B:477:GLU:OE2	1:B:479:SER:N	2.38	0.55
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.86	0.55
3:E:22:LEU:HD11	3:E:31:MET:SD	2.46	0.55
1:A:314:GLY:HA2	1:A:318:ILE:CD1	2.37	0.55
3:E:15:TRP:CD1	3:E:56:ILE:HD13	2.41	0.55
1:B:33:GLN:HE22	1:B:130:ALA:HB1	1.72	0.55
3:F:111:HIS:CE1	3:F:132:GLU:OE2	2.59	0.55
1:A:76:GLU:OE2	1:B:76:GLU:HG2	2.06	0.55
1:B:310:TYR:CZ	1:B:336:LYS:HD2	2.41	0.55
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.55
1:B:185:LYS:O	1:B:189:SER:HB2	2.06	0.55
1:B:314:GLY:HA2	1:B:318:ILE:CD1	2.37	0.55
1:B:230:GLU:C	1:B:233:PRO:HD2	2.27	0.55
1:B:140:GLN:O	1:B:144:GLU:HG2	2.07	0.55
3:E:57:GLU:O	3:E:61:GLU:HG3	2.06	0.55
2:D:146:ASN:HD22	2:D:197:ARG:HE	1.56	0.54
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.90	0.54
1:A:209:GLU:OE2	1:A:246:HIS:ND1	2.39	0.54
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.89	0.54
1:A:230:GLU:C	1:A:233:PRO:HD2	2.28	0.54
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.43	0.54
3:E:35:PHE:CE1	3:E:39:HIS:HD2	2.26	0.54
1:B:436:LEU:HB3	3:F:167:GLN:NE2	2.22	0.54
2:C:306:ASP:O	2:C:310:SER:HB2	2.08	0.54
1:B:438:VAL:HG12	3:F:164:VAL:HG21	1.90	0.54
2:D:156:GLU:OE2	2:D:156:GLU:HA	2.09	0.53
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.05	0.53
3:E:165:HIS:ND1	3:E:166:LEU:N	2.57	0.53
1:A:252:GLN:CA	1:A:252:GLN:NE2	2.68	0.53
3:E:98:MET:CE	3:E:110:ILE:HB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:ND2	1:B:41:ASN:N	2.54	0.53
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.89	0.53
2:C:261:ARG:NE	2:C:285:GLN:HE22	1.98	0.53
1:B:438:VAL:HG12	3:F:164:VAL:CG2	2.38	0.53
2:D:319:ASN:OD1	3:F:78:ARG:HD3	2.08	0.53
3:F:68:LYS:HG3	3:F:72:PHE:CD2	2.43	0.53
3:E:132:GLU:CA	3:E:132:GLU:OE2	2.50	0.53
1:A:438:VAL:HG12	3:E:164:VAL:CG2	2.39	0.53
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.09	0.53
2:C:146:ASN:HD22	2:C:197:ARG:HE	1.57	0.53
1:A:114:GLU:O	1:A:144:GLU:HG3	2.09	0.53
1:A:269:THR:HG22	3:E:148:TYR:HE1	1.72	0.52
3:F:46:SER:OG	3:F:48:GLU:HG2	2.09	0.52
3:F:153:GLU:H	3:F:153:GLU:CD	2.12	0.52
1:A:403:ILE:HG22	1:A:406:MET:HG3	1.91	0.52
2:D:336:MET:HE2	2:D:356:LEU:HD11	1.91	0.52
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.44	0.52
1:B:29:HIS:CD2	1:B:61:LYS:HA	2.44	0.52
1:A:83:GLN:HG2	6:A:5091:HOH:O	2.09	0.52
3:E:46:SER:OG	3:E:48:GLU:HG2	2.10	0.52
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.45	0.52
1:B:313:TRP:CZ3	1:B:318:ILE:HD11	2.45	0.52
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.90	0.52
1:B:393:ARG:NH1	6:B:5051:HOH:O	2.39	0.52
2:C:153:LEU:C	2:C:153:LEU:HD12	2.30	0.52
1:A:123:MET:HE1	1:A:197:ALA:HA	1.91	0.52
1:B:198:VAL:O	1:B:202:LEU:HG	2.09	0.52
3:E:61:GLU:HB3	3:E:121:PRO:HD3	1.92	0.52
2:C:75:LYS:HB3	2:C:80:ARG:O	2.09	0.52
1:A:107:SER:HB3	1:A:155:ASN:ND2	2.24	0.52
1:B:118:ILE:HD13	1:B:145:ILE:HG12	1.92	0.52
2:C:33:ASN:HD22	2:C:33:ASN:C	2.13	0.52
1:B:110:LEU:O	1:B:114:GLU:HG2	2.10	0.52
1:A:33:GLN:HA	1:A:131:ALA:HB3	1.92	0.52
1:B:30:ARG:HD3	1:B:30:ARG:C	2.29	0.52
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.10	0.52
1:B:196:ASP:HB2	3:F:140:MET:SD	2.51	0.51
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.91	0.51
1:A:192:PHE:CE2	1:A:204:LEU:HA	2.45	0.51
1:B:526:PHE:HE2	3:F:165:HIS:CD2	2.27	0.51
1:A:33:GLN:HE22	1:A:130:ALA:HB1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:TRP:CZ3	1:A:318:ILE:HD11	2.46	0.51
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.45	0.51
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.10	0.51
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.09	0.51
1:A:221:THR:HG22	1:A:233:PRO:HA	1.92	0.51
2:C:21:LEU:HD22	2:D:4:LEU:HD21	1.92	0.51
1:B:107:SER:HB3	1:B:155:ASN:ND2	2.26	0.51
3:F:98:MET:HE2	3:F:110:ILE:HD12	1.93	0.51
1:A:380:TYR:CE2	1:A:388:GLU:OE1	2.64	0.51
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.44	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.93	0.51
2:D:336:MET:HE1	2:D:356:LEU:HD11	1.92	0.51
2:D:143:GLU:HG2	2:D:144:PHE:CE1	2.46	0.50
1:A:206:LEU:HD11	1:A:321:LEU:CD1	2.41	0.50
1:A:109:PHE:O	1:A:112:VAL:HG12	2.11	0.50
1:B:516:ASN:C	1:B:516:ASN:HD22	2.15	0.50
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.92	0.50
1:A:118:ILE:CG1	1:A:144:GLU:HB3	2.39	0.50
1:A:477:GLU:OE2	1:A:479:SER:N	2.40	0.50
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.95	0.50
1:B:221:THR:HG22	1:B:233:PRO:HA	1.92	0.50
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.29	0.50
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.94	0.50
2:C:365:GLU:CA	2:C:365:GLU:OE1	2.59	0.50
3:F:41:THR:O	3:F:44:ARG:CD	2.60	0.50
3:F:15:TRP:CD1	3:F:56:ILE:HD13	2.47	0.50
3:E:162:ARG:CZ	3:E:164:VAL:HG12	2.41	0.50
3:E:41:THR:O	3:E:44:ARG:CD	2.60	0.50
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.12	0.50
1:A:196:ASP:HB2	3:E:140:MET:SD	2.51	0.50
2:C:143:GLU:HG2	2:C:144:PHE:CE1	2.47	0.49
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.12	0.49
3:E:153:GLU:H	3:E:153:GLU:CD	2.15	0.49
1:B:352:ALA:CA	1:B:404:PRO:HB2	2.27	0.49
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.43	0.49
2:C:235:TRP:CD1	2:C:235:TRP:C	2.84	0.49
2:D:365:GLU:OE1	2:D:365:GLU:CA	2.60	0.49
1:A:313:TRP:O	1:A:318:ILE:HG13	2.13	0.49
3:F:162:ARG:CZ	3:F:164:VAL:HG12	2.43	0.49
2:C:4:LEU:HD21	2:D:21:LEU:HD22	1.93	0.49
3:E:4:LEU:HG	3:E:4:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.94	0.49
1:B:207:VAL:HG11	1:B:275:PHE:HA	1.94	0.49
2:D:54:VAL:O	2:D:55:TYR:HB2	2.12	0.49
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.48	0.49
2:C:143:GLU:HG2	2:C:144:PHE:CD1	2.48	0.49
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.48	0.49
1:B:526:PHE:CE2	3:F:165:HIS:HD2	2.30	0.49
1:B:284:PRO:HB3	1:B:342:ALA:HB1	1.95	0.49
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.93	0.49
1:B:302:VAL:HG12	1:B:376:TYR:OH	2.13	0.49
2:D:143:GLU:HG2	2:D:144:PHE:CD1	2.47	0.49
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.94	0.49
1:A:207:VAL:HG22	1:A:313:TRP:HZ2	1.78	0.49
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.48	0.49
1:A:302:VAL:HG12	1:A:376:TYR:OH	2.13	0.48
1:A:123:MET:CE	1:A:197:ALA:HA	2.42	0.48
2:D:33:ASN:C	2:D:33:ASN:ND2	2.66	0.48
1:B:268:ASN:HD21	1:B:327:GLU:H	1.59	0.48
1:B:313:TRP:O	1:B:318:ILE:HG13	2.13	0.48
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.60	0.48
1:B:438:VAL:HB	3:F:164:VAL:HG23	1.96	0.48
1:B:186:ARG:HA	2:D:73:THR:OG1	2.13	0.48
2:C:277:THR:HB	2:C:278:PRO:HD3	1.94	0.48
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.14	0.48
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.32	0.48
2:D:324:TRP:O	2:D:327:PRO:HD2	2.13	0.48
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.49	0.48
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.47	0.48
1:B:382:HIS:O	1:B:386:ILE:HG13	2.14	0.48
2:D:146:ASN:ND2	2:D:197:ARG:NH2	2.57	0.48
2:D:235:TRP:CD1	2:D:235:TRP:C	2.87	0.48
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.14	0.48
1:B:380:TYR:CE2	1:B:388:GLU:OE1	2.67	0.48
2:C:54:VAL:O	2:C:55:TYR:HB2	2.13	0.48
1:B:252:GLN:HE21	1:B:252:GLN:CA	2.24	0.48
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.14	0.47
1:A:252:GLN:HE21	1:A:252:GLN:CA	2.18	0.47
1:A:204:LEU:HG	1:A:205:GLN:HG3	1.96	0.47
1:B:413:HIS:HD2	1:B:428:SER:OG	1.98	0.47
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.96	0.47
1:B:406:MET:O	1:B:410:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.96	0.47
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.14	0.47
3:F:35:PHE:CE1	3:F:39:HIS:HD2	2.32	0.47
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.96	0.47
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.79	0.47
3:E:130:ASP:OD1	3:E:133:ARG:NH1	2.47	0.47
1:A:382:HIS:O	1:A:386:ILE:HG13	2.14	0.47
1:A:49:LYS:CE	3:E:144:ASN:HD22	2.28	0.47
1:A:413:HIS:HD2	1:A:428:SER:OG	1.97	0.47
1:A:406:MET:O	1:A:410:GLU:HG3	2.13	0.47
2:D:82:SER:O	2:D:168:ARG:NH2	2.48	0.47
3:E:159:ARG:HG3	3:E:161:VAL:HG12	1.97	0.47
1:A:198:VAL:O	1:A:202:LEU:HG	2.14	0.47
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.27	0.47
2:D:306:ASP:O	2:D:310:SER:HB2	2.14	0.47
1:A:373:GLU:OE2	1:A:377:PRO:HA	2.15	0.47
2:D:75:LYS:HB3	2:D:80:ARG:O	2.15	0.47
1:B:440:GLU:OE1	3:F:162:ARG:NH1	2.39	0.47
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.97	0.47
1:B:417:ILE:HG13	1:B:468:ASN:HB2	1.97	0.47
3:E:150:THR:CG2	3:E:154:GLU:HG2	2.45	0.47
1:A:439:HIS:CG	3:E:161:VAL:HG21	2.50	0.47
2:D:157:TYR:O	2:D:160:PHE:HB3	2.15	0.46
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.97	0.46
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.50	0.46
1:B:65:LYS:HD2	2:D:117:TRP:HB2	1.96	0.46
2:C:146:ASN:ND2	2:C:197:ARG:NH2	2.58	0.46
1:A:430:ALA:HA	6:A:5054:HOH:O	2.15	0.46
1:B:302:VAL:HG12	1:B:376:TYR:CZ	2.50	0.46
1:A:108:ASN:HD21	1:A:175:ARG:CD	2.28	0.46
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.79	0.46
1:A:195:GLY:HA2	6:C:5060:HOH:O	2.14	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.51	0.46
2:C:80:ARG:HB2	6:C:5062:HOH:O	2.15	0.46
1:B:313:TRP:CE3	1:B:318:ILE:HD11	2.51	0.46
1:B:75:ASP:OD2	1:B:146:ARG:NH1	2.48	0.46
1:A:268:ASN:HD21	1:A:327:GLU:H	1.62	0.46
2:C:318:ARG:NH2	6:C:5034:HOH:O	2.48	0.46
1:A:302:VAL:HG12	1:A:376:TYR:CZ	2.51	0.46
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.48	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CG	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.50	0.46
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.16	0.46
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.98	0.46
1:B:207:VAL:O	1:B:211:CYS:HB3	2.16	0.46
1:A:186:ARG:HD3	1:A:186:ARG:C	2.36	0.46
2:D:348:ASP:OD2	2:D:350:GLU:HB3	2.15	0.45
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.51	0.45
1:B:484:GLU:OE1	3:F:6:ILE:N	2.46	0.45
1:B:186:ARG:HD3	1:B:186:ARG:C	2.36	0.45
1:A:186:ARG:HD2	1:A:277:THR:HG23	1.99	0.45
1:B:393:ARG:HB3	1:B:402:PHE:CD2	2.51	0.45
2:C:80:ARG:HG3	3:E:132:GLU:OE1	2.16	0.45
1:B:202:LEU:HD22	1:B:206:LEU:HD23	1.99	0.45
1:B:109:PHE:O	1:B:112:VAL:HG12	2.16	0.45
1:A:516:ASN:C	1:A:516:ASN:HD22	2.18	0.45
3:F:66:VAL:HG12	3:F:70:ARG:HH21	1.80	0.45
1:B:43:ARG:HD2	1:B:43:ARG:C	2.37	0.45
1:B:108:ASN:HD21	1:B:175:ARG:CD	2.29	0.45
1:A:202:LEU:HD22	1:A:206:LEU:HD23	1.98	0.45
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.52	0.45
1:A:417:ILE:HG13	1:A:468:ASN:HB2	1.98	0.45
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.62	0.45
2:C:33:ASN:ND2	2:C:33:ASN:C	2.69	0.45
2:D:184:PHE:O	2:D:187:ILE:HG22	2.17	0.45
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.51	0.45
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.49	0.45
1:A:212:PHE:O	1:A:216:LEU:HB3	2.16	0.45
1:B:373:GLU:OE2	1:B:377:PRO:HA	2.17	0.45
1:A:113:GLY:HA2	1:A:188:PHE:HB3	1.99	0.45
2:D:143:GLU:O	2:D:147:ARG:HB3	2.17	0.45
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.14	0.45
3:F:159:ARG:HG3	3:F:161:VAL:HG12	1.98	0.44
3:E:115:ARG:NH1	3:E:132:GLU:OE1	2.48	0.44
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.98	0.44
1:A:283:THR:HB	1:A:284:PRO:HD3	1.99	0.44
1:B:283:THR:HB	1:B:284:PRO:HD3	1.98	0.44
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.99	0.44
3:F:33:LYS:O	3:F:37:MET:HG2	2.18	0.44
1:B:123:MET:HE1	1:B:197:ALA:HA	1.99	0.44
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.35	0.44
3:E:98:MET:HA	3:E:98:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:ASP:HA	2:C:307:PRO:HD3	1.86	0.44
1:B:44:THR:HG23	1:B:127:SER:HA	2.00	0.44
1:A:124:LEU:HB3	1:A:137:TYR:CE1	2.53	0.44
1:B:65:LYS:HB3	2:D:117:TRP:CD2	2.53	0.44
1:A:163:GLN:HG2	6:A:5012:HOH:O	2.16	0.44
2:C:256:PHE:HA	2:C:332:LEU:HD21	1.99	0.44
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.53	0.44
1:A:207:VAL:HG11	1:A:275:PHE:HA	1.99	0.44
1:A:313:TRP:CE3	1:A:318:ILE:HD11	2.52	0.44
1:B:207:VAL:HG22	1:B:313:TRP:HZ2	1.79	0.44
2:C:157:TYR:O	2:C:160:PHE:HB3	2.18	0.44
2:C:247:SER:O	2:C:251:VAL:HB	2.18	0.44
3:E:98:MET:HE2	3:E:110:ILE:HD12	1.99	0.43
1:A:291:GLU:OE1	1:A:343:HIS:HE1	2.01	0.43
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.53	0.43
1:B:212:PHE:O	1:B:216:LEU:HB3	2.18	0.43
2:C:144:PHE:CZ	2:C:342:LEU:HD23	2.54	0.43
2:C:143:GLU:O	2:C:147:ARG:HB3	2.17	0.43
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.52	0.43
1:B:348:LEU:HD23	1:B:387:TYR:CE2	2.53	0.43
1:B:403:ILE:HD12	1:B:515:LEU:CD1	2.49	0.43
1:A:348:LEU:HD23	1:A:387:TYR:CE2	2.54	0.43
1:A:451:GLN:HB2	3:E:152:LEU:HD11	2.00	0.43
3:E:161:VAL:HG23	3:E:162:ARG:N	2.33	0.43
2:C:184:PHE:O	2:C:187:ILE:HG22	2.18	0.43
3:F:161:VAL:HG23	3:F:162:ARG:N	2.34	0.43
3:F:6:ILE:HG22	3:F:7:HIS:ND1	2.33	0.43
1:A:403:ILE:HD12	1:A:515:LEU:CD1	2.48	0.43
3:F:150:THR:CG2	3:F:154:GLU:HG2	2.48	0.43
1:A:352:ALA:CA	1:A:404:PRO:HB2	2.25	0.43
2:D:80:ARG:HG3	3:F:132:GLU:OE1	2.19	0.43
3:F:22:LEU:HD13	3:F:28:ALA:HA	2.00	0.43
1:A:393:ARG:HB3	1:A:402:PHE:CD2	2.54	0.43
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.02	0.43
3:E:98:MET:HE3	3:E:98:MET:HB2	1.95	0.43
1:A:435:THR:HG22	1:A:449:SER:O	2.18	0.43
1:B:297:LYS:HG2	1:B:371:TRP:CE2	2.53	0.43
1:A:43:ARG:HD2	1:A:43:ARG:C	2.38	0.43
1:B:243:GLU:OE1	1:B:246:HIS:ND1	2.52	0.43
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.54	0.43
1:B:102:THR:OG1	1:B:293:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:68:LYS:HG3	3:E:72:PHE:CD2	2.54	0.42
2:D:78:GLY:O	3:F:115:ARG:HD3	2.18	0.42
2:C:82:SER:O	2:C:168:ARG:NH2	2.52	0.42
2:D:306:ASP:HA	2:D:307:PRO:HD3	1.88	0.42
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.54	0.42
2:D:141:ARG:HD2	2:D:204:VAL:HG21	2.02	0.42
2:D:277:THR:HB	2:D:278:PRO:HD3	2.00	0.42
3:E:15:TRP:CZ3	3:E:18:LYS:HD3	2.55	0.42
1:A:393:ARG:NH1	1:A:393:ARG:CG	2.80	0.42
2:D:310:SER:O	2:D:314:ARG:HG3	2.20	0.42
1:B:69:ARG:O	1:B:73:VAL:HG23	2.20	0.42
3:F:168:SER:HA	3:F:169:PRO:HD2	1.91	0.42
2:C:338:LEU:CB	6:C:5175:HOH:O	2.64	0.42
2:D:153:LEU:HD12	2:D:154:PHE:N	2.34	0.42
1:B:516:ASN:ND2	1:B:516:ASN:O	2.48	0.42
3:F:120:PRO:HD3	3:F:128:PHE:CG	2.55	0.42
2:C:201:ALA:HA	2:C:207:PHE:HB3	2.02	0.42
2:D:145:ILE:O	2:D:149:TRP:HB3	2.19	0.42
2:C:126:GLY:O	2:C:130:ASP:HB2	2.20	0.42
2:D:324:TRP:C	2:D:327:PRO:HD2	2.39	0.42
3:E:98:MET:HE3	3:E:110:ILE:HG21	2.02	0.42
1:B:137:TYR:O	1:B:141:VAL:HG23	2.19	0.42
1:B:393:ARG:HG3	1:B:393:ARG:HH11	1.84	0.42
1:B:435:THR:HG22	1:B:449:SER:O	2.20	0.42
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.54	0.42
3:F:11:THR:HG22	3:F:12:ARG:N	2.34	0.42
1:A:116:ASN:CG	1:A:189:SER:HA	2.41	0.42
1:A:186:ARG:CZ	1:A:277:THR:HG23	2.50	0.42
1:A:360:ARG:HD2	1:A:489:ARG:NH2	2.35	0.42
3:F:33:LYS:HD2	3:F:117:ALA:HA	2.02	0.42
2:D:297:ASP:O	2:D:301:ASN:HB3	2.20	0.42
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.53	0.42
1:B:365:ASP:C	1:B:365:ASP:OD2	2.58	0.42
1:A:84:ASP:HB3	1:B:81:SER:OG	2.20	0.42
3:F:15:TRP:CZ3	3:F:18:LYS:HD3	2.55	0.42
1:A:344:HIS:HE1	1:A:376:TYR:CE2	2.38	0.42
2:D:275:ASN:C	2:D:278:PRO:HD2	2.39	0.42
2:C:262:ARG:HA	2:C:266:GLN:HB3	2.02	0.42
1:B:44:THR:CG2	1:B:127:SER:HA	2.50	0.41
1:B:437:ARG:NH1	1:B:454:GLU:OE2	2.49	0.41
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.50	0.41
1:A:143:ASP:O	1:A:146:ARG:HB3	2.20	0.41
2:C:348:ASP:OD2	2:C:350:GLU:HB3	2.20	0.41
1:A:516:ASN:O	1:A:516:ASN:ND2	2.49	0.41
1:B:115:TYR:OH	2:D:173:ASP:HA	2.20	0.41
1:B:121:THR:HG21	1:B:140:GLN:CG	2.50	0.41
3:F:98:MET:HE2	3:F:98:MET:HA	2.01	0.41
1:B:125:TRP:C	1:B:125:TRP:CD1	2.94	0.41
2:C:300:TYR:CD1	2:C:370:ARG:HG3	2.56	0.41
1:B:192:PHE:O	1:B:200:CYS:HB3	2.21	0.41
1:A:297:LYS:HG2	1:A:371:TRP:CE2	2.56	0.41
1:A:445:MET:CE	1:A:526:PHE:HB2	2.51	0.41
1:B:18:ARG:O	2:D:129:ALA:HA	2.20	0.41
2:D:42:ARG:HB2	2:D:99:ARG:HG3	2.01	0.41
1:B:206:LEU:HA	1:B:206:LEU:HD12	1.90	0.41
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.89	0.41
1:B:31:TRP:CZ2	2:D:210:SER:HA	2.55	0.41
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.91	0.41
3:F:98:MET:CE	3:F:98:MET:HA	2.51	0.41
1:A:393:ARG:HG3	1:A:393:ARG:NH1	2.35	0.41
2:C:297:ASP:O	2:C:301:ASN:HB3	2.20	0.41
1:A:137:TYR:O	1:A:141:VAL:HG23	2.21	0.41
1:B:121:THR:HG21	1:B:140:GLN:HG2	2.03	0.41
2:C:266:GLN:NE2	2:C:281:ILE:HG22	2.36	0.41
1:B:18:ARG:HH11	1:B:18:ARG:HG3	1.85	0.41
2:D:201:ALA:HA	2:D:207:PHE:HB3	2.02	0.41
2:D:247:SER:O	2:D:251:VAL:HB	2.21	0.41
2:D:165:GLN:OE1	2:D:239:PHE:HA	2.21	0.41
3:E:36:ARG:NH2	3:E:119:LYS:HD2	2.36	0.41
1:B:360:ARG:HD2	1:B:489:ARG:NH2	2.35	0.41
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.56	0.41
1:A:209:GLU:HA	1:A:213:THR:HB	2.02	0.40
3:E:4:LEU:CG	3:E:4:LEU:O	2.69	0.40
3:E:22:LEU:HD13	3:E:28:ALA:HA	2.03	0.40
1:A:146:ARG:HB2	2:C:106:HIS:NE2	2.34	0.40
1:B:20:PRO:HG3	2:D:129:ALA:HB2	2.03	0.40
1:A:510:ASP:O	1:A:514:ARG:HG3	2.21	0.40
1:B:124:LEU:HB3	1:B:137:TYR:CE1	2.55	0.40
2:D:308:GLU:HG3	2:D:308:GLU:O	2.22	0.40
2:D:147:ARG:HD2	2:D:148:TYR:CE1	2.56	0.40
1:A:69:ARG:O	1:A:73:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.57	0.40
1:B:252:GLN:NE2	1:B:252:GLN:CA	2.70	0.40
3:F:74:GLU:O	3:F:78:ARG:HG3	2.22	0.40
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/527 (97%)	481 (94%)	25 (5%)	3 (1%)	30	43
1	B	508/527 (96%)	479 (94%)	27 (5%)	2 (0%)	39	56
2	C	386/389 (99%)	368 (95%)	16 (4%)	2 (0%)	34	48
2	D	384/389 (99%)	363 (94%)	18 (5%)	3 (1%)	24	35
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100	100
3	F	166/170 (98%)	162 (98%)	4 (2%)	0	100	100
All	All	2117/2172 (98%)	2014 (95%)	93 (4%)	10 (0%)	34	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	386	ALA
2	C	64	ALA
2	D	64	ALA
1	A	40	LYS
1	B	40	LYS
2	D	251	VAL
1	A	94	ARG
1	B	284	PRO

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Mol	Chain	Res	Type
2	C	251	VAL
1	A	284	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/442 (98%)	411 (95%)	21 (5%)	31	48
1	B	432/442 (98%)	411 (95%)	21 (5%)	31	48
2	C	322/323 (100%)	310 (96%)	12 (4%)	41	62
2	D	320/323 (99%)	308 (96%)	12 (4%)	40	60
3	E	144/147 (98%)	134 (93%)	10 (7%)	19	30
3	F	145/147 (99%)	136 (94%)	9 (6%)	23	35
All	All	1795/1824 (98%)	1710 (95%)	85 (5%)	32	50

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	30	ARG
1	A	41	ASN
1	A	43	ARG
1	A	90	ASN
1	A	125	TRP
1	A	144	GLU
1	A	186	ARG
1	A	213	THR
1	A	252	GLN
1	A	279	GLN
1	A	302	VAL
1	A	311	GLU
1	A	334	ASP
1	A	393	ARG
1	A	403	ILE

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Mol	Chain	Res	Type
1	A	435	THR
1	A	442	ASN
1	A	477	GLU
1	A	504	ASP
1	A	516	ASN
1	B	21	THR
1	B	30	ARG
1	B	41	ASN
1	B	43	ARG
1	B	90	ASN
1	B	125	TRP
1	B	186	ARG
1	B	213	THR
1	B	252	GLN
1	B	269	THR
1	B	279	GLN
1	B	302	VAL
1	B	311	GLU
1	B	334	ASP
1	B	393	ARG
1	B	403	ILE
1	B	435	THR
1	B	442	ASN
1	B	477	GLU
1	B	504	ASP
1	B	516	ASN
2	C	33	ASN
2	C	35	MET
2	C	80	ARG
2	C	153	LEU
2	C	168	ARG
2	C	173	ASP
2	C	179	LEU
2	C	266	GLN
2	C	308	GLU
2	C	311	ASP
2	C	365	GLU
2	C	378	ASP
2	D	33	ASN
2	D	35	MET
2	D	80	ARG
2	D	153	LEU

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Mol	Chain	Res	Type
2	D	168	ARG
2	D	173	ASP
2	D	179	LEU
2	D	266	GLN
2	D	308	GLU
2	D	311	ASP
2	D	365	GLU
2	D	378	ASP
3	E	7	HIS
3	E	11	THR
3	E	23	ASN
3	E	24	THR
3	E	44	ARG
3	E	46	SER
3	E	125	VAL
3	E	132	GLU
3	E	154	GLU
3	E	165	HIS
3	F	7	HIS
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	46	SER
3	F	125	VAL
3	F	132	GLU
3	F	154	GLU
3	F	165	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	116	ASN
1	A	133	GLN
1	A	155	ASN
1	A	168	HIS
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	B	41	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	116	ASN
1	B	155	ASN
1	B	168	HIS
1	B	227	ASN
1	B	249	ASN
1	B	252	GLN
1	B	268	ASN
1	B	273	ASN
1	B	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	382	HIS
1	B	412	ASN
1	B	413	HIS
1	B	439	HIS
1	B	442	ASN
1	B	527	ASN
2	C	98	HIS
2	C	132	GLN
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN

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Mol	Chain	Res	Type
2	C	301	ASN
2	D	33	ASN
2	D	98	HIS
2	D	146	ASN
2	D	155	ASN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
2	D	301	ASN
3	E	39	HIS
3	E	45	ASN
3	E	111	HIS
3	E	144	ASN
3	E	167	GLN
3	F	39	HIS
3	F	45	ASN
3	F	111	HIS
3	F	144	ASN
3	F	167	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	511/527 (96%)	0.28	33 (6%) 22 22	22, 42, 71, 88	0
1	B	510/527 (96%)	0.24	37 (7%) 18 18	25, 41, 74, 87	0
2	C	388/389 (99%)	-0.29	0 100 100	19, 28, 47, 65	0
2	D	386/389 (99%)	0.62	38 (9%) 10 9	27, 53, 84, 89	0
3	E	166/170 (97%)	-0.30	1 (0%) 90 90	18, 32, 51, 68	0
3	F	168/170 (98%)	1.05	31 (18%) 2 2	42, 62, 83, 92	0
All	All	2129/2172 (98%)	0.24	140 (6%) 22 22	18, 41, 77, 92	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	380	ILE	6.4
1	B	264	ALA	6.2
1	A	310	TYR	5.7
2	D	353	THR	5.1
2	D	205	PRO	4.9
1	A	316	ILE	4.9
1	B	259	ASN	4.7
1	A	326	VAL	4.7
2	D	82	SER	4.6
1	A	315	GLY	4.5
2	D	375	ALA	4.2
3	F	22	LEU	4.2
1	B	261	PRO	4.1
3	F	28	ALA	4.1
3	F	80	LYS	3.9
3	F	4(A)	LEU	3.9
1	B	31	TRP	3.9
1	B	53	ALA	3.9
1	B	265	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	328	SER	3.8
3	F	102	LYS	3.8
2	D	83	TRP	3.8
3	F	72	PHE	3.7
1	A	318	ILE	3.7
2	D	365	GLU	3.7
1	B	257	ILE	3.7
1	A	337	GLN	3.6
1	B	119	ALA	3.6
3	F	83	PHE	3.5
1	B	55	GLU	3.5
3	F	101	ALA	3.5
1	B	193	ILE	3.5
3	F	30	GLU	3.4
1	B	35	PHE	3.4
3	F	100	ALA	3.4
3	F	103	ASP	3.4
1	B	194	SER	3.3
3	F	27	LYS	3.3
1	B	187	VAL	3.3
1	A	338	ASP	3.3
1	A	263	SER	3.3
2	D	167	ALA	3.2
1	A	321	LEU	3.2
2	D	354	ALA	3.2
3	F	23	ASN	3.1
3	F	67	LEU	3.1
1	B	54	ASN	3.1
2	D	349	LYS	3.1
1	B	191	GLY	3.1
3	F	25	LEU	3.0
1	A	19	ALA	3.0
2	D	170	ALA	3.0
1	B	57	LYS	3.0
2	D	382	LYS	3.0
2	D	356	LEU	3.0
2	D	166	GLY	3.0
1	B	320	ARG	2.9
1	A	262	ALA	2.9
2	D	381	VAL	2.9
2	D	44	LYS	2.9
2	D	2	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	352	ILE	2.9
1	A	189	SER	2.9
2	D	206	GLY	2.9
1	A	434	SER	2.8
1	B	325	GLY	2.8
2	D	357	TYR	2.8
2	D	377	ARG	2.8
1	B	493	LYS	2.8
1	A	314	GLY	2.8
3	F	74	GLU	2.8
1	B	192	PHE	2.7
1	A	113	GLY	2.7
1	A	17	ASN	2.7
2	D	45	ARG	2.7
1	B	59	GLN	2.7
2	D	378	ASP	2.7
1	A	192	PHE	2.7
1	B	141	VAL	2.6
3	F	35	PHE	2.6
2	D	244	SER	2.6
3	F	142	LEU	2.6
1	B	23	VAL	2.6
1	B	260	ASP	2.6
2	D	270	PRO	2.6
1	A	55	GLU	2.5
3	F	26	GLU	2.5
3	F	97	LYS	2.5
1	A	204	LEU	2.5
2	D	72	TRP	2.5
3	F	138	ARG	2.5
1	B	189	SER	2.5
1	B	263	SER	2.5
1	A	141	VAL	2.5
3	E	102	LYS	2.5
1	B	188	PHE	2.4
1	B	40	LYS	2.4
3	F	84	GLY	2.4
1	A	257	ILE	2.4
3	F	87	ALA	2.4
1	B	117	ALA	2.4
2	D	385	LEU	2.3
1	A	340	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	327	GLU	2.3
3	F	145	LEU	2.3
1	A	118	ILE	2.3
1	B	115	TYR	2.3
1	B	255	VAL	2.3
2	D	84	GLY	2.3
3	F	60	LEU	2.3
1	A	54	ASN	2.2
2	D	73	THR	2.2
2	D	81	PRO	2.2
2	D	141	ARG	2.2
1	B	248	ALA	2.2
3	F	82	ALA	2.2
3	F	20	ALA	2.2
3	F	21	GLN	2.2
1	A	213	THR	2.2
2	D	179	LEU	2.1
2	D	87	THR	2.1
1	A	106	VAL	2.1
1	A	392	ALA	2.1
1	A	433	ALA	2.1
1	B	46	TYR	2.1
3	F	170	HIS	2.1
3	F	90	VAL	2.1
2	D	224	TYR	2.1
1	A	112	VAL	2.1
1	B	319	GLY	2.1
1	B	116	ASN	2.1
2	D	203	ILE	2.1
1	B	190	ASP	2.1
3	F	118	TYR	2.1
2	D	207	PHE	2.1
1	A	311	GLU	2.0
1	A	265	LYS	2.0
1	A	320	ARG	2.0
2	D	172	SER	2.0
2	D	383	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FE2	B	5003	1/1	0.87	0.18	0.88	58,58,58,58	0
5	CA	A	5005	1/1	0.98	0.10	-1.89	53,53,53,53	0
4	FE2	A	5001	1/1	0.96	0.12	-2.48	56,56,56,56	0
5	CA	C	5006	1/1	0.93	0.08	-	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.