



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:00 AM UTC

PDB ID : 5TMF / pdb_00005tmf
Title : Re-refinement of thermus thermophilus RNA polymerase
Authors : Wang, J.
Deposited on : 2016-10-12
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

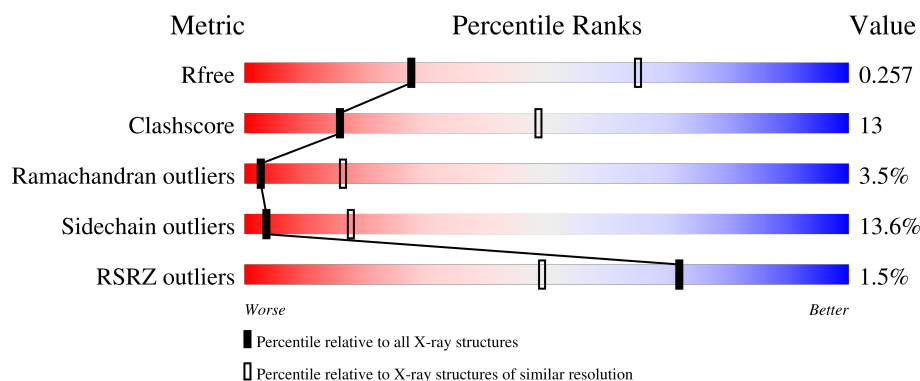
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	315	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	

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Mol	Chain	Length	Quality of chain
5	F	423	2% 57% 21% 17%

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
7	NE6	C	1201	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28078 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1816	1159	315	339	3			
1	B	238	Total	C	N	O	S	0	0	0
			1863	1188	322	350	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1504	Total	C	N	O	S	0	0	0
			11864	7518	2091	2219	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLU	VAL	conflict	UNP Q72ID6
E	92	ILE	LEU	conflict	UNP Q72ID6
E	95	GLY	VAL	conflict	UNP Q72ID6

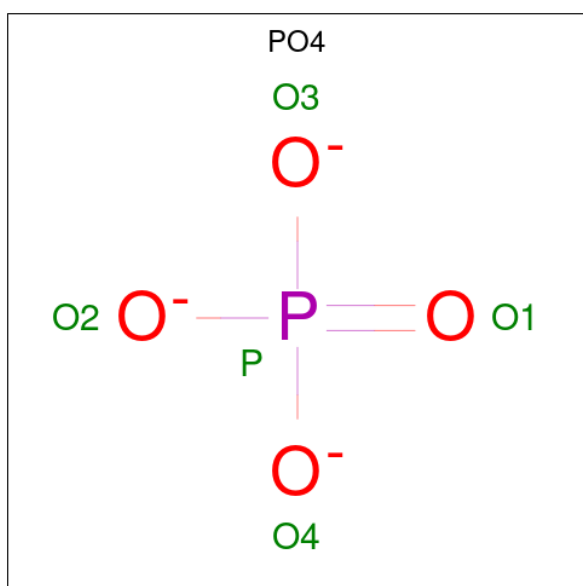
- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	351	Total	C	N	O	S	0	0	0
			2844	1794	515	531	4			

There is a discrepancy between the modelled and reference sequences:

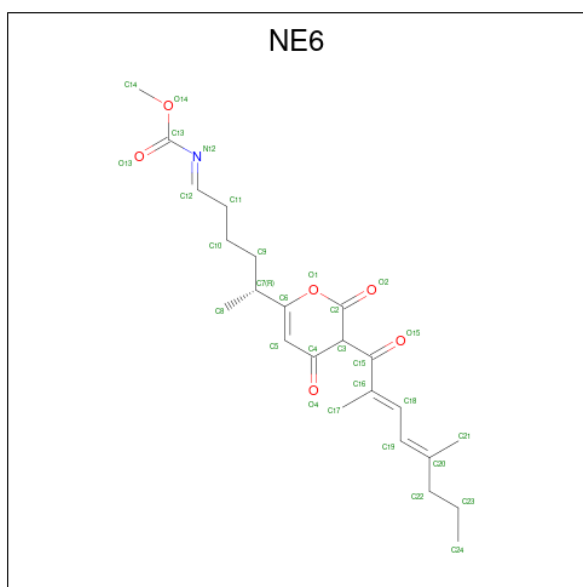
Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is methyl [(1E,5R)-5-{(3S)-3-[(2E,4E)-2,5-dimethylocta-2,4-dienoyl]-2,4-dioxo-3,4-dihydro-2H-pyran-6-yl}hexylidene]carbamate (CCD ID: NE6) (formula: C₂₃H₃₁NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			30	23	1	6		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Mg	0	0
			2	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	O	0	0
			2	2		
10	B	3	Total	O	0	0
			3	3		
10	C	23	Total	O	0	0
			23	23		
10	D	20	Total	O	0	0
			20	20		

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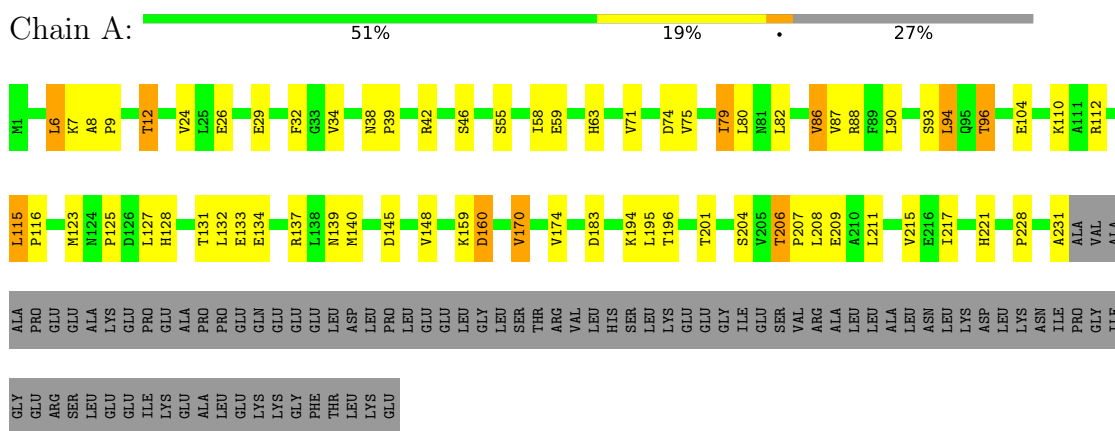
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	1	Total	O	0	0
			1	1		

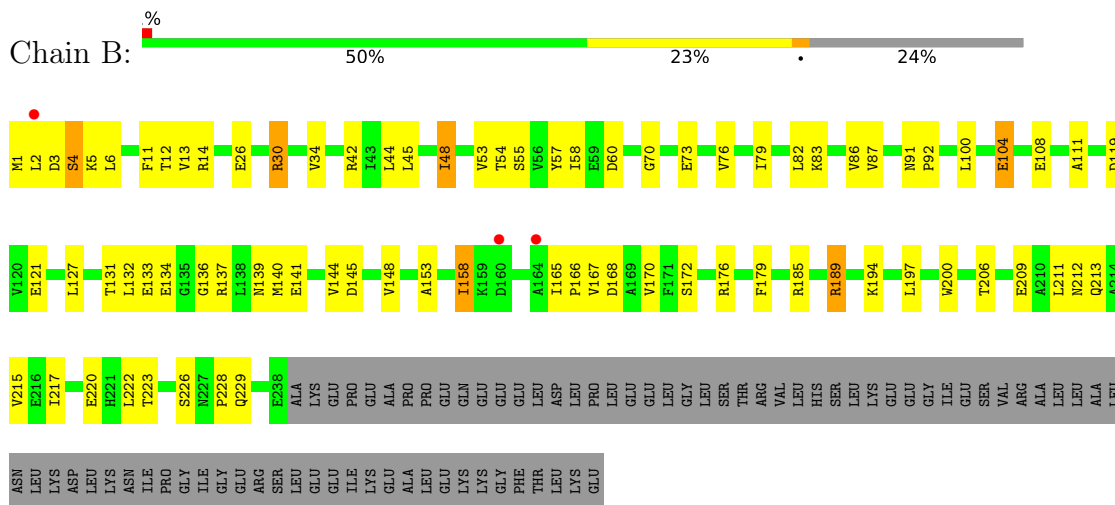
3 Residue-property plots

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.

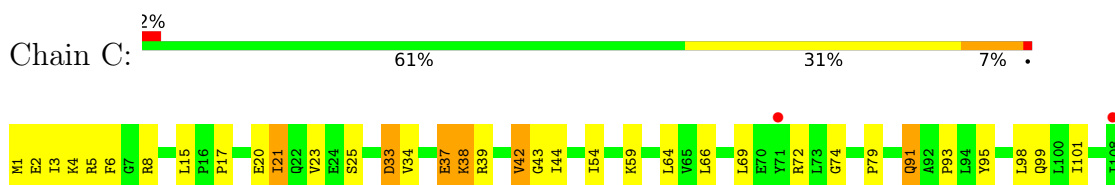
- Molecule 1: DNA-directed RNA polymerase subunit alpha



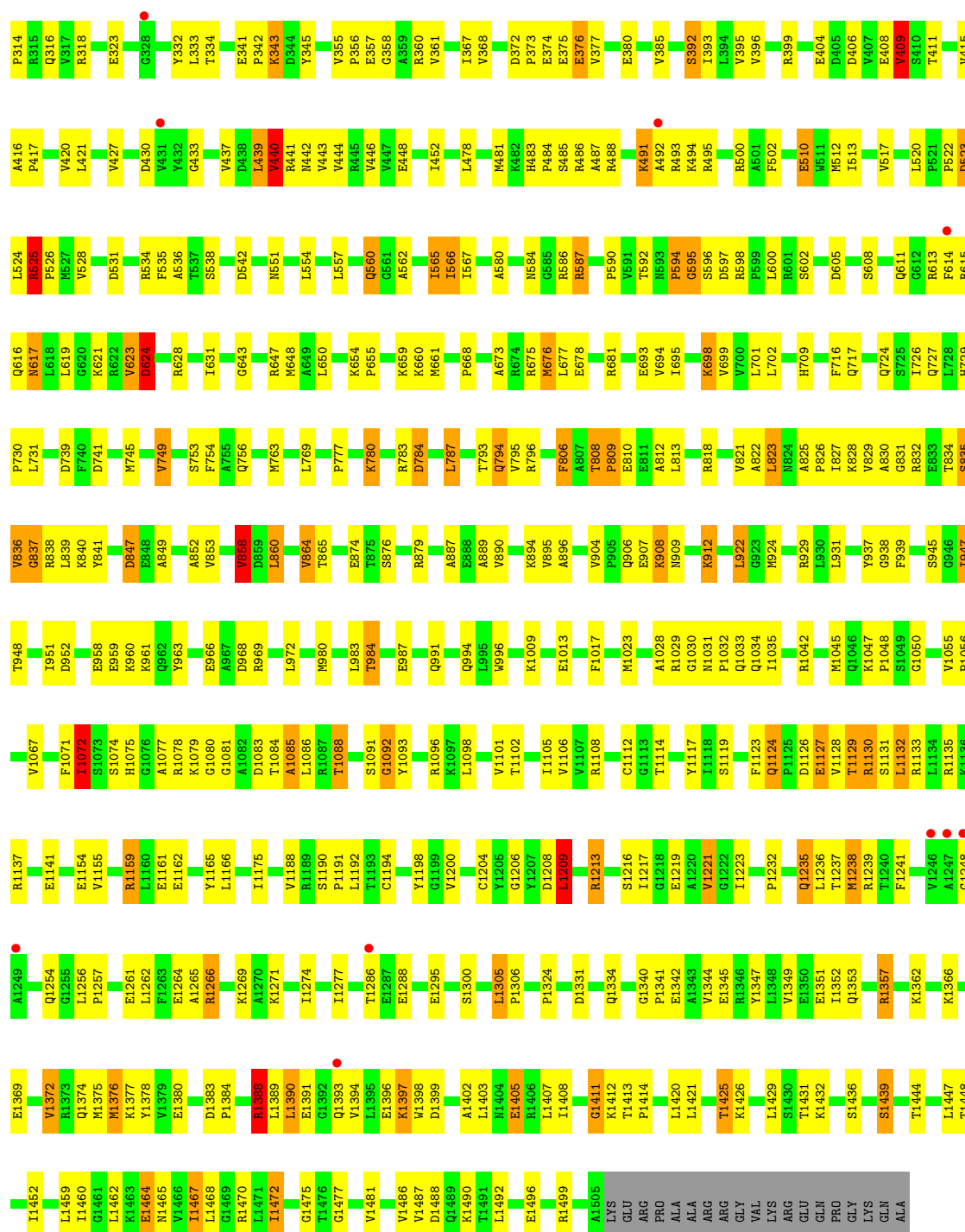
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta





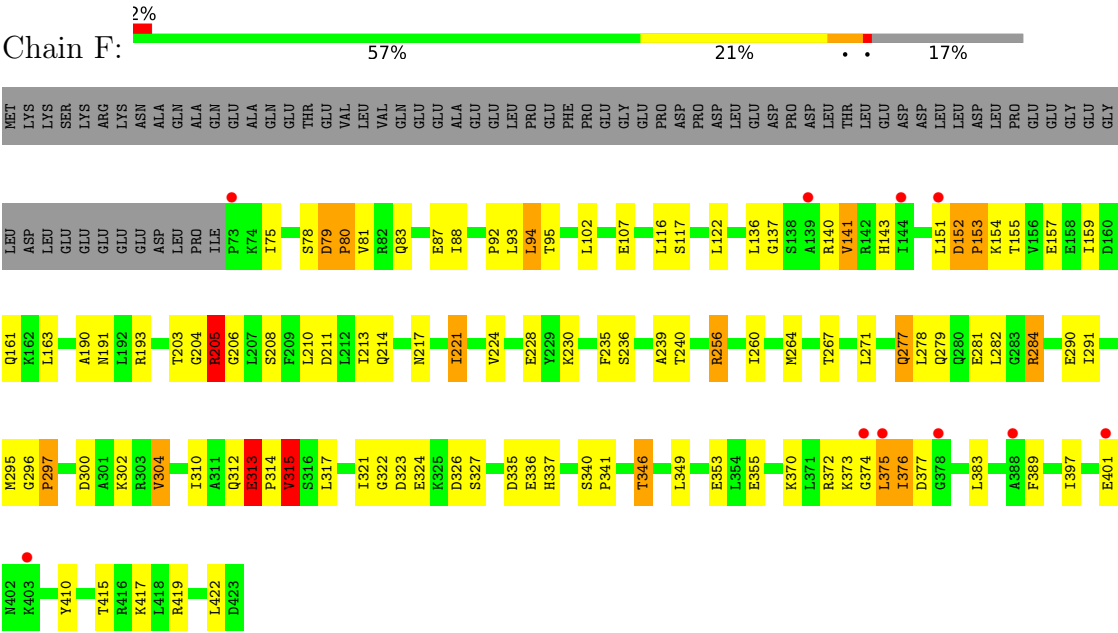


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 67% 21% 8%



- Molecule 5: RNA polymerase sigma factor SigA



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	235.09Å 235.09Å 250.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.80 – 3.00 46.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.80-3.00) 96.1 (46.80-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.234 0.203 , 0.257	Depositor DCC
R_{free} test set	1177 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.956 for H, K, L 0.044 for -H-K, K, -L	Depositor
Outliers	0 of 150767 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28078	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: MG, NE6, PO4, ZN

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	0.55	0/1848	0.91	0/2512
1	B	0.56	0/1896	0.87	0/2579
2	C	0.61	0/8997	0.97	26/12164 (0.2%)
3	D	0.62	0/12073	0.95	22/16324 (0.1%)
4	E	0.53	0/783	0.96	5/1054 (0.5%)
5	F	0.54	0/2890	0.97	8/3888 (0.2%)
All	All	0.60	0/28487	0.95	61/38521 (0.2%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	749	VAL	N-CA-C	7.50	115.58	108.15
3	D	624	ASP	N-CA-C	7.32	120.69	111.69
2	C	684	PHE	N-CA-C	7.10	118.67	111.07
2	C	903	SER	CA-C-N	6.97	127.00	119.89
2	C	903	SER	C-N-CA	6.97	127.00	119.89
3	D	415	VAL	N-CA-C	6.97	117.32	108.82
4	E	57	ASP	CA-C-N	6.93	126.56	119.56
4	E	57	ASP	C-N-CA	6.93	126.56	119.56
5	F	312	GLN	N-CA-C	6.80	119.72	110.55
5	F	376	ILE	N-CA-C	6.64	118.44	106.61
3	D	1340	GLY	CA-C-N	6.62	128.12	119.84
3	D	1340	GLY	C-N-CA	6.62	128.12	119.84
2	C	441	VAL	CB-CA-C	6.43	116.78	111.05
2	C	494	TYR	N-CA-C	6.30	119.81	109.85
5	F	315	VAL	N-CA-C	6.18	117.55	109.58
3	D	355	VAL	CA-C-N	6.17	126.14	119.78
3	D	355	VAL	C-N-CA	6.17	126.14	119.78
3	D	172	PRO	CA-C-N	6.08	127.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	172	PRO	C-N-CA	6.08	127.44	119.84
2	C	163	ILE	N-CA-C	6.07	114.65	107.73
5	F	313	GLU	CA-C-N	5.94	141.25	127.00
5	F	313	GLU	C-N-CA	5.94	141.25	127.00
3	D	909	ASN	N-CA-C	5.77	117.37	111.14
2	C	985	GLY	CA-C-N	5.67	125.58	119.85
2	C	985	GLY	C-N-CA	5.67	125.58	119.85
3	D	623	VAL	N-CA-C	5.66	116.83	108.45
2	C	188	LYS	N-CA-C	-5.61	106.43	113.28
2	C	118	ILE	CA-C-N	5.59	125.52	119.76
2	C	118	ILE	C-N-CA	5.59	125.52	119.76
2	C	310	LEU	N-CA-C	-5.59	105.19	111.28
3	D	494	LYS	N-CA-C	-5.54	105.78	112.54
2	C	163	ILE	CA-C-N	5.49	126.70	119.84
2	C	163	ILE	C-N-CA	5.49	126.70	119.84
2	C	858	MET	CA-C-N	5.46	125.78	119.93
2	C	858	MET	C-N-CA	5.46	125.78	119.93
3	D	525	ARG	N-CA-C	-5.36	97.97	109.81
2	C	418	LEU	N-CA-C	5.30	117.74	109.52
2	C	908	GLY	N-CA-C	5.30	125.74	113.18
3	D	1388	ARG	N-CA-C	5.28	117.68	109.60
4	E	13	VAL	N-CA-C	5.27	116.44	108.96
3	D	1397	LYS	N-CA-C	-5.21	103.79	111.81
3	D	276	ASP	N-CA-C	5.20	116.63	110.97
2	C	583	LEU	N-CA-C	5.16	118.36	111.75
5	F	79	ASP	CA-C-N	5.16	126.29	119.84
5	F	79	ASP	C-N-CA	5.16	126.29	119.84
3	D	1092	GLY	CA-C-N	5.14	127.16	120.28
3	D	1092	GLY	C-N-CA	5.14	127.16	120.28
4	E	45	ARG	CA-C-N	5.13	125.12	119.89
4	E	45	ARG	C-N-CA	5.13	125.12	119.89
2	C	699	PHE	CA-C-N	-5.12	114.60	123.25
2	C	699	PHE	C-N-CA	-5.12	114.60	123.25
2	C	419	THR	N-CA-C	5.11	121.68	110.80
3	D	341	GLU	CA-C-N	5.11	125.04	119.78
3	D	341	GLU	C-N-CA	5.11	125.04	119.78
5	F	313	GLU	C-N-CD	-5.11	109.37	120.60
3	D	749	VAL	CB-CA-C	-5.10	106.24	111.08
2	C	1081	VAL	CA-C-N	5.06	125.50	120.14
2	C	1081	VAL	C-N-CA	5.06	125.50	120.14
3	D	837	GLY	N-CA-C	-5.06	98.63	113.30
2	C	718	GLY	CA-C-N	5.05	124.98	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	718	GLY	C-N-CA	5.05	124.98	119.78

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	1816	0	1871	44	0
1	B	1863	0	1914	42	0
2	C	8829	0	8933	287	0
3	D	11864	0	12094	354	0
4	E	769	0	775	18	0
5	F	2844	0	2926	57	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
7	C	30	0	30	5	0
8	D	2	0	0	0	0
9	D	2	0	0	0	0
10	A	2	0	0	0	0
10	B	3	0	0	0	0
10	C	23	0	0	3	0
10	D	20	0	0	4	0
10	F	1	0	0	1	0
All	All	28078	0	28543	750	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (750) 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)
3:D:1265:ALA:HA	3:D:1266:ARG:CB	1.72	1.19
3:D:613:ARG:HB3	3:D:614:PHE:HA	1.21	1.18
2:C:23:VAL:HA	2:C:121:MET:HE1	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:PRO:HA	2:C:117:HIS:HB2	1.31	1.06
2:C:93:PRO:HA	2:C:117:HIS:CB	1.85	1.06
3:D:1085:ALA:HA	3:D:1088:THR:HG22	1.39	1.04
3:D:586:ARG:O	3:D:587:ARG:HG3	1.59	1.02
2:C:21:ILE:HD12	2:C:21:ILE:H	1.25	1.02
3:D:1265:ALA:HA	3:D:1266:ARG:HB3	1.00	0.99
3:D:520:LEU:O	3:D:525:ARG:NH1	2.00	0.94
3:D:1213:ARG:HG2	3:D:1213:ARG:HH11	1.30	0.93
3:D:1265:ALA:CA	3:D:1266:ARG:HB3	1.96	0.92
3:D:64:LYS:HD3	5:F:376:ILE:HG21	1.52	0.92
2:C:737:LEU:O	2:C:739:GLU:N	2.04	0.90
3:D:631:ILE:HG21	3:D:745:MET:HG3	1.53	0.90
3:D:1126:ASP:HA	3:D:1130:ARG:H	1.37	0.88
2:C:776:SER:HA	2:C:780:GLU:HB2	1.55	0.87
2:C:881:ASN:H	2:C:881:ASN:HD22	1.21	0.86
2:C:1084:SER:HB2	7:C:1201:NE6:O15	1.74	0.86
5:F:256:ARG:NH2	5:F:310:ILE:O	2.09	0.85
3:D:613:ARG:HB3	3:D:614:PHE:CA	2.06	0.84
3:D:836:VAL:H	3:D:837:GLY:HA3	1.41	0.84
3:D:358:GLY:HA2	3:D:385:VAL:O	1.77	0.83
1:B:2:LEU:N	1:B:3:ASP:HA	1.93	0.83
3:D:1124:GLN:HE21	3:D:1124:GLN:HA	1.41	0.83
3:D:206:ARG:HB2	3:D:392:SER:O	1.77	0.83
3:D:584:ASN:OD1	3:D:590:PRO:HD2	1.78	0.83
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.61	0.82
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.60	0.82
2:C:95:TYR:CE2	2:C:114:PHE:HB3	2.14	0.81
3:D:783:ARG:HH11	3:D:783:ARG:HG2	1.44	0.81
2:C:243:ARG:HB3	2:C:244:PRO:HA	1.63	0.81
2:C:550:LEU:HD22	2:C:905:ILE:HD11	1.62	0.81
2:C:396:ASP:H	2:C:406:HIS:HD2	1.29	0.81
2:C:219:GLN:HA	2:C:222:MET:HG2	1.63	0.81
3:D:64:LYS:HB2	5:F:376:ILE:HG13	1.61	0.80
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.63	0.80
3:D:95:LEU:HD21	3:D:517:VAL:HG23	1.64	0.80
2:C:1058:ASP:OD2	2:C:1084:SER:HB3	1.82	0.80
3:D:374:GLU:O	3:D:376:GLU:HG3	1.82	0.80
1:B:153:ALA:HB1	1:B:166:PRO:HB2	1.62	0.80
3:D:192:ALA:HB1	3:D:193:PRO:CD	2.13	0.79
3:D:702:LEU:HB3	3:D:745:MET:HE3	1.65	0.79
2:C:486:MET:HE3	2:C:491:GLU:HA	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1388:ARG:HH21	3:D:1390:LEU:HB3	1.47	0.78
3:D:1397:LYS:C	3:D:1398:TRP:HE3	1.91	0.77
3:D:822:ALA:O	3:D:823:LEU:HB3	1.83	0.77
3:D:1208:ASP:O	3:D:1209:LEU:HB2	1.83	0.77
2:C:266:ARG:HH11	2:C:266:ARG:HB2	1.49	0.77
3:D:613:ARG:CB	3:D:614:PHE:HA	2.11	0.77
3:D:1397:LYS:C	3:D:1398:TRP:CE3	2.63	0.77
5:F:79:ASP:N	5:F:80:PRO:HD2	1.99	0.76
5:F:92:PRO:HG2	5:F:193:ARG:HH11	1.49	0.76
2:C:720:GLU:HB3	2:C:760:SER:HA	1.67	0.76
5:F:205:ARG:HG2	5:F:205:ARG:HH11	1.50	0.76
7:C:1201:NE6:C21	3:D:1467:ILE:HD11	2.16	0.75
3:D:1394:VAL:HG21	10:D:1713:HOH:O	1.86	0.75
2:C:258:TYR:HA	2:C:264:PRO:HB3	1.69	0.75
1:A:104:GLU:HG3	1:A:137:ARG:HG2	1.68	0.74
3:D:1137:ARG:HG2	3:D:1141:GLU:OE2	1.87	0.74
3:D:1394:VAL:CG2	10:D:1713:HOH:O	2.36	0.73
3:D:65:ARG:HG2	5:F:375:LEU:HD23	1.69	0.73
2:C:553:ASP:OD1	2:C:843:HIS:HD2	1.71	0.73
5:F:151:LEU:C	5:F:153:PRO:HD3	2.14	0.73
2:C:93:PRO:HA	2:C:117:HIS:HB3	1.69	0.72
2:C:164:PRO:HA	2:C:266:ARG:HB3	1.71	0.72
3:D:1091:SER:C	3:D:1093:TYR:H	1.95	0.72
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.71	0.72
3:D:491:LYS:O	3:D:493:ARG:N	2.22	0.72
1:A:115:LEU:HD13	1:A:116:PRO:HD2	1.72	0.72
3:D:1265:ALA:CA	3:D:1266:ARG:CB	2.58	0.71
2:C:676:ILE:HG13	2:C:676:ILE:O	1.91	0.71
1:B:70:GLY:HA3	1:B:136:GLY:HA3	1.73	0.71
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.71	0.71
3:D:729:HIS:HD2	3:D:731:LEU:H	1.37	0.70
7:C:1201:NE6:H21A	3:D:1467:ILE:HD11	1.74	0.70
2:C:738:ASP:O	2:C:740:GLU:N	2.24	0.70
3:D:984:THR:HG22	3:D:987:GLU:H	1.54	0.70
3:D:1397:LYS:HB2	3:D:1398:TRP:CZ3	2.26	0.70
3:D:1031:ASN:H	3:D:1034:GLN:HE21	1.39	0.70
2:C:93:PRO:CA	2:C:117:HIS:HB2	2.15	0.70
3:D:45:PHE:O	3:D:86:ARG:NH2	2.25	0.70
2:C:881:ASN:H	2:C:881:ASN:ND2	1.88	0.69
3:D:65:ARG:O	3:D:66:GLN:HB3	1.93	0.69
3:D:1398:TRP:HD1	3:D:1402:ALA:HB2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:ARG:HD3	5:F:375:LEU:HA	1.74	0.69
2:C:266:ARG:HB2	2:C:266:ARG:NH1	2.07	0.69
2:C:689:VAL:HG22	2:C:870:ILE:HB	1.73	0.69
2:C:751:PRO:HG3	2:C:796:GLU:HA	1.73	0.69
7:C:1201:NE6:C20	3:D:1467:ILE:HD11	2.23	0.69
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.75	0.69
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.32	0.68
2:C:317:VAL:N	2:C:318:PRO:HD3	2.08	0.68
2:C:1105:LYS:O	2:C:1106:ASP:HB2	1.94	0.68
3:D:613:ARG:HA	3:D:615:ARG:N	2.08	0.68
3:D:416:ALA:HB1	3:D:417:PRO:HA	1.76	0.68
3:D:613:ARG:HA	3:D:615:ARG:H	1.59	0.67
5:F:291:ILE:HG23	5:F:304:VAL:HG11	1.76	0.67
3:D:137:PRO:O	3:D:138:LYS:HB2	1.95	0.67
2:C:559:LEU:HD12	2:C:559:LEU:C	2.20	0.67
3:D:836:VAL:N	3:D:837:GLY:HA3	2.09	0.67
2:C:21:ILE:HD12	2:C:21:ILE:N	2.06	0.67
2:C:187:ASN:HD22	2:C:189:ARG:HG3	1.60	0.66
2:C:1015:LEU:HA	5:F:335:ASP:HB2	1.77	0.66
2:C:380:ALA:HA	2:C:383:ARG:HG2	1.78	0.66
2:C:626:ARG:HG3	2:C:629:TYR:CD1	2.30	0.66
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.77	0.66
3:D:535:PHE:O	5:F:314:PRO:HB2	1.94	0.66
3:D:1232:PRO:O	3:D:1235:GLN:HG3	1.94	0.66
3:D:1465:ASN:HD22	3:D:1470:ARG:HD3	1.60	0.66
1:A:231:ALA:HB3	1:B:14:ARG:HB3	1.75	0.66
2:C:198:ARG:HD3	2:C:228:ALA:HA	1.76	0.66
3:D:48:ARG:HB3	3:D:48:ARG:CZ	2.26	0.66
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.31	0.66
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.78	0.65
3:D:631:ILE:HG21	3:D:745:MET:CG	2.25	0.65
1:A:133:GLU:OE2	2:C:610:ARG:NH2	2.30	0.65
2:C:305:PRO:HA	2:C:308:ARG:HG2	1.78	0.65
3:D:699:VAL:HG12	3:D:717:GLN:HB3	1.76	0.65
5:F:152:ASP:N	5:F:153:PRO:HD3	2.12	0.65
2:C:710:ILE:HD13	2:C:790:LEU:HB2	1.79	0.64
3:D:178:LEU:O	3:D:181:ASP:N	2.29	0.64
2:C:396:ASP:H	2:C:406:HIS:CD2	2.12	0.64
3:D:1398:TRP:CD1	3:D:1402:ALA:HB2	2.31	0.64
2:C:23:VAL:HA	2:C:121:MET:CE	2.22	0.64
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:557:LEU:HD22	3:D:566:ILE:HD11	1.80	0.64
2:C:876:VAL:H	2:C:877:PRO:HD2	1.62	0.64
2:C:776:SER:CA	2:C:780:GLU:HB2	2.28	0.64
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.80	0.64
2:C:581:THR:N	2:C:584:GLU:OE2	2.29	0.64
3:D:1353:GLN:O	3:D:1357:ARG:HG2	1.98	0.64
2:C:738:ASP:HB2	2:C:744:ARG:HH21	1.63	0.64
2:C:266:ARG:NH2	2:C:271:GLU:O	2.30	0.63
3:D:1091:SER:C	3:D:1093:TYR:N	2.56	0.63
3:D:1213:ARG:HH11	3:D:1213:ARG:CG	2.07	0.63
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.80	0.63
1:A:71:VAL:HG22	1:A:132:LEU:CD2	2.29	0.63
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.32	0.63
5:F:117:SER:HB2	5:F:122:LEU:O	1.98	0.63
1:A:206:THR:HB	1:A:209:GLU:HG3	1.81	0.63
1:A:42:ARG:NH2	2:C:857:ASP:OD1	2.31	0.62
3:D:44:LEU:O	3:D:525:ARG:NH2	2.33	0.62
3:D:141:ILE:HG22	3:D:142:LEU:H	1.63	0.62
3:D:1105:ILE:HD11	3:D:1374:GLN:CD	2.25	0.61
2:C:762:LYS:HG3	2:C:786:LYS:HD2	1.81	0.61
3:D:376:GLU:OE2	3:D:377:VAL:N	2.28	0.61
5:F:94:LEU:HG	5:F:190:ALA:HB1	1.82	0.61
1:A:96:THR:HB	1:A:145:ASP:OD2	1.99	0.61
2:C:274:ARG:HA	2:C:277:ALA:HB3	1.81	0.61
2:C:626:ARG:HG3	2:C:629:TYR:HD1	1.65	0.61
2:C:181:VAL:HG12	2:C:182:VAL:H	1.65	0.61
3:D:675:ARG:O	3:D:678:GLU:HG2	2.00	0.61
1:A:128:HIS:HE1	1:A:131:THR:HG23	1.66	0.61
3:D:1217:ILE:HD12	3:D:1217:ILE:H	1.66	0.61
3:D:1377:LYS:HD2	3:D:1378:TYR:CZ	2.36	0.60
2:C:122:THR:HG22	2:C:123:GLU:H	1.65	0.60
2:C:1115:LEU:HB3	3:D:85:VAL:HG23	1.82	0.60
1:A:58:ILE:HG12	1:A:140:MET:HE2	1.83	0.60
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.01	0.60
2:C:469:THR:HG23	2:C:538:GLN:HE21	1.66	0.60
2:C:426:ASP:O	2:C:428:ARG:N	2.35	0.60
2:C:1018:GLN:HG3	2:C:1060:ILE:HD11	1.84	0.59
3:D:592:THR:HG23	3:D:600:LEU:HD21	1.83	0.59
4:E:83:ASP:C	4:E:85:LEU:H	2.10	0.59
1:A:86:VAL:HG22	1:A:123:MET:HB2	1.83	0.59
3:D:211:VAL:HG23	3:D:345:TYR:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:525:ARG:N	3:D:526:PRO:HD3	2.17	0.59
2:C:368:THR:H	2:C:369:PRO:HD3	1.67	0.59
3:D:1397:LYS:HE3	3:D:1432:LYS:HE3	1.85	0.59
1:B:111:ALA:HB2	1:B:127:LEU:HB3	1.83	0.59
5:F:321:ILE:O	5:F:323:ASP:N	2.35	0.59
3:D:1393:GLN:OE1	3:D:1398:TRP:HH2	1.85	0.59
2:C:626:ARG:CG	2:C:629:TYR:HD1	2.15	0.59
3:D:586:ARG:O	3:D:587:ARG:CG	2.44	0.59
1:B:30:ARG:NH1	2:C:854:PRO:HB3	2.18	0.59
3:D:849:ALA:O	3:D:852:ALA:HB3	2.02	0.59
2:C:243:ARG:HA	2:C:245:GLY:H	1.66	0.59
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.84	0.58
5:F:155:THR:O	5:F:159:ILE:HG12	2.02	0.58
1:B:133:GLU:HG2	1:B:134:GLU:H	1.68	0.58
2:C:926:PHE:CE2	2:C:960:GLU:HG3	2.38	0.58
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.38	0.58
3:D:795:VAL:HG12	3:D:876:SER:HB3	1.84	0.58
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.85	0.58
3:D:1261:GLU:O	3:D:1265:ALA:HB2	2.03	0.58
2:C:685:GLU:O	2:C:686:ASP:HB2	2.03	0.58
3:D:1262:LEU:HD13	3:D:1352:ILE:HG13	1.86	0.58
3:D:1256:LEU:N	3:D:1257:PRO:HD2	2.19	0.58
2:C:186:VAL:HG23	2:C:187:ASN:H	1.69	0.57
3:D:780:LYS:HD2	3:D:912:LYS:HG3	1.86	0.57
2:C:325:ILE:HD12	2:C:325:ILE:H	1.68	0.57
3:D:836:VAL:H	3:D:837:GLY:CA	2.15	0.57
3:D:1042:ARG:HB3	3:D:1045:MET:HE3	1.86	0.57
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.87	0.57
7:C:1201:NE6:H21A	3:D:1467:ILE:CD1	2.34	0.57
1:B:57:TYR:O	1:B:140:MET:HB2	2.05	0.57
2:C:550:LEU:CD2	2:C:905:ILE:HD11	2.34	0.57
2:C:878:SER:HB3	3:D:1029:ARG:HD2	1.86	0.57
3:D:1465:ASN:HD21	3:D:1470:ARG:HH11	1.50	0.57
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.40	0.56
3:D:112:ILE:HG22	3:D:512:MET:CE	2.35	0.56
3:D:1397:LYS:O	3:D:1398:TRP:CE3	2.57	0.56
4:E:26:ARG:O	4:E:30:LEU:HB2	2.05	0.56
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.88	0.56
2:C:1078:GLU:HG2	2:C:1079:PRO:HD2	1.87	0.56
3:D:191:LEU:HD13	3:D:393:ILE:HD12	1.87	0.56
3:D:484:PRO:HG2	3:D:488:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:560:GLN:HG2	5:F:221:ILE:HG21	1.87	0.56
3:D:834:THR:HG22	3:D:835:SER:N	2.20	0.56
1:A:75:VAL:O	1:A:79:ILE:HD12	2.06	0.56
2:C:575:GLN:HE21	2:C:670:GLN:HG3	1.69	0.56
2:C:895:TYR:HB2	2:C:991:GLN:HG3	1.87	0.56
3:D:853:VAL:HG12	3:D:858:VAL:HG12	1.86	0.56
3:D:433:GLY:HA3	3:D:446:VAL:HG13	1.87	0.56
1:A:128:HIS:CE1	1:A:131:THR:HG23	2.40	0.56
3:D:367:ILE:HB	3:D:377:VAL:HG12	1.87	0.56
3:D:673:ALA:O	3:D:676:MET:HB3	2.05	0.56
4:E:40:LEU:HD13	4:E:67:GLU:HG2	1.87	0.56
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.88	0.56
10:C:1311:HOH:O	3:D:952:ASP:HB2	2.05	0.56
3:D:1397:LYS:HB2	3:D:1398:TRP:HZ3	1.66	0.56
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.06	0.56
2:C:1004:LYS:HG2	2:C:1005:MET:N	2.19	0.56
2:C:175:GLU:HB3	2:C:183:SER:HB2	1.87	0.55
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.89	0.55
2:C:740:GLU:N	2:C:740:GLU:CD	2.64	0.55
3:D:847:ASP:OD1	3:D:847:ASP:N	2.31	0.55
3:D:1366:LYS:HA	3:D:1369:GLU:OE1	2.06	0.55
2:C:317:VAL:H	2:C:318:PRO:HD3	1.72	0.55
2:C:98:LEU:O	2:C:99:GLN:HB3	2.07	0.55
2:C:987:ILE:HA	3:D:948:THR:HG21	1.88	0.55
3:D:64:LYS:CB	5:F:376:ILE:HG13	2.36	0.55
2:C:263:ASP:OD1	2:C:264:PRO:HD3	2.07	0.55
3:D:565:ILE:HG13	3:D:566:ILE:N	2.21	0.55
3:D:822:ALA:O	3:D:823:LEU:CB	2.54	0.55
3:D:1462:LEU:HB3	3:D:1472:ILE:HD11	1.87	0.55
4:E:50:THR:C	4:E:52:GLU:H	2.14	0.55
2:C:463:GLU:CD	2:C:463:GLU:H	2.15	0.55
2:C:501:THR:HB	2:C:532:MET:HE3	1.87	0.55
3:D:613:ARG:HH21	3:D:617:ASN:H	1.55	0.55
1:A:211:LEU:O	1:A:215:VAL:HG23	2.07	0.55
3:D:661:MET:HE1	3:D:677:LEU:HD21	1.89	0.55
2:C:881:ASN:HD22	2:C:881:ASN:N	1.89	0.54
1:A:88:ARG:HG2	1:A:204:SER:HA	1.88	0.54
2:C:150:PRO:HA	2:C:158:TYR:HD2	1.72	0.54
2:C:369:PRO:HD2	2:C:371:LYS:HG3	1.88	0.54
2:C:750:LYS:HG3	3:D:681:ARG:HH21	1.71	0.54
1:A:228:PRO:HA	1:B:11:PHE:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:689:VAL:CG2	2:C:870:ILE:HB	2.38	0.54
5:F:78:SER:C	5:F:80:PRO:HD2	2.32	0.54
2:C:265:ARG:HD3	2:C:268:ASP:OD2	2.08	0.54
3:D:190:GLU:HA	3:D:196:VAL:HA	1.89	0.54
3:D:534:ARG:HH21	5:F:313:GLU:HB3	1.72	0.54
3:D:192:ALA:CB	3:D:193:PRO:CD	2.86	0.54
3:D:580:ALA:O	3:D:584:ASN:HB2	2.08	0.54
3:D:584:ASN:CB	3:D:602:SER:HB3	2.37	0.54
3:D:1127:GLU:HG2	3:D:1133:ARG:HD2	1.90	0.54
3:D:1219:GLU:HG2	3:D:1221:VAL:HG23	1.90	0.54
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.90	0.53
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.90	0.53
3:D:187:LYS:HA	3:D:199:LEU:O	2.08	0.53
3:D:525:ARG:O	3:D:525:ARG:HG3	2.07	0.53
3:D:1262:LEU:HA	3:D:1265:ALA:HB2	1.91	0.53
2:C:352:ALA:HA	2:C:355:VAL:HB	1.91	0.53
3:D:202:VAL:O	3:D:395:VAL:HA	2.08	0.53
3:D:584:ASN:OD1	3:D:590:PRO:CD	2.53	0.53
3:D:701:LEU:HD22	3:D:763:MET:HE2	1.89	0.53
3:D:835:SER:N	3:D:838:ARG:HE	2.07	0.53
1:A:71:VAL:HG22	1:A:132:LEU:HD22	1.89	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.91	0.53
3:D:784:ASP:OD1	3:D:784:ASP:N	2.41	0.53
1:B:137:ARG:HH22	1:B:139:ASN:HB2	1.74	0.53
2:C:628:PHE:H	2:C:638:ASP:HB2	1.73	0.53
2:C:1051:GLU:HB2	2:C:1055:LEU:HD12	1.91	0.52
3:D:586:ARG:NH2	3:D:1444:THR:HG21	2.23	0.52
3:D:179:VAL:C	3:D:181:ASP:H	2.16	0.52
2:C:838:LYS:HD2	2:C:846:LYS:HE2	1.92	0.52
2:C:838:LYS:HG3	2:C:997:LEU:HD12	1.90	0.52
5:F:372:ARG:O	5:F:373:LYS:HG3	2.09	0.52
3:D:65:ARG:O	3:D:66:GLN:CB	2.57	0.52
2:C:91:GLN:HB2	2:C:118:ILE:C	2.35	0.52
2:C:775:ARG:HB3	2:C:780:GLU:HG3	1.91	0.52
3:D:562:ALA:HB3	3:D:567:ILE:HD11	1.92	0.52
3:D:611:GLN:HB3	3:D:613:ARG:HG3	1.91	0.52
3:D:823:LEU:HD12	3:D:837:GLY:HA2	1.91	0.52
4:E:46:PRO:HB2	4:E:57:ASP:HB3	1.92	0.52
5:F:136:LEU:HB3	5:F:140:ARG:HG2	1.91	0.52
2:C:368:THR:N	2:C:369:PRO:CD	2.73	0.52
2:C:691:SER:HA	2:C:858:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:367:ILE:HB	3:D:377:VAL:CG1	2.40	0.52
3:D:887:ALA:HA	3:D:896:ALA:HB2	1.91	0.52
3:D:1079:LYS:HB3	3:D:1239:ARG:HH22	1.74	0.52
3:D:1305:LEU:HB2	3:D:1306:PRO:HD2	1.91	0.52
1:A:217:ILE:O	1:A:221:HIS:HD2	1.93	0.52
2:C:95:TYR:CD2	2:C:114:PHE:HB3	2.44	0.52
2:C:504:GLU:HB2	2:C:509:ALA:HB2	1.90	0.52
2:C:649:VAL:CG2	2:C:653:ASP:HB2	2.40	0.51
3:D:1031:ASN:OD1	3:D:1034:GLN:HG3	2.10	0.51
5:F:214:GLN:HA	5:F:214:GLN:OE1	2.10	0.51
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.91	0.51
2:C:59:LYS:H	2:C:59:LYS:HD2	1.75	0.51
2:C:1041:GLU:HG2	3:D:1472:ILE:CD1	2.40	0.51
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.91	0.51
3:D:729:HIS:CD2	3:D:731:LEU:H	2.24	0.51
3:D:808:THR:O	3:D:809:PRO:C	2.53	0.51
3:D:837:GLY:H	3:D:840:LYS:HB3	1.76	0.51
5:F:372:ARG:HG2	5:F:401:GLU:OE2	2.10	0.51
2:C:194:VAL:O	2:C:196:LEU:N	2.43	0.51
2:C:521:PRO:HG3	3:D:1072:ILE:HD11	1.91	0.51
2:C:685:GLU:HG3	3:D:739:ASP:HB2	1.92	0.51
2:C:810:ASP:OD1	2:C:811:PRO:HD3	2.11	0.51
2:C:853:LEU:HD12	2:C:858:MET:HE2	1.92	0.51
2:C:1019:GLN:HE22	3:D:621:LYS:HG2	1.75	0.51
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.92	0.51
3:D:212:ARG:HD3	3:D:342:PRO:HB3	1.93	0.51
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.93	0.51
3:D:945:SER:OG	3:D:947:ILE:HG23	2.11	0.51
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.50	0.51
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.92	0.51
3:D:777:PRO:HG2	3:D:912:LYS:HG2	1.92	0.51
2:C:317:VAL:N	2:C:318:PRO:CD	2.73	0.51
5:F:372:ARG:HD3	5:F:383:LEU:HD23	1.93	0.51
2:C:193:LEU:O	2:C:194:VAL:C	2.54	0.50
2:C:674:VAL:HB	2:C:869:VAL:HG22	1.93	0.50
3:D:823:LEU:HA	3:D:836:VAL:HB	1.93	0.50
2:C:368:THR:N	2:C:369:PRO:HD3	2.27	0.50
2:C:709:GLU:HG2	2:C:824:ARG:HG2	1.93	0.50
5:F:282:LEU:HD23	5:F:284:ARG:HE	1.75	0.50
1:B:212:ASN:O	1:B:215:VAL:HG22	2.10	0.50
2:C:175:GLU:HG2	2:C:176:VAL:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:628:PHE:H	2:C:638:ASP:CB	2.24	0.50
3:D:1380:GLU:HB2	3:D:1420:LEU:HD12	1.93	0.50
2:C:208:ALA:HB1	2:C:221:LEU:HD21	1.92	0.50
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.93	0.50
3:D:223:LEU:HB2	3:D:333:LEU:HB2	1.93	0.50
3:D:525:ARG:N	3:D:526:PRO:CD	2.74	0.50
1:A:34:VAL:HB	1:B:42:ARG:NH1	2.26	0.50
2:C:261:ILE:HG22	2:C:262:ALA:H	1.76	0.50
2:C:422:ARG:O	2:C:423:ALA:C	2.54	0.50
3:D:272:LEU:HG	3:D:282:TYR:HE1	1.77	0.50
3:D:1009:LYS:O	3:D:1013:GLU:HG2	2.11	0.50
3:D:1411:GLY:O	3:D:1413:THR:N	2.44	0.50
2:C:181:VAL:HG12	2:C:182:VAL:N	2.27	0.50
2:C:588:VAL:HG13	2:C:593:ALA:HB3	1.93	0.50
2:C:851:LYS:HE3	2:C:853:LEU:HD23	1.93	0.50
5:F:205:ARG:HG2	5:F:205:ARG:NH1	2.23	0.50
5:F:370:LYS:HA	5:F:374:GLY:HA3	1.94	0.50
2:C:136:ILE:CD1	2:C:392:SER:HB2	2.42	0.49
3:D:87:ARG:HB3	3:D:523:ASP:HB3	1.94	0.49
2:C:17:PRO:O	2:C:20:GLU:HB2	2.12	0.49
2:C:194:VAL:O	2:C:197:LEU:HG	2.12	0.49
3:D:1465:ASN:ND2	3:D:1470:ARG:HD3	2.26	0.49
3:D:876:SER:OG	3:D:879:ARG:HG2	2.12	0.49
2:C:122:THR:HG22	2:C:123:GLU:N	2.27	0.49
2:C:683:ASN:HD22	2:C:683:ASN:C	2.20	0.49
3:D:1050:GLY:HA2	3:D:1241:PHE:HE2	1.76	0.49
2:C:342:ASP:HA	2:C:345:ARG:HD2	1.94	0.49
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.93	0.49
2:C:575:GLN:HG3	2:C:670:GLN:HG3	1.94	0.49
2:C:670:GLN:HG2	2:C:699:PHE:CE2	2.47	0.49
3:D:433:GLY:HA3	3:D:446:VAL:CG1	2.42	0.49
5:F:204:GLY:C	5:F:206:GLY:H	2.21	0.49
2:C:242:LEU:HD13	2:C:254:VAL:HG11	1.94	0.49
5:F:210:LEU:HA	5:F:213:ILE:HD12	1.94	0.49
2:C:211:LEU:HD22	2:C:308:ARG:HH12	1.77	0.49
3:D:937:TYR:O	3:D:938:GLY:C	2.55	0.49
4:E:41:GLU:O	4:E:42:PRO:C	2.56	0.49
2:C:251:ASP:N	2:C:251:ASP:OD1	2.44	0.49
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.38	0.49
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.93	0.49
1:A:174:VAL:HA	1:A:201:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HB	1:A:209:GLU:CG	2.41	0.49
1:B:176:ARG:HD2	1:B:200:TRP:CZ3	2.47	0.49
2:C:395:LYS:HE2	2:C:403:SER:HB3	1.95	0.49
1:B:206:THR:HB	1:B:209:GLU:H	1.77	0.48
3:D:907:GLU:O	3:D:908:LYS:C	2.54	0.48
5:F:277:GLN:N	5:F:277:GLN:HE21	2.10	0.48
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.12	0.48
2:C:846:LYS:HD3	3:D:741:ASP:HB2	1.94	0.48
2:C:910:LYS:O	2:C:911:GLU:C	2.56	0.48
3:D:186:VAL:HG12	3:D:187:LYS:H	1.78	0.48
2:C:99:GLN:HA	2:C:110:GLU:H	1.77	0.48
1:A:26:GLU:HB3	1:A:194:LYS:HG3	1.94	0.48
2:C:418:LEU:O	2:C:420:ARG:N	2.47	0.48
2:C:428:ARG:O	2:C:429:ASP:HB2	2.11	0.48
2:C:469:THR:HG23	2:C:538:GLN:NE2	2.28	0.48
3:D:631:ILE:HG22	3:D:726:ILE:HB	1.96	0.48
4:E:37:ASN:H	4:E:37:ASN:ND2	2.11	0.48
2:C:198:ARG:NH1	2:C:203:ASP:HB3	2.29	0.48
2:C:559:LEU:HD12	2:C:559:LEU:O	2.14	0.48
2:C:958:THR:OG1	2:C:961:GLU:HG2	2.14	0.48
2:C:25:SER:OG	2:C:335:THR:HB	2.13	0.48
2:C:649:VAL:HG22	2:C:653:ASP:HB2	1.94	0.48
3:D:835:SER:H	3:D:838:ARG:HE	1.62	0.48
3:D:959:GLU:HB3	3:D:963:TYR:HE2	1.78	0.48
3:D:1128:VAL:O	3:D:1129:THR:C	2.56	0.48
1:A:195:LEU:HD12	1:A:196:THR:N	2.29	0.48
1:B:2:LEU:H	1:B:3:ASP:HA	1.73	0.48
2:C:843:HIS:HE1	2:C:887:GLU:OE1	1.97	0.48
3:D:64:LYS:HB2	5:F:376:ILE:CG1	2.38	0.48
3:D:440:VAL:HG23	3:D:441:ARG:H	1.79	0.48
3:D:829:VAL:O	3:D:831:GLY:N	2.47	0.48
3:D:984:THR:CG2	3:D:987:GLU:H	2.25	0.48
1:B:58:ILE:HD13	1:B:140:MET:CB	2.43	0.48
3:D:64:LYS:CD	5:F:376:ILE:HG21	2.34	0.48
3:D:783:ARG:HG2	3:D:783:ARG:NH1	2.22	0.48
3:D:835:SER:HB2	3:D:838:ARG:HG3	1.96	0.48
3:D:259:VAL:HG21	3:D:270:LEU:HA	1.96	0.48
3:D:1165:TYR:HE2	3:D:1206:GLY:HA2	1.77	0.48
2:C:606:VAL:HG12	2:C:611:ILE:HG12	1.96	0.47
2:C:1030:GLN:OE1	3:D:628:ARG:HB2	2.14	0.47
2:C:1055:LEU:HG	2:C:1079:PRO:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:794:GLN:HB3	3:D:1017:PHE:CZ	2.49	0.47
3:D:1208:ASP:O	3:D:1209:LEU:CB	2.56	0.47
2:C:639:GLN:HA	2:C:657:ASP:O	2.14	0.47
2:C:808:ARG:O	2:C:810:ASP:N	2.44	0.47
5:F:239:ALA:O	5:F:240:THR:C	2.57	0.47
3:D:1028:ALA:O	3:D:1029:ARG:HB2	2.14	0.47
3:D:1436:SER:O	3:D:1439:SER:N	2.44	0.47
1:A:139:ASN:C	1:A:139:ASN:OD1	2.57	0.47
2:C:358:ARG:HE	2:C:372:LEU:HA	1.78	0.47
2:C:985:GLY:HA3	10:D:1703:HOH:O	2.13	0.47
3:D:502:PHE:CZ	3:D:1452:ILE:HD12	2.50	0.47
2:C:91:GLN:CB	2:C:119:PRO:HA	2.44	0.47
2:C:740:GLU:CD	2:C:740:GLU:H	2.23	0.47
3:D:166:GLN:HG2	3:D:396:VAL:HG23	1.96	0.47
3:D:212:ARG:HA	3:D:343:LYS:O	2.14	0.47
3:D:806:PHE:CE1	3:D:812:ALA:HA	2.50	0.47
3:D:834:THR:HG23	3:D:838:ARG:HD2	1.97	0.47
3:D:864:VAL:HG13	3:D:865:THR:N	2.30	0.47
3:D:1074:SER:O	3:D:1077:ALA:HB3	2.15	0.47
3:D:1078:ARG:O	3:D:1079:LYS:C	2.57	0.47
2:C:563:ASN:O	2:C:566:THR:HB	2.15	0.47
2:C:1100:GLN:HG3	2:C:1102:LEU:HD21	1.97	0.47
3:D:1213:ARG:HG2	3:D:1213:ARG:NH1	2.08	0.47
2:C:42:VAL:HG13	2:C:43:GLY:N	2.30	0.47
3:D:1124:GLN:HA	3:D:1124:GLN:NE2	2.21	0.47
2:C:1071:ILE:O	3:D:659:LYS:HD3	2.14	0.47
2:C:1105:LYS:O	2:C:1106:ASP:CB	2.63	0.47
3:D:112:ILE:HG22	3:D:512:MET:HE3	1.97	0.47
3:D:195:VAL:O	3:D:196:VAL:HG22	2.15	0.47
3:D:1377:LYS:HD2	3:D:1378:TYR:CE2	2.50	0.47
5:F:224:VAL:HG23	5:F:235:PHE:HZ	1.80	0.47
2:C:195:LEU:HB3	2:C:238:LEU:HD22	1.98	0.46
2:C:712:ALA:HB3	2:C:821:GLU:HG2	1.97	0.46
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.96	0.46
3:D:1124:GLN:HG2	3:D:1135:ARG:HG2	1.95	0.46
3:D:1464:GLU:O	3:D:1467:ILE:HG22	2.15	0.46
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.97	0.46
2:C:803:THR:HG22	2:C:825:VAL:HG13	1.97	0.46
1:A:6:LEU:HD23	1:A:6:LEU:N	2.29	0.46
3:D:536:ALA:HA	5:F:315:VAL:O	2.14	0.46
3:D:1405:GLU:HB3	3:D:1414:PRO:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:421:GLU:O	2:C:423:ALA:N	2.49	0.46
3:D:1236:LEU:O	3:D:1237:THR:C	2.58	0.46
3:D:108:VAL:HG12	3:D:109:PRO:HA	1.96	0.46
3:D:1397:LYS:HB2	3:D:1398:TRP:CE3	2.51	0.46
2:C:795:GLY:O	2:C:796:GLU:HB2	2.15	0.46
3:D:65:ARG:HB2	5:F:376:ILE:HG12	1.98	0.46
2:C:676:ILE:HG12	2:C:988:VAL:HG13	1.98	0.46
2:C:830:LYS:HB2	2:C:830:LYS:HE3	1.79	0.46
3:D:783:ARG:HH11	3:D:783:ARG:CG	2.21	0.46
3:D:821:VAL:HG12	3:D:822:ALA:N	2.31	0.46
3:D:1048:PRO:HA	3:D:1079:LYS:HE2	1.98	0.46
3:D:709:HIS:C	3:D:709:HIS:CD2	2.94	0.46
3:D:980:MET:HE2	3:D:980:MET:HA	1.97	0.46
3:D:1190:SER:OG	3:D:1191:PRO:HD2	2.16	0.46
2:C:72:ARG:HH11	2:C:112:GLU:CD	2.24	0.46
2:C:679:PHE:CE2	2:C:853:LEU:HD11	2.51	0.46
2:C:876:VAL:N	2:C:877:PRO:HD2	2.29	0.46
1:B:1:MET:HB3	1:B:2:LEU:H	1.56	0.45
1:B:133:GLU:HG2	1:B:134:GLU:N	2.30	0.45
2:C:115:LEU:HD13	2:C:373:VAL:HG12	1.97	0.45
2:C:627:ARG:HA	2:C:627:ARG:HD3	1.61	0.45
3:D:1192:LEU:HD23	3:D:1192:LEU:HA	1.75	0.45
3:D:1264:GLU:OE1	3:D:1425:THR:HB	2.16	0.45
3:D:1399:ASP:O	3:D:1403:LEU:HD13	2.16	0.45
3:D:1492:LEU:HD11	4:E:74:VAL:HG21	1.98	0.45
1:A:79:ILE:O	1:A:80:LEU:C	2.57	0.45
2:C:72:ARG:HG3	2:C:95:TYR:HB2	1.98	0.45
2:C:151:ASP:HB3	2:C:154:ARG:HB3	1.98	0.45
2:C:1007:ALA:HB2	3:D:648:MET:HG3	1.99	0.45
3:D:116:LEU:O	3:D:150:ARG:NH2	2.48	0.45
5:F:191:ASN:HA	10:F:501:HOH:O	2.16	0.45
2:C:375:SER:O	2:C:378:LEU:N	2.49	0.45
2:C:640:ARG:O	2:C:656:ALA:HA	2.16	0.45
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.98	0.45
3:D:660:LYS:HG3	3:D:694:VAL:HG23	1.97	0.45
2:C:654:LEU:HG	2:C:655:LEU:N	2.31	0.45
3:D:108:VAL:CG1	3:D:109:PRO:HA	2.47	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.86	0.45
2:C:91:GLN:HB2	2:C:119:PRO:HA	1.99	0.45
2:C:184:MET:HG3	2:C:193:LEU:HD13	1.98	0.45
2:C:595:LEU:HD11	2:C:623:TYR:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.75	0.45
3:D:240:GLU:HB3	3:D:241:ILE:H	1.56	0.45
3:D:493:ARG:HH21	3:D:1390:LEU:HB2	1.82	0.45
3:D:631:ILE:CG2	3:D:745:MET:HG3	2.35	0.45
2:C:637:LEU:HA	2:C:659:PRO:HB3	1.99	0.45
3:D:1394:VAL:HG22	10:D:1713:HOH:O	2.11	0.45
4:E:52:GLU:CD	4:E:52:GLU:N	2.75	0.45
5:F:79:ASP:N	5:F:80:PRO:CD	2.75	0.45
1:A:160:ASP:OD1	1:A:160:ASP:N	2.30	0.45
2:C:109:LYS:H	2:C:109:LYS:HG2	1.64	0.45
2:C:333:ILE:HG13	2:C:333:ILE:O	2.17	0.45
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.41	0.45
2:C:1055:LEU:HD22	2:C:1066:ALA:HB2	1.97	0.45
1:B:57:TYR:HB3	1:B:141:GLU:HB2	1.97	0.45
2:C:575:GLN:NE2	2:C:670:GLN:HG3	2.31	0.45
3:D:596:SER:C	3:D:598:ARG:H	2.25	0.45
2:C:166:PRO:HB2	2:C:168:ARG:H	1.81	0.45
3:D:1031:ASN:H	3:D:1034:GLN:NE2	2.11	0.45
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.99	0.45
5:F:335:ASP:OD1	5:F:337:HIS:N	2.50	0.45
2:C:923:GLU:O	2:C:927:GLY:HA3	2.17	0.45
3:D:238:PRO:HB3	3:D:318:ARG:HA	1.98	0.45
3:D:838:ARG:HD3	3:D:874:GLU:OE2	2.17	0.45
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.60	0.44
2:C:222:MET:O	2:C:223:ASP:HB2	2.17	0.44
2:C:243:ARG:HB3	2:C:244:PRO:CA	2.42	0.44
2:C:759:THR:HA	2:C:786:LYS:O	2.17	0.44
2:C:1118:LYS:HG2	2:C:1119:ARG:H	1.82	0.44
3:D:95:LEU:HA	3:D:551:ASN:HD21	1.82	0.44
3:D:889:ALA:O	3:D:929:ARG:NH1	2.50	0.44
2:C:166:PRO:HD2	2:C:169:GLY:HA3	1.98	0.44
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.42	0.44
3:D:1071:PHE:O	3:D:1072:ILE:C	2.61	0.44
3:D:1393:GLN:HE22	3:D:1398:TRP:HZ3	1.64	0.44
1:B:3:ASP:HB3	1:B:4:SER:H	1.70	0.44
3:D:48:ARG:HB3	3:D:48:ARG:NH1	2.31	0.44
2:C:302:VAL:O	2:C:305:PRO:HD2	2.17	0.44
2:C:498:GLN:OE1	3:D:1067:VAL:HG13	2.17	0.44
2:C:1016:ILE:O	3:D:87:ARG:NH2	2.50	0.44
3:D:584:ASN:H	3:D:602:SER:CB	2.30	0.44
3:D:1030:GLY:HA2	3:D:1034:GLN:NE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1345:GLU:O	3:D:1349:VAL:HG23	2.18	0.44
4:E:50:THR:C	4:E:52:GLU:N	2.75	0.44
2:C:177:GLU:HG2	2:C:178:PRO:HD2	1.99	0.44
3:D:106:LYS:HA	3:D:106:LYS:HD3	1.82	0.44
3:D:304:LEU:O	3:D:305:ALA:HB2	2.17	0.44
3:D:699:VAL:HB	3:D:716:PHE:O	2.18	0.44
3:D:834:THR:CG2	3:D:835:SER:N	2.80	0.44
3:D:983:LEU:HD23	3:D:983:LEU:HA	1.69	0.44
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.16	0.44
3:D:1468:LEU:HD23	3:D:1468:LEU:C	2.43	0.44
1:A:183:ASP:HA	2:C:938:LYS:HE3	2.00	0.44
2:C:15:LEU:CD2	2:C:457:ALA:HB1	2.46	0.44
2:C:304:LEU:HB3	2:C:305:PRO:CD	2.45	0.44
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.53	0.44
3:D:1048:PRO:HD3	3:D:1075:HIS:CD2	2.53	0.44
1:A:42:ARG:NH1	1:B:34:VAL:HB	2.32	0.44
3:D:86:ARG:O	3:D:523:ASP:HB2	2.18	0.44
3:D:586:ARG:HH22	3:D:1444:THR:HG21	1.81	0.44
3:D:1353:GLN:HA	3:D:1353:GLN:OE1	2.18	0.44
5:F:277:GLN:HE21	5:F:277:GLN:H	1.66	0.44
1:B:185:ARG:HA	1:B:189:ARG:O	2.18	0.44
2:C:553:ASP:OD1	2:C:843:HIS:CD2	2.60	0.44
2:C:589:ARG:HH11	2:C:589:ARG:HG3	1.83	0.44
2:C:710:ILE:CG2	2:C:823:VAL:HB	2.48	0.44
3:D:756:GLN:NE2	4:E:61:GLU:OE2	2.46	0.44
2:C:64:LEU:HD23	2:C:359:MET:HE3	1.99	0.44
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.18	0.44
1:B:55:SER:HA	1:B:167:VAL:HG23	2.00	0.43
2:C:474:VAL:HG11	2:C:529:VAL:HG12	2.00	0.43
3:D:960:LYS:O	3:D:961:LYS:C	2.60	0.43
3:D:1033:GLN:N	3:D:1033:GLN:CD	2.76	0.43
4:E:41:GLU:O	4:E:44:GLU:HG2	2.17	0.43
5:F:205:ARG:HH11	5:F:205:ARG:CG	2.26	0.43
2:C:99:GLN:H	2:C:110:GLU:HB2	1.83	0.43
2:C:274:ARG:HE	2:C:285:LEU:HD22	1.83	0.43
3:D:1254:GLN:O	3:D:1257:PRO:HG2	2.18	0.43
2:C:266:ARG:NH1	2:C:273:GLY:H	2.15	0.43
2:C:399:ASN:HB2	2:C:400:PRO:HD2	2.01	0.43
3:D:1425:THR:HG22	3:D:1426:LYS:N	2.34	0.43
5:F:291:ILE:CG2	5:F:304:VAL:HG11	2.45	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:LEU:O	3:D:127:LEU:HB2	2.18	0.43
3:D:693:GLU:HA	4:E:48:MET:HE1	2.01	0.43
1:A:12:THR:HB	1:B:229:GLN:HB3	1.99	0.43
1:B:144:VAL:HG12	1:B:145:ASP:N	2.34	0.43
3:D:538:SER:N	5:F:317:LEU:HD12	2.34	0.43
3:D:1465:ASN:ND2	3:D:1470:ARG:HH11	2.16	0.43
1:A:206:THR:HG22	1:A:208:LEU:N	2.32	0.43
2:C:177:GLU:HB3	2:C:181:VAL:H	1.84	0.43
2:C:740:GLU:OE2	2:C:740:GLU:HA	2.17	0.43
2:C:904:PRO:HA	10:C:1305:HOH:O	2.18	0.43
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.85	0.43
2:C:6:PHE:HB3	2:C:908:GLY:HA2	2.00	0.43
3:D:1031:ASN:HB2	3:D:1032:PRO:CD	2.48	0.43
3:D:1079:LYS:HB3	3:D:1239:ARG:NH2	2.33	0.43
1:A:46:SER:HB3	2:C:856:GLU:CD	2.44	0.43
1:B:226:SER:O	1:B:228:PRO:HD3	2.19	0.43
2:C:607:ASP:C	2:C:609:ASN:H	2.25	0.43
3:D:1079:LYS:H	3:D:1079:LYS:HG2	1.64	0.43
3:D:1117:TYR:CD1	3:D:1117:TYR:C	2.97	0.43
5:F:296:GLY:HA3	5:F:297:PRO:HD3	1.82	0.43
1:B:144:VAL:CG1	1:B:145:ASP:N	2.81	0.43
2:C:266:ARG:H	2:C:266:ARG:HG3	1.62	0.43
2:C:722:ILE:HD12	2:C:722:ILE:H	1.83	0.43
3:D:1123:PHE:HB3	3:D:1132:LEU:HG	2.01	0.43
3:D:1154:GLU:HA	3:D:1159:ARG:HA	2.01	0.43
2:C:612:VAL:HG22	2:C:622:GLU:HG3	2.01	0.43
2:C:693:GLU:O	2:C:697:ARG:HG3	2.18	0.43
3:D:272:LEU:HD12	3:D:279:VAL:HB	2.00	0.43
3:D:523:ASP:O	3:D:526:PRO:HG3	2.18	0.43
1:B:58:ILE:HD13	1:B:140:MET:HB3	2.01	0.42
1:B:108:GLU:HG3	1:B:131:THR:HG22	2.01	0.42
2:C:254:VAL:O	2:C:257:VAL:HB	2.18	0.42
2:C:422:ARG:O	2:C:424:GLY:N	2.52	0.42
2:C:953:VAL:CG1	2:C:966:LEU:HD13	2.47	0.42
3:D:136:ASP:HA	3:D:137:PRO:HD3	1.87	0.42
3:D:860:LEU:O	3:D:876:SER:HB2	2.19	0.42
3:D:1331:ASP:HB3	3:D:1334:GLN:HB2	2.01	0.42
2:C:681:GLY:HA2	3:D:939:PHE:CE2	2.53	0.42
2:C:1054:THR:HG22	2:C:1082:PRO:HB3	2.01	0.42
3:D:80:VAL:HG23	3:D:80:VAL:O	2.19	0.42
3:D:247:GLU:HA	3:D:248:PRO:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:729:HIS:CD2	3:D:730:PRO:HD2	2.54	0.42
3:D:1378:TYR:CE2	3:D:1394:VAL:HG22	2.53	0.42
5:F:153:PRO:HB2	5:F:154:LYS:H	1.59	0.42
5:F:271:LEU:HD23	5:F:295:MET:HE3	2.01	0.42
1:A:29:GLU:O	1:A:32:PHE:HB2	2.18	0.42
1:B:58:ILE:HD13	1:B:140:MET:HB2	2.00	0.42
2:C:676:ILE:O	3:D:948:THR:HG22	2.20	0.42
3:D:86:ARG:C	3:D:523:ASP:HB2	2.43	0.42
3:D:1124:GLN:HE21	3:D:1124:GLN:CA	2.22	0.42
4:E:41:GLU:OE1	4:E:42:PRO:HD2	2.19	0.42
1:A:112:ARG:HB3	1:A:125:PRO:HB2	2.01	0.42
3:D:96:ALA:HB3	3:D:554:LEU:CD2	2.49	0.42
3:D:367:ILE:HG22	3:D:368:VAL:HG23	2.01	0.42
3:D:835:SER:H	3:D:838:ARG:NE	2.16	0.42
5:F:137:GLY:HA3	5:F:141:VAL:HG13	2.00	0.42
2:C:274:ARG:NE	2:C:285:LEU:HD13	2.33	0.42
2:C:939:ARG:NH2	10:C:1302:HOH:O	2.49	0.42
3:D:616:GLN:HB3	3:D:617:ASN:H	1.55	0.42
3:D:793:THR:HG21	3:D:906:GLN:HG2	2.01	0.42
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.01	0.42
3:D:1194:CYS:HB2	3:D:1204:CYS:CB	2.50	0.42
1:B:220:GLU:O	1:B:223:THR:OG1	2.36	0.42
2:C:184:MET:HE1	2:C:186:VAL:HG13	2.01	0.42
2:C:280:LYS:HA	2:C:280:LYS:HD3	1.89	0.42
2:C:738:ASP:CB	2:C:744:ARG:HH21	2.31	0.42
2:C:985:GLY:HA2	2:C:986:PRO:HD3	1.74	0.42
3:D:244:GLU:HG2	3:D:245:LEU:H	1.85	0.42
3:D:439:LEU:H	3:D:439:LEU:HG	1.63	0.42
3:D:594:PRO:O	3:D:595:GLY:C	2.62	0.42
3:D:966:GLU:HG2	3:D:969:ARG:HH12	1.83	0.42
2:C:157:ARG:HG3	2:C:158:TYR:H	1.85	0.42
2:C:501:THR:HA	2:C:502:PRO:HD3	1.89	0.42
2:C:1019:GLN:O	2:C:1020:PRO:C	2.63	0.42
3:D:864:VAL:CG1	3:D:865:THR:N	2.83	0.42
3:D:1166:LEU:HD23	3:D:1166:LEU:HA	1.87	0.42
3:D:698:LYS:HA	3:D:756:GLN:HE22	1.84	0.42
3:D:809:PRO:HB2	3:D:810:GLU:H	1.66	0.42
3:D:1447:LEU:O	3:D:1448:THR:C	2.62	0.42
5:F:217:ASN:O	5:F:221:ILE:HD12	2.20	0.42
2:C:172:ILE:HG23	2:C:184:MET:HE3	2.01	0.42
3:D:825:ALA:HA	3:D:826:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1362:LYS:HE3	3:D:1362:LYS:HB2	1.88	0.42
2:C:1042:ALA:HB2	3:D:1223:ILE:HG22	2.01	0.42
3:D:987:GLU:O	3:D:991:GLN:HB2	2.19	0.42
3:D:1397:LYS:CA	3:D:1398:TRP:HE3	2.32	0.42
4:E:30:LEU:CD2	4:E:63:TRP:HB3	2.49	0.42
5:F:116:LEU:HD22	5:F:163:LEU:HD22	2.01	0.42
2:C:54:ILE:HG23	2:C:66:LEU:HB3	2.02	0.41
2:C:198:ARG:HH21	2:C:231:PRO:HB3	1.85	0.41
2:C:214:TYR:HE1	2:C:311:PHE:HB3	1.85	0.41
2:C:443:THR:HG23	2:C:444:PRO:N	2.35	0.41
2:C:517:ARG:HG3	2:C:522:VAL:HG21	2.02	0.41
2:C:37:GLU:HG3	2:C:38:LYS:HG3	2.01	0.41
2:C:252:LYS:HB3	2:C:256:TYR:HD1	1.85	0.41
2:C:313:LEU:C	2:C:315:ALA:H	2.27	0.41
2:C:685:GLU:OE1	3:D:783:ARG:HD2	2.20	0.41
2:C:1059:ASP:OD1	2:C:1059:ASP:C	2.63	0.41
3:D:312:ARG:HB3	3:D:313:MET:H	1.76	0.41
3:D:698:LYS:HA	3:D:756:GLN:NE2	2.35	0.41
5:F:415:THR:HG22	5:F:417:LYS:HG3	2.01	0.41
1:B:104:GLU:HA	1:B:132:LEU:HD22	2.03	0.41
2:C:1118:LYS:HD2	3:D:22:SER:O	2.21	0.41
3:D:485:SER:HB3	3:D:486:ARG:H	1.65	0.41
3:D:1436:SER:O	3:D:1439:SER:HB3	2.21	0.41
3:D:821:VAL:HG11	3:D:827:ILE:HD11	2.03	0.41
3:D:1475:GLY:C	3:D:1477:GLY:H	2.28	0.41
1:A:195:LEU:HD12	1:A:196:THR:H	1.84	0.41
2:C:111:ASP:HB3	2:C:112:GLU:H	1.53	0.41
2:C:890:LEU:HG	2:C:901:TYR:CD1	2.55	0.41
2:C:1012:PRO:HD3	2:C:1026:GLN:HG2	2.02	0.41
3:D:1256:LEU:N	3:D:1257:PRO:CD	2.84	0.41
2:C:462:ASP:OD1	2:C:462:ASP:C	2.63	0.41
2:C:751:PRO:HB3	2:C:794:PRO:HA	2.02	0.41
2:C:759:THR:HB	2:C:785:VAL:HB	2.03	0.41
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.84	0.41
3:D:356:PRO:O	3:D:358:GLY:N	2.54	0.41
3:D:525:ARG:H	3:D:526:PRO:CD	2.33	0.41
2:C:720:GLU:CB	2:C:759:THR:O	2.69	0.41
2:C:957:LYS:HB3	2:C:961:GLU:HG3	2.02	0.41
3:D:191:LEU:HD12	3:D:195:VAL:HB	2.01	0.41
3:D:224:ARG:HH11	3:D:332:TYR:HB2	1.86	0.41
3:D:266:GLU:HB2	3:D:314:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1101:VAL:CG1	3:D:1102:THR:HG23	2.51	0.41
2:C:674:VAL:HG11	2:C:992:MET:HB2	2.03	0.41
3:D:137:PRO:HB2	3:D:138:LYS:H	1.50	0.41
3:D:408:GLU:O	3:D:409:VAL:HG22	2.21	0.41
3:D:1130:ARG:HD2	3:D:1130:ARG:HA	1.76	0.41
3:D:1295:GLU:HG2	3:D:1300:SER:OG	2.21	0.41
2:C:394:PHE:O	2:C:395:LYS:C	2.62	0.41
2:C:953:VAL:HB	2:C:962:GLN:HG2	2.03	0.41
3:D:179:VAL:C	3:D:181:ASP:N	2.79	0.41
3:D:230:TRP:HE1	3:D:233:LYS:HG2	1.86	0.41
3:D:417:PRO:HB3	3:D:430:ASP:O	2.21	0.41
3:D:676:MET:HE2	3:D:676:MET:HB2	1.84	0.41
3:D:931:LEU:HA	3:D:931:LEU:HD23	1.87	0.41
5:F:370:LYS:O	5:F:375:LEU:N	2.54	0.41
1:B:211:LEU:O	1:B:212:ASN:C	2.64	0.41
2:C:233:GLU:HA	2:C:236:ILE:HD12	2.03	0.41
3:D:272:LEU:C	3:D:274:ARG:H	2.27	0.41
3:D:452:ILE:HD12	3:D:452:ILE:H	1.86	0.41
3:D:821:VAL:CG1	3:D:822:ALA:N	2.83	0.41
4:E:46:PRO:CB	4:E:57:ASP:HB3	2.51	0.41
1:A:38:ASN:O	1:A:39:PRO:C	2.64	0.40
1:B:179:PHE:HB3	1:B:197:LEU:HD13	2.03	0.40
1:B:213:GLN:O	1:B:217:ILE:HG13	2.21	0.40
2:C:21:ILE:H	2:C:21:ILE:CD1	2.00	0.40
2:C:907:ASP:O	2:C:908:GLY:O	2.39	0.40
3:D:879:ARG:NH1	3:D:904:VAL:C	2.79	0.40
3:D:1376:MET:HE3	3:D:1421:LEU:HA	2.02	0.40
1:A:94:LEU:HD22	1:A:96:THR:H	1.87	0.40
1:A:170:VAL:HG11	2:C:696:LYS:HB3	2.04	0.40
1:A:201:THR:OG1	1:A:207:PRO:HD3	2.22	0.40
1:B:45:LEU:HD23	1:B:45:LEU:HA	1.93	0.40
1:B:91:ASN:HA	1:B:92:PRO:HD3	1.93	0.40
2:C:1112:PHE:O	2:C:1113:GLU:C	2.65	0.40
4:E:30:LEU:HD23	4:E:63:TRP:HB3	2.02	0.40
2:C:218:VAL:HG23	2:C:311:PHE:CZ	2.56	0.40
4:E:62:THR:O	4:E:63:TRP:C	2.64	0.40
5:F:419:ARG:O	5:F:422:LEU:HD12	2.21	0.40
2:C:15:LEU:HD21	2:C:457:ALA:HB1	2.04	0.40
2:C:311:PHE:HA	2:C:314:THR:OG1	2.22	0.40
2:C:722:ILE:HD12	2:C:722:ILE:N	2.36	0.40
2:C:728:HIS:NE2	2:C:730:SER:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:905:ILE:HG23	2:C:906:PHE:HD1	1.87	0.40
1:A:63:HIS:CB	2:C:799:ILE:HD11	2.51	0.40
2:C:421:GLU:C	2:C:423:ALA:H	2.30	0.40
2:C:974:LEU:HD23	2:C:974:LEU:HA	1.86	0.40
3:D:372:ASP:HB2	3:D:373:PRO:HD2	2.04	0.40
3:D:616:GLN:O	3:D:617:ASN:HB3	2.22	0.40
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	2.03	0.40
5:F:300:ASP:O	5:F:304:VAL:HG23	2.21	0.40
5:F:346:THR:O	5:F:349:LEU:N	2.54	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	229/315 (73%)	211 (92%)	17 (7%)	1 (0%)	30	65
1	B	236/315 (75%)	218 (92%)	16 (7%)	2 (1%)	16	50
2	C	1117/1119 (100%)	928 (83%)	151 (14%)	38 (3%)	3	17
3	D	1502/1524 (99%)	1228 (82%)	208 (14%)	66 (4%)	2	12
4	E	93/99 (94%)	71 (76%)	16 (17%)	6 (6%)	1	5
5	F	349/423 (82%)	302 (86%)	36 (10%)	11 (3%)	3	18
All	All	3526/3795 (93%)	2958 (84%)	444 (13%)	124 (4%)	3	16

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	42	VAL
2	C	194	VAL
2	C	195	LEU

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Mol	Chain	Res	Type
2	C	223	ASP
2	C	261	ILE
2	C	419	THR
2	C	422	ARG
2	C	423	ALA
2	C	738	ASP
2	C	739	GLU
2	C	808	ARG
2	C	908	GLY
3	D	137	PRO
3	D	173	PRO
3	D	192	ALA
3	D	196	VAL
3	D	357	GLU
3	D	409	VAL
3	D	492	ALA
3	D	525	ARG
3	D	587	ARG
3	D	809	PRO
3	D	823	LEU
3	D	830	ALA
3	D	858	VAL
3	D	1209	LEU
3	D	1238	MET
3	D	1407	LEU
3	D	1412	LYS
4	E	51	LEU
5	F	80	PRO
5	F	322	GLY
5	F	377	ASP
1	B	4	SER
2	C	215	GLY
2	C	296	GLY
2	C	369	PRO
2	C	429	ASP
2	C	796	GLU
2	C	809	GLY
2	C	1113	GLU
3	D	138	LYS
3	D	177	ALA
3	D	205	TYR
3	D	265	GLU

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Mol	Chain	Res	Type
3	D	304	LEU
3	D	316	GLN
3	D	375	GLU
3	D	442	ASN
3	D	491	LYS
3	D	594	PRO
3	D	595	GLY
3	D	1080	GLY
3	D	1129	THR
3	D	1266	ARG
4	E	79	LEU
5	F	153	PRO
2	C	37	GLU
2	C	110	GLU
2	C	156	GLY
2	C	263	ASP
2	C	363	SER
2	C	1106	ASP
3	D	110	SER
3	D	142	LEU
3	D	305	ALA
3	D	437	VAL
3	D	617	ASN
3	D	787	LEU
3	D	1072	ILE
3	D	1341	PRO
3	D	1391	GLU
3	D	1408	ILE
4	E	54	LEU
5	F	205	ARG
5	F	389	PHE
1	A	59	GLU
2	C	33	ASP
2	C	79	PRO
2	C	218	VAL
2	C	427	VAL
2	C	1010	THR
2	C	1057	SER
3	D	69	GLU
3	D	178	LEU
3	D	245	LEU
3	D	248	PRO

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Mol	Chain	Res	Type
3	D	250	LEU
3	D	278	PRO
3	D	285	PRO
3	D	487	ALA
3	D	510	GLU
3	D	668	PRO
3	D	698	LYS
3	D	835	SER
3	D	1092	GLY
3	D	1390	LEU
1	B	158	ILE
2	C	181	VAL
2	C	288	ARG
2	C	735	ARG
2	C	876	VAL
3	D	227	LEU
3	D	255	GLU
4	E	42	PRO
4	E	84	ARG
5	F	75	ILE
3	D	1085	ALA
5	F	346	THR
3	D	808	THR
3	D	1081	GLY
5	F	297	PRO
2	C	74	GLY
2	C	166	PRO
2	C	376	ARG
3	D	287	GLY
3	D	440	VAL
3	D	836	VAL
3	D	1248	GLY
3	D	1411	GLY
4	E	4	PRO
5	F	152	ASP
3	D	303	PRO
5	F	141	VAL

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	202/273 (74%)	181 (90%)	21 (10%)	7	28
1	B	206/273 (76%)	183 (89%)	23 (11%)	6	24
2	C	941/941 (100%)	804 (85%)	137 (15%)	3	15
3	D	1264/1279 (99%)	1089 (86%)	175 (14%)	3	17
4	E	83/87 (95%)	74 (89%)	9 (11%)	6	26
5	F	306/371 (82%)	263 (86%)	43 (14%)	3	16
All	All	3002/3224 (93%)	2594 (86%)	408 (14%)	3	17

All (408) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	LYS
1	A	12	THR
1	A	55	SER
1	A	74	ASP
1	A	79	ILE
1	A	86	VAL
1	A	87	VAL
1	A	90	LEU
1	A	93	SER
1	A	94	LEU
1	A	96	THR
1	A	110	LYS
1	A	115	LEU
1	A	127	LEU
1	A	134	GLU
1	A	148	VAL
1	A	159	LYS
1	A	160	ASP
1	A	170	VAL
1	A	206	THR
1	B	5	LYS
1	B	6	LEU
1	B	12	THR
1	B	13	VAL
1	B	30	ARG

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Mol	Chain	Res	Type
1	B	48	ILE
1	B	53	VAL
1	B	54	THR
1	B	60	ASP
1	B	73	GLU
1	B	76	VAL
1	B	86	VAL
1	B	87	VAL
1	B	100	LEU
1	B	104	GLU
1	B	119	ASP
1	B	121	GLU
1	B	148	VAL
1	B	158	ILE
1	B	165	ILE
1	B	170	VAL
1	B	172	SER
1	B	189	ARG
2	C	1	MET
2	C	2	GLU
2	C	3	ILE
2	C	4	LYS
2	C	5	ARG
2	C	8	ARG
2	C	21	ILE
2	C	33	ASP
2	C	34	VAL
2	C	38	LYS
2	C	39	ARG
2	C	44	ILE
2	C	69	LEU
2	C	91	GLN
2	C	101	ILE
2	C	109	LYS
2	C	110	GLU
2	C	113	VAL
2	C	118	ILE
2	C	140	ILE
2	C	157	ARG
2	C	159	ILE
2	C	161	SER
2	C	165	LEU

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Mol	Chain	Res	Type
2	C	167	LYS
2	C	179	ASN
2	C	182	VAL
2	C	184	MET
2	C	186	VAL
2	C	202	TYR
2	C	205	GLU
2	C	221	LEU
2	C	230	ARG
2	C	233	GLU
2	C	240	THR
2	C	251	ASP
2	C	256	TYR
2	C	261	ILE
2	C	263	ASP
2	C	265	ARG
2	C	266	ARG
2	C	268	ASP
2	C	274	ARG
2	C	289	THR
2	C	290	LEU
2	C	302	VAL
2	C	304	LEU
2	C	308	ARG
2	C	317	VAL
2	C	322	VAL
2	C	325	ILE
2	C	333	ILE
2	C	335	THR
2	C	341	THR
2	C	355	VAL
2	C	365	ASP
2	C	367	LEU
2	C	372	LEU
2	C	382	ILE
2	C	391	LEU
2	C	392	SER
2	C	393	GLN
2	C	394	PHE
2	C	413	LEU
2	C	419	THR
2	C	426	ASP

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Mol	Chain	Res	Type
2	C	430	VAL
2	C	441	VAL
2	C	442	GLU
2	C	443	THR
2	C	464	LEU
2	C	469	THR
2	C	474	VAL
2	C	489	THR
2	C	503	LEU
2	C	554	ASP
2	C	559	LEU
2	C	569	VAL
2	C	572	ILE
2	C	583	LEU
2	C	584	GLU
2	C	589	ARG
2	C	592	LEU
2	C	595	LEU
2	C	600	ASP
2	C	606	VAL
2	C	610	ARG
2	C	613	VAL
2	C	616	GLU
2	C	625	LEU
2	C	627	ARG
2	C	637	LEU
2	C	640	ARG
2	C	643	VAL
2	C	645	VAL
2	C	670	GLN
2	C	672	VAL
2	C	673	LEU
2	C	674	VAL
2	C	676	ILE
2	C	683	ASN
2	C	690	ILE
2	C	699	PHE
2	C	715	THR
2	C	717	LEU
2	C	720	GLU
2	C	722	ILE
2	C	724	ARG

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Mol	Chain	Res	Type
2	C	729	LEU
2	C	736	ASP
2	C	739	GLU
2	C	740	GLU
2	C	750	LYS
2	C	754	ILE
2	C	756	VAL
2	C	768	THR
2	C	784	ASP
2	C	799	ILE
2	C	804	VAL
2	C	816	LYS
2	C	822	VAL
2	C	830	LYS
2	C	838	LYS
2	C	856	GLU
2	C	869	VAL
2	C	881	ASN
2	C	905	ILE
2	C	988	VAL
2	C	989	VAL
2	C	1000	MET
2	C	1001	VAL
2	C	1002	GLU
2	C	1004	LYS
2	C	1058	ASP
2	C	1076	VAL
2	C	1099	VAL
2	C	1113	GLU
3	D	3	LYS
3	D	5	VAL
3	D	6	ARG
3	D	10	ILE
3	D	12	LEU
3	D	20	SER
3	D	32	ILE
3	D	35	ARG
3	D	48	ARG
3	D	64	LYS
3	D	65	ARG
3	D	80	VAL
3	D	81	THR

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Mol	Chain	Res	Type
3	D	85	VAL
3	D	97	THR
3	D	108	VAL
3	D	111	LYS
3	D	126	VAL
3	D	131	LYS
3	D	141	ILE
3	D	143	ASN
3	D	152	LEU
3	D	153	LEU
3	D	156	GLU
3	D	163	TYR
3	D	171	LEU
3	D	185	VAL
3	D	186	VAL
3	D	190	GLU
3	D	191	LEU
3	D	196	VAL
3	D	199	LEU
3	D	204	LEU
3	D	211	VAL
3	D	241	ILE
3	D	252	ARG
3	D	265	GLU
3	D	270	LEU
3	D	271	VAL
3	D	311	LEU
3	D	323	GLU
3	D	334	THR
3	D	343	LYS
3	D	360	ARG
3	D	361	VAL
3	D	376	GLU
3	D	380	GLU
3	D	392	SER
3	D	399	ARG
3	D	404	GLU
3	D	406	ASP
3	D	409	VAL
3	D	411	THR
3	D	420	VAL
3	D	421	LEU

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Mol	Chain	Res	Type
3	D	427	VAL
3	D	439	LEU
3	D	440	VAL
3	D	443	VAL
3	D	444	VAL
3	D	448	GLU
3	D	478	LEU
3	D	481	MET
3	D	495	ARG
3	D	500	ARG
3	D	510	GLU
3	D	513	ILE
3	D	523	ASP
3	D	524	LEU
3	D	528	VAL
3	D	531	ASP
3	D	542	ASP
3	D	560	GLN
3	D	565	ILE
3	D	566	ILE
3	D	597	ASP
3	D	605	ASP
3	D	608	SER
3	D	619	LEU
3	D	623	VAL
3	D	624	ASP
3	D	647	ARG
3	D	650	LEU
3	D	676	MET
3	D	695	ILE
3	D	724	GLN
3	D	749	VAL
3	D	753	SER
3	D	754	PHE
3	D	769	LEU
3	D	780	LYS
3	D	784	ASP
3	D	794	GLN
3	D	796	ARG
3	D	806	PHE
3	D	813	LEU
3	D	818	ARG

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Mol	Chain	Res	Type
3	D	828	LYS
3	D	832	ARG
3	D	839	LEU
3	D	847	ASP
3	D	858	VAL
3	D	860	LEU
3	D	864	VAL
3	D	894	LYS
3	D	908	LYS
3	D	912	LYS
3	D	922	LEU
3	D	924	MET
3	D	947	ILE
3	D	951	ILE
3	D	958	GLU
3	D	968	ASP
3	D	972	LEU
3	D	984	THR
3	D	994	GLN
3	D	1035	ILE
3	D	1055	VAL
3	D	1072	ILE
3	D	1083	ASP
3	D	1084	THR
3	D	1086	LEU
3	D	1088	THR
3	D	1096	ARG
3	D	1098	LEU
3	D	1119	SER
3	D	1124	GLN
3	D	1127	GLU
3	D	1130	ARG
3	D	1131	SER
3	D	1132	LEU
3	D	1155	VAL
3	D	1159	ARG
3	D	1161	GLU
3	D	1162	GLU
3	D	1175	ILE
3	D	1188	VAL
3	D	1198	TYR
3	D	1200	VAL

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Mol	Chain	Res	Type
3	D	1209	LEU
3	D	1213	ARG
3	D	1216	SER
3	D	1221	VAL
3	D	1235	GLN
3	D	1238	MET
3	D	1269	LYS
3	D	1277	ILE
3	D	1286	THR
3	D	1288	GLU
3	D	1305	LEU
3	D	1342	GLU
3	D	1344	VAL
3	D	1357	ARG
3	D	1372	VAL
3	D	1376	MET
3	D	1388	ARG
3	D	1389	LEU
3	D	1396	GLU
3	D	1405	GLU
3	D	1425	THR
3	D	1429	LEU
3	D	1431	THR
3	D	1439	SER
3	D	1459	LEU
3	D	1460	ILE
3	D	1464	GLU
3	D	1467	ILE
3	D	1472	ILE
3	D	1481	VAL
3	D	1486	VAL
3	D	1487	VAL
3	D	1488	ASP
3	D	1490	LYS
3	D	1496	GLU
3	D	1499	ARG
4	E	32	ARG
4	E	37	ASN
4	E	40	LEU
4	E	51	LEU
4	E	52	GLU
4	E	61	GLU

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Mol	Chain	Res	Type
4	E	82	GLU
4	E	83	ASP
4	E	92	ILE
5	F	81	VAL
5	F	83	GLN
5	F	87	GLU
5	F	88	ILE
5	F	93	LEU
5	F	94	LEU
5	F	95	THR
5	F	102	LEU
5	F	107	GLU
5	F	143	HIS
5	F	157	GLU
5	F	161	GLN
5	F	203	THR
5	F	205	ARG
5	F	221	ILE
5	F	228	GLU
5	F	230	LYS
5	F	236	SER
5	F	256	ARG
5	F	260	ILE
5	F	264	MET
5	F	267	THR
5	F	277	GLN
5	F	278	LEU
5	F	279	GLN
5	F	281	GLU
5	F	284	ARG
5	F	290	GLU
5	F	302	LYS
5	F	304	VAL
5	F	313	GLU
5	F	315	VAL
5	F	324	GLU
5	F	326	ASP
5	F	327	SER
5	F	336	GLU
5	F	340	SER
5	F	341	PRO
5	F	353	GLU

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Mol	Chain	Res	Type
5	F	355	GLU
5	F	375	LEU
5	F	397	ILE
5	F	410	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	81	ASN
1	A	156	HIS
1	A	163	ASN
1	A	188	GLN
1	A	221	HIS
1	B	81	ASN
1	B	95	GLN
1	B	128	HIS
1	B	180	GLN
1	B	213	GLN
1	B	221	HIS
2	C	41	ASN
2	C	179	ASN
2	C	187	ASN
2	C	204	GLN
2	C	406	HIS
2	C	565	GLN
2	C	575	GLN
2	C	683	ASN
2	C	829	GLN
2	C	834	GLN
2	C	843	HIS
2	C	881	ASN
2	C	920	GLN
2	C	969	GLN
3	D	302	GLN
3	D	352	ASN
3	D	442	ASN
3	D	483	HIS
3	D	560	GLN
3	D	611	GLN
3	D	640	HIS
3	D	680	GLN

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Mol	Chain	Res	Type
3	D	703	ASN
3	D	714	GLN
3	D	727	GLN
3	D	729	HIS
3	D	756	GLN
3	D	845	ASN
3	D	855	HIS
3	D	906	GLN
3	D	973	GLN
3	D	994	GLN
3	D	1034	GLN
3	D	1116	ASN
3	D	1124	GLN
3	D	1195	GLN
3	D	1202	GLN
3	D	1323	GLN
3	D	1333	HIS
3	D	1359	GLN
3	D	1442	ASN
3	D	1465	ASN
4	E	28	GLN
4	E	29	GLN
4	E	33	HIS
4	E	37	ASN
4	E	86	GLN
5	F	83	GLN
5	F	175	HIS
5	F	218	GLN
5	F	254	GLN
5	F	269	ASN
5	F	277	GLN
5	F	280	GLN
5	F	312	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
6	PO4	A	401	-	4,4,4	0.89	0	6,6,6	0.69	0
7	NE6	C	1201	-	30,30,30	3.83	7 (23%)	28,39,39	2.68	6 (21%)
6	PO4	D	1603	-	4,4,4	0.97	0	6,6,6	0.31	0

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
7	NE6	C	1201	-	1/1/9/13	11/26/46/46	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1201	NE6	C11-C12	-16.72	1.33	1.49
7	C	1201	NE6	O4-C4	9.68	1.36	1.22
7	C	1201	NE6	O14-C13	4.55	1.44	1.33
7	C	1201	NE6	C5-C4	-3.76	1.39	1.46
7	C	1201	NE6	C3-C15	-2.62	1.48	1.53
7	C	1201	NE6	O2-C2	2.12	1.26	1.21
7	C	1201	NE6	C5-C6	2.00	1.40	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1201	NE6	O14-C13-N12	8.70	119.82	108.66
7	C	1201	NE6	O1-C6-C7	6.68	117.22	111.35
7	C	1201	NE6	O1-C2-O2	6.61	123.11	116.94
7	C	1201	NE6	O14-C13-O13	-2.60	115.92	122.36
7	C	1201	NE6	C21-C20-C22	2.55	119.65	115.23
7	C	1201	NE6	C2-O1-C6	2.24	123.91	120.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	1201	NE6	C3

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1201	NE6	O1-C6-C7-C8
7	C	1201	NE6	O1-C6-C7-C9
7	C	1201	NE6	C9-C10-C11-C12
7	C	1201	NE6	C3-C15-C16-C17
7	C	1201	NE6	C3-C15-C16-C18
7	C	1201	NE6	O15-C15-C16-C17
7	C	1201	NE6	C16-C18-C19-C20
7	C	1201	NE6	O15-C15-C16-C18
7	C	1201	NE6	C21-C20-C22-C23
7	C	1201	NE6	C5-C6-C7-C8
7	C	1201	NE6	C19-C20-C22-C23

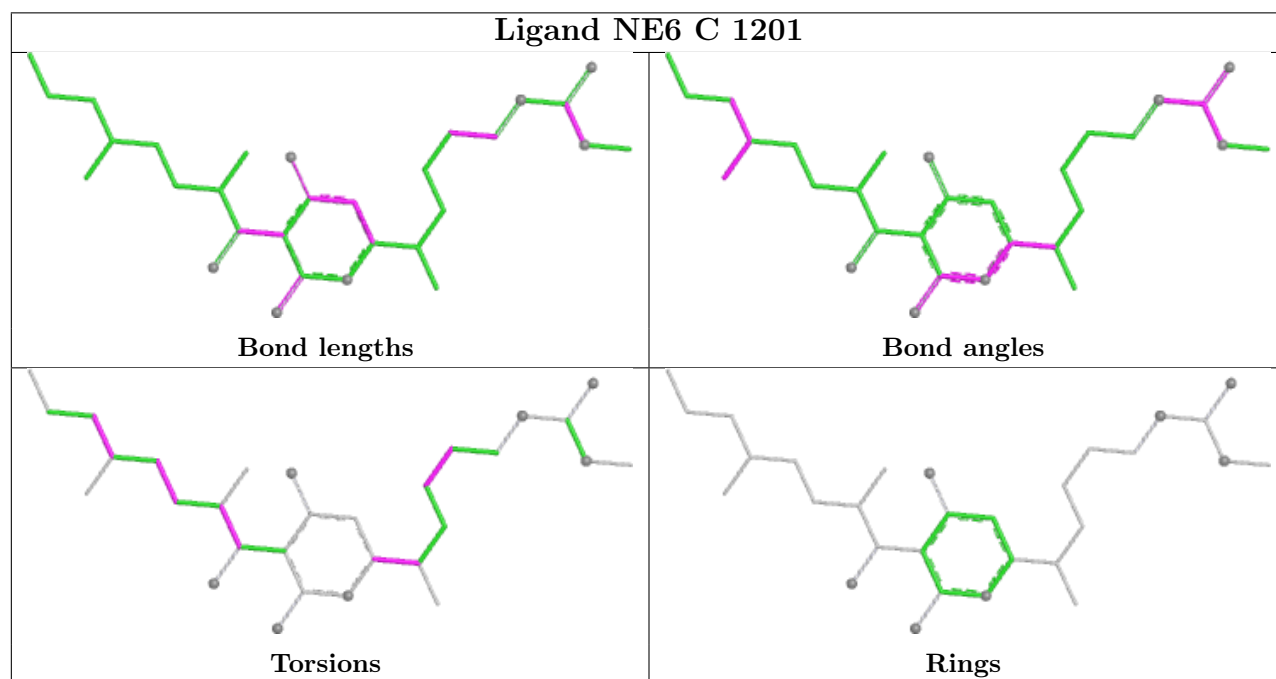
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1201	NE6	5	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	231/315 (73%)	-0.63	0 100 100	67, 96, 155, 259	0
1	B	238/315 (75%)	-0.30	3 (1%) 75 53	82, 145, 226, 248	0
2	C	1119/1119 (100%)	-0.32	18 (1%) 70 47	56, 104, 253, 323	0
3	D	1504/1524 (98%)	-0.38	21 (1%) 73 51	56, 106, 251, 301	0
4	E	95/99 (95%)	-0.37	0 100 100	82, 129, 203, 210	0
5	F	351/423 (82%)	-0.23	10 (2%) 55 32	78, 129, 236, 277	0
All	All	3538/3795 (93%)	-0.36	52 (1%) 72 49	56, 111, 246, 323	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	614	PHE	4.3
3	D	283	PHE	4.2
5	F	144	ILE	4.1
5	F	375	LEU	3.8
3	D	242	LEU	3.7
3	D	243	ALA	3.5
3	D	1247	ALA	3.3
3	D	431	VAL	3.3
2	C	269	LEU	3.1
2	C	71	TYR	3.0
3	D	225	LEU	2.9
5	F	151	LEU	2.9
3	D	492	ALA	2.8
2	C	170	PRO	2.8
2	C	165	LEU	2.7
2	C	217	LEU	2.7
5	F	73	PRO	2.7
3	D	1246	VAL	2.7
2	C	226	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	328	GLY	2.6
3	D	179	VAL	2.6
3	D	303	PRO	2.6
3	D	1248	GLY	2.5
3	D	147	VAL	2.5
2	C	289	THR	2.5
3	D	1286	THR	2.4
2	C	302	VAL	2.4
2	C	311	PHE	2.4
3	D	180	LYS	2.4
5	F	139	ALA	2.3
2	C	662	GLU	2.3
1	B	2	LEU	2.3
2	C	108	ILE	2.3
2	C	729	LEU	2.2
2	C	208	ALA	2.2
3	D	291	LEU	2.2
1	B	160	ASP	2.2
3	D	270	LEU	2.2
2	C	168	ARG	2.2
2	C	370	ALA	2.1
3	D	1393	GLN	2.1
5	F	388	ALA	2.1
5	F	374	GLY	2.1
3	D	298	VAL	2.1
2	C	196	LEU	2.1
3	D	1249	ALA	2.1
1	B	164	ALA	2.1
2	C	114	PHE	2.0
5	F	401	GLU	2.0
2	C	290	LEU	2.0
5	F	378	GLY	2.0
5	F	403	LYS	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](#)

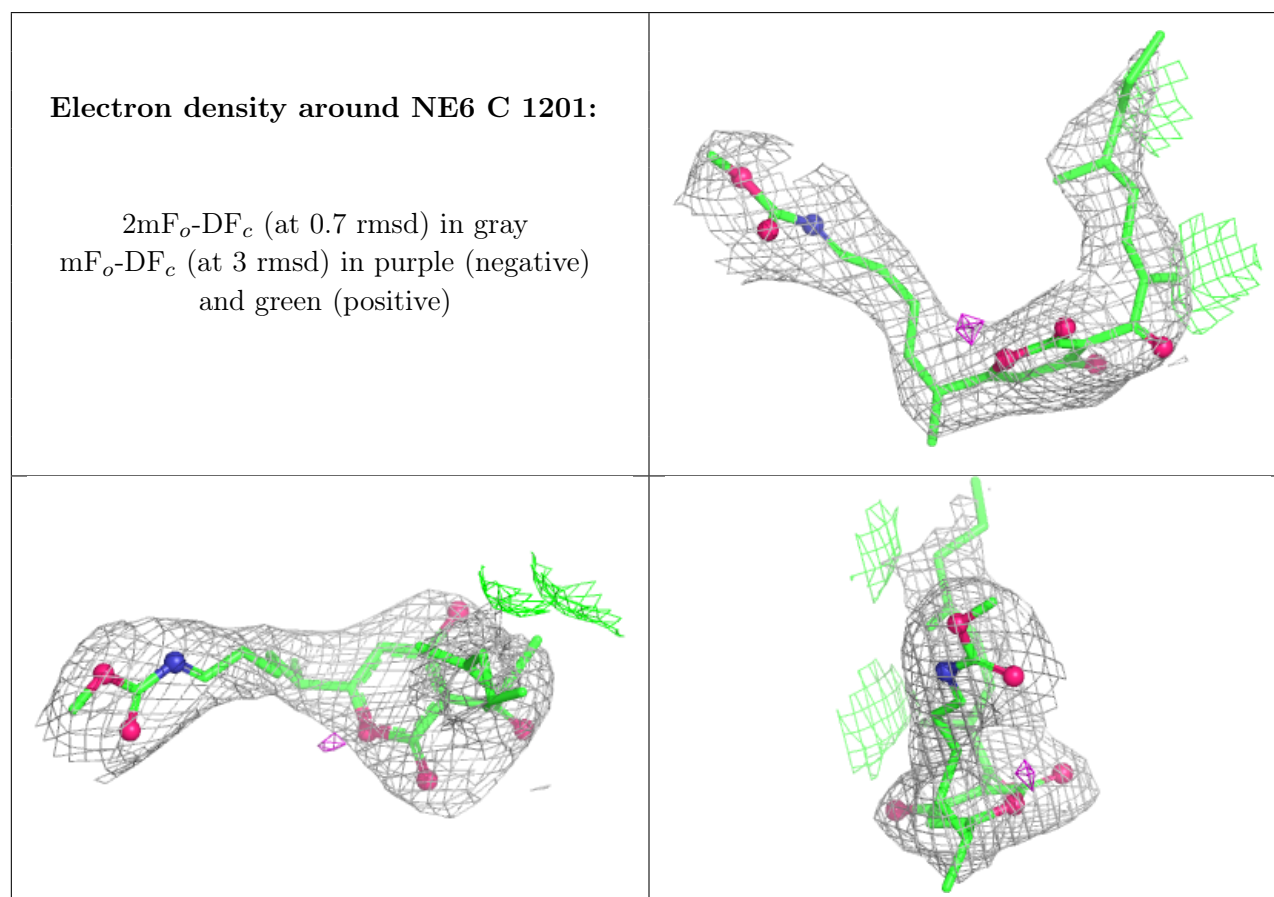
There are no oligosaccharides in this entry.

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
6	PO4	D	1603	5/5	0.78	0.16	143,144,156,163	0
9	MG	D	1604	1/1	0.84	0.26	101,101,101,101	0
6	PO4	A	401	5/5	0.95	0.10	122,124,129,130	0
9	MG	D	1605	1/1	0.95	0.07	98,98,98,98	0
7	NE6	C	1201	30/30	0.96	0.11	76,92,105,115	0
8	ZN	D	1601	1/1	1.00	0.02	104,104,104,104	0
8	ZN	D	1602	1/1	1.00	0.01	84,84,84,84	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 [i](#)

There are no such residues in this entry.