



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 PM UTC

PDB ID : 3H8A / pdb_00003h8a
Title : Crystal structure of E. coli enolase bound to its cognate RNase E recognition domain
Authors : Nurmohamed, S.; Luisi, B.F.
Deposited on : 2009-04-29
Resolution : 1.90 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

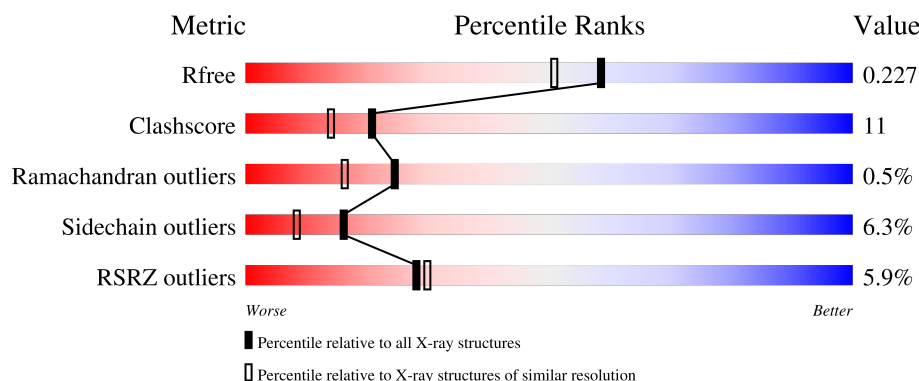
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	432	<div> <div>6%</div> <div>85% 12% .</div> </div>
1	B	432	<div> <div>6%</div> <div>78% 17% 5%</div> </div>
1	C	432	<div> <div>11%</div> <div>79% 16% .</div> </div>
1	D	432	<div> <div>4%</div> <div>80% 18% .</div> </div>
2	E	28	<div> <div>7%</div> <div>61% 36% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	28	<div><div></div><div>25%</div><div>46%</div><div>39%</div><div>•</div><div>11%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14368 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3187	2000	544	630	13			
1	B	430	Total	C	N	O	S	0	0	0
			3178	1992	541	632	13			
1	C	430	Total	C	N	O	S	0	0	0
			3186	1997	544	632	13			
1	D	431	Total	C	N	O	S	0	0	0
			3163	1980	541	629	13			

- Molecule 2 is a protein called RNase E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	28	Total	C	N	O	S	0	0	0
			213	139	37	36	1			
2	F	25	Total	C	N	O	S	0	0	0
			187	122	31	33	1			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	382	Total	O	0	0
			382	382		
4	B	268	Total	O	0	0
			268	268		

Continued on next page...

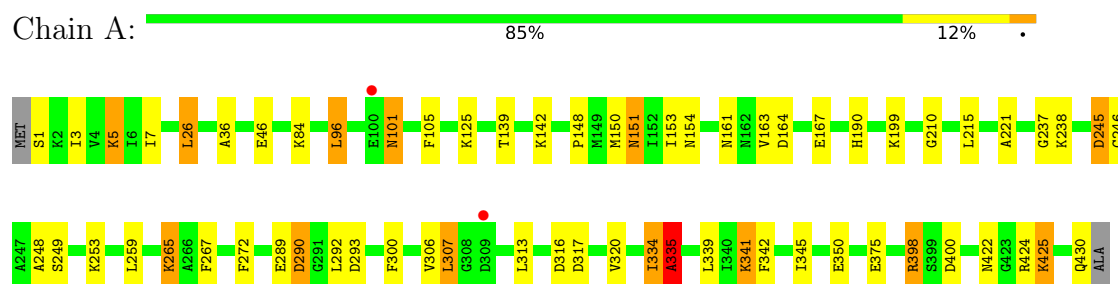
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	247	Total 247	O 247	0	0
4	D	293	Total 293	O 293	0	0
4	E	34	Total 34	O 34	0	0
4	F	28	Total 28	O 28	0	0

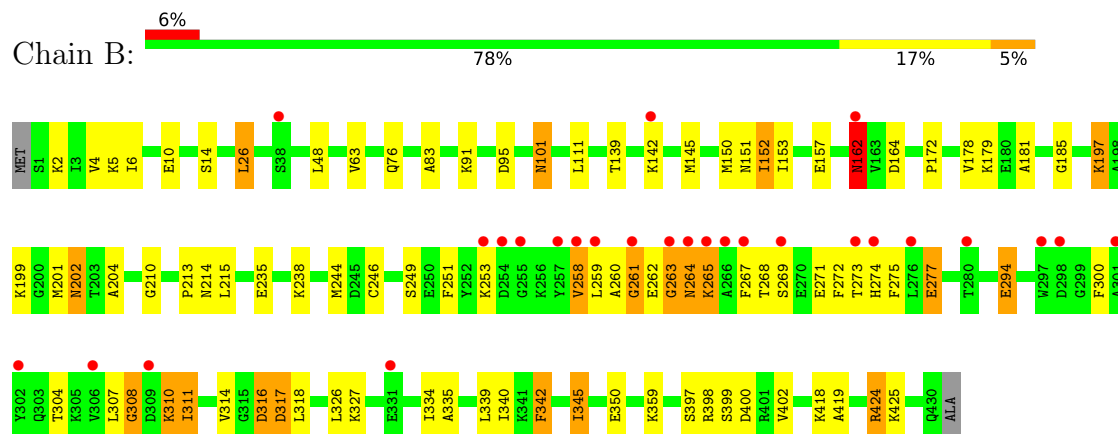
3 Residue-property plots

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.

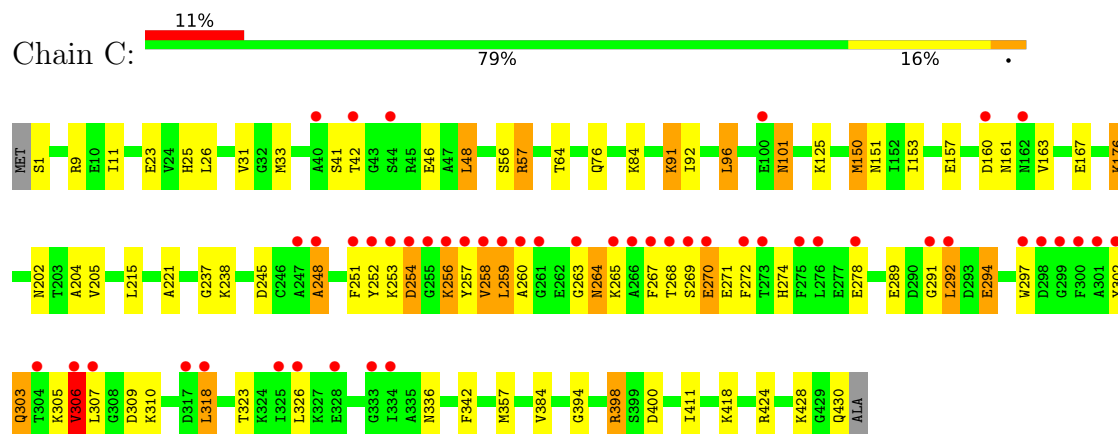
• Molecule 1: Enolase



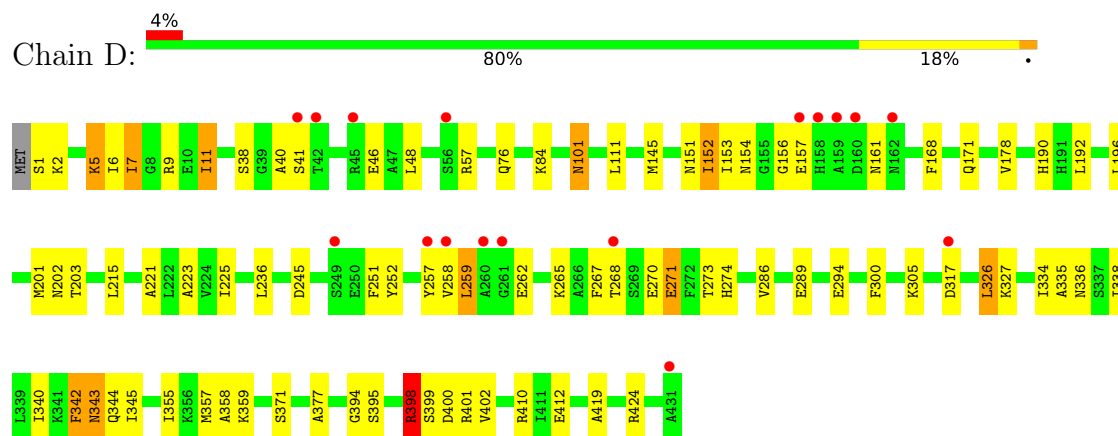
• Molecule 1: Enolase



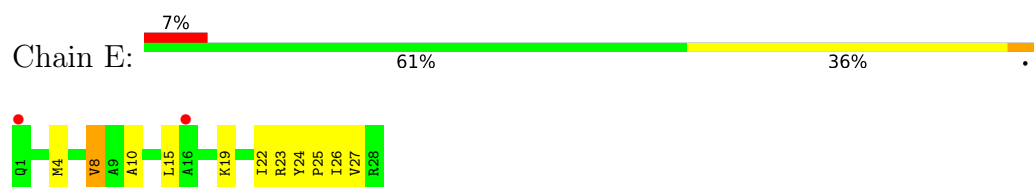
• Molecule 1: Enolase



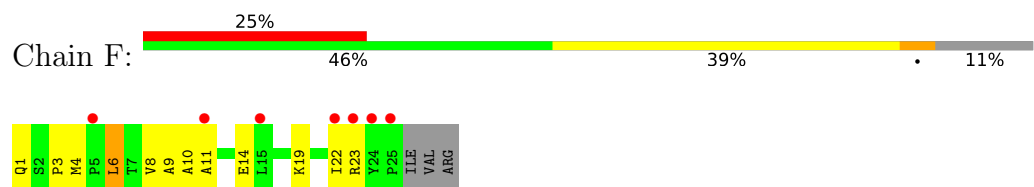
- Molecule 1: Enolase



- Molecule 2: RNase E



- Molecule 2: RNase E



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.88Å 110.21Å 160.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 1.90 24.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.89-1.90) 99.3 (24.89-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.226 0.183 , 0.227	Depositor DCC
R_{free} test set	7228 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14368	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.20	18/3232 (0.6%)	0.97	2/4354 (0.0%)
1	B	1.14	8/3220 (0.2%)	1.03	7/4340 (0.2%)
1	C	1.19	5/3228 (0.2%)	1.04	10/4348 (0.2%)
1	D	1.22	17/3204 (0.5%)	1.03	6/4322 (0.1%)
2	E	1.16	0/219	0.91	0/300
2	F	1.59	4/193 (2.1%)	1.15	0/265
All	All	1.19	52/13296 (0.4%)	1.02	25/17929 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	336	ASN	C-O	-9.79	1.16	1.23
1	D	336	ASN	C-O	-7.78	1.15	1.24
1	A	153	ILE	C-O	-7.21	1.16	1.24
1	B	153	ILE	C-O	-7.09	1.17	1.24
1	D	57	ARG	C-O	-7.05	1.16	1.24
1	B	152	ILE	C-O	-6.83	1.16	1.24
1	B	397	SER	C-O	-6.83	1.15	1.23
1	A	161	ASN	C-O	-6.73	1.15	1.23
1	D	394	GLY	C-O	-6.65	1.17	1.23
1	A	246	CYS	C-O	-6.57	1.15	1.24
1	D	342	PHE	C-O	-6.25	1.16	1.24
1	A	163	VAL	C-O	-6.23	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	PHE	C-O	-6.20	1.16	1.24
1	A	320	VAL	C-O	-6.19	1.16	1.24
1	C	153	ILE	C-O	-6.17	1.17	1.24
1	D	38	SER	C-O	-6.16	1.16	1.23
1	D	271	GLU	C-O	-6.14	1.16	1.24
1	A	245	ASP	C-O	-6.12	1.17	1.24
1	D	340	ILE	C-O	-6.09	1.17	1.24
1	A	139	THR	CA-CB	6.03	1.60	1.53
1	A	334	ILE	C-O	-5.98	1.17	1.24
1	C	150	MET	C-O	-5.97	1.17	1.24
1	A	341	LYS	C-O	-5.95	1.17	1.23
1	A	151	ASN	C-O	-5.89	1.16	1.23
2	F	6	LEU	C-O	-5.78	1.17	1.24
1	D	358	ALA	C-O	-5.76	1.17	1.24
1	A	398	ARG	C-O	-5.73	1.16	1.24
1	A	317	ASP	C-O	-5.72	1.17	1.24
1	D	11	ILE	C-O	-5.67	1.17	1.24
2	F	11	ALA	C-O	-5.65	1.17	1.24
1	A	290	ASP	C-O	-5.61	1.16	1.23
1	B	340	ILE	C-O	-5.61	1.17	1.24
1	D	152	ILE	CA-C	5.60	1.58	1.52
2	F	14	GLU	C-O	-5.58	1.17	1.24
1	D	274	HIS	C-O	-5.50	1.17	1.24
1	C	398	ARG	C-O	-5.46	1.17	1.24
1	A	154	ASN	C-O	-5.44	1.17	1.24
1	B	345	ILE	C-O	-5.44	1.17	1.23
1	B	14	SER	C-O	-5.35	1.17	1.24
1	D	335	ALA	C-O	-5.35	1.17	1.24
1	A	335	ALA	C-O	-5.34	1.17	1.24
1	D	343	ASN	C-O	-5.25	1.17	1.24
1	D	398	ARG	C-O	-5.21	1.17	1.24
2	F	4	MET	C-O	-5.15	1.18	1.23
1	B	316	ASP	C-O	-5.14	1.17	1.24
1	A	46	GLU	C-O	-5.11	1.17	1.23
1	C	151	ASN	C-O	-5.09	1.17	1.23
1	D	377	ALA	CA-CB	5.08	1.60	1.53
1	A	292	LEU	C-O	-5.04	1.17	1.23
1	D	345	ILE	C-O	-5.03	1.17	1.24
1	D	152	ILE	C-O	-5.01	1.18	1.23
1	A	248	ALA	CA-CB	-5.00	1.44	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	LYS	N-CA-C	-9.19	101.22	111.14
1	D	161	ASN	N-CA-CB	8.94	125.37	111.24
1	C	306	VAL	N-CA-C	8.41	118.98	110.23
1	D	161	ASN	N-CA-C	-8.25	97.24	108.38
1	C	394	GLY	N-CA-C	6.90	119.08	112.04
1	B	265	LYS	N-CA-C	-6.70	100.11	110.10
1	B	258	VAL	N-CA-C	6.38	116.81	107.37
1	B	162	ASN	N-CA-C	5.68	118.98	112.57
1	B	263	GLY	N-CA-C	-5.61	108.13	115.47
1	D	394	GLY	N-CA-C	5.59	118.86	111.70
1	B	314	VAL	N-CA-C	5.57	116.75	108.23
1	C	205	VAL	N-CA-C	5.55	117.81	109.20
1	A	36	ALA	CA-C-N	-5.43	114.99	120.21
1	A	36	ALA	C-N-CA	-5.43	114.99	120.21
1	D	157	GLU	N-CA-C	5.36	119.67	113.18
1	C	161	ASN	N-CA-CB	5.33	119.29	110.97
1	C	303	GLN	N-CA-C	5.32	117.77	111.33
1	C	258	VAL	N-CA-C	5.30	115.48	107.80
1	C	160	ASP	N-CA-C	-5.23	95.51	107.48
1	C	163	VAL	CA-C-N	5.20	129.39	120.71
1	C	163	VAL	C-N-CA	5.20	129.39	120.71
1	B	264	ASN	N-CA-C	-5.18	106.91	113.23
1	D	273	THR	N-CA-C	5.12	117.26	111.11
1	D	223	ALA	N-CA-C	5.11	116.54	111.07
1	B	308	GLY	N-CA-C	5.08	120.03	113.27

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	156	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3187	0	3212	33	0
1	B	3178	0	3180	73	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3186	0	3205	84	0
1	D	3163	0	3152	94	0
2	E	213	0	227	13	0
2	F	187	0	194	21	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	382	0	0	5	0
4	B	268	0	0	6	0
4	C	247	0	0	9	0
4	D	293	0	0	11	0
4	E	34	0	0	2	0
4	F	28	0	0	3	0
All	All	14368	0	13170	292	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 11.

All (292) 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:B:268:THR:CG2	1:B:271:GLU:HG3	1.35	1.54
1:C:33:MET:HE3	2:F:9:ALA:CB	1.55	1.34
1:C:33:MET:CE	2:F:9:ALA:HB3	1.58	1.31
1:C:302:TYR:O	1:C:306:VAL:HG23	1.39	1.22
1:B:268:THR:HG22	1:B:271:GLU:CG	1.73	1.17
1:D:5:LYS:HZ1	2:F:23:ARG:CD	1.62	1.12
1:C:259:LEU:N	1:C:259:LEU:HD23	1.63	1.09
1:B:268:THR:CG2	1:B:271:GLU:CG	2.30	1.07
1:C:323:THR:HA	1:C:357:MET:HE1	1.38	1.05
1:D:327:LYS:CB	1:D:357:MET:HE1	1.89	1.03
1:B:268:THR:HG23	1:B:271:GLU:H	1.24	1.00
1:B:268:THR:HG22	1:B:271:GLU:HG3	0.99	0.99
1:C:326:LEU:HD23	1:C:357:MET:HE3	1.43	0.97
1:D:101:ASN:HD22	1:D:101:ASN:H	1.02	0.97
1:C:258:VAL:C	1:C:259:LEU:HD23	1.89	0.97
1:D:327:LYS:HA	1:D:357:MET:HE2	1.43	0.97
1:C:259:LEU:N	1:C:259:LEU:CD2	2.30	0.95
1:B:5:LYS:HZ1	2:E:23:ARG:HG3	1.34	0.91
1:D:152:ILE:HG13	4:D:737:HOH:O	1.71	0.89
1:B:5:LYS:NZ	2:E:23:ARG:HG3	1.87	0.89
1:A:422:ASN:HB3	1:A:425:LYS:HD3	1.54	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:LYS:CA	1:D:357:MET:CE	2.51	0.88
1:C:33:MET:HE3	2:F:9:ALA:HB3	0.89	0.88
1:D:5:LYS:HE2	1:D:7:ILE:HD11	1.53	0.88
1:D:327:LYS:HA	1:D:357:MET:CE	2.03	0.88
1:D:5:LYS:CD	1:D:7:ILE:HD11	2.04	0.86
1:D:268:THR:HG23	1:D:271:GLU:H	1.41	0.86
1:B:268:THR:HG21	1:B:271:GLU:HG3	1.53	0.85
1:D:399:SER:HA	1:D:402:VAL:HG22	1.58	0.84
1:D:5:LYS:HZ1	2:F:23:ARG:HD2	1.39	0.84
1:D:5:LYS:HB3	1:D:5:LYS:HZ3	1.42	0.84
1:D:252:TYR:CD1	1:D:257:TYR:CE1	2.65	0.83
1:C:270:GLU:O	1:C:274:HIS:HD2	1.60	0.83
1:B:277:GLU:HG3	1:B:307:LEU:HD21	1.59	0.83
1:D:101:ASN:HB3	4:D:613:HOH:O	1.79	0.83
1:C:270:GLU:O	1:C:274:HIS:CD2	2.32	0.82
1:D:5:LYS:CE	1:D:7:ILE:HD11	2.09	0.82
1:D:327:LYS:CA	1:D:357:MET:HE1	2.11	0.81
1:D:5:LYS:NZ	2:F:23:ARG:CD	2.43	0.81
1:D:327:LYS:CB	1:D:357:MET:CE	2.59	0.81
1:B:268:THR:HG23	1:B:271:GLU:HG3	1.59	0.80
1:C:424:ARG:HH11	1:C:430:GLN:NE2	1.79	0.80
1:C:91:LYS:HD3	4:C:902:HOH:O	1.81	0.79
1:D:268:THR:HG22	1:D:271:GLU:HB2	1.64	0.78
1:B:263:GLY:O	1:B:264:ASN:HB3	1.84	0.78
1:D:101:ASN:HD22	1:D:101:ASN:N	1.81	0.78
1:D:252:TYR:CD1	1:D:257:TYR:CZ	2.72	0.78
1:C:258:VAL:C	1:C:259:LEU:CD2	2.59	0.76
1:C:326:LEU:CD2	1:C:357:MET:HE3	2.16	0.75
1:D:5:LYS:NZ	2:F:23:ARG:NE	2.35	0.75
1:D:101:ASN:H	1:D:101:ASN:ND2	1.80	0.74
1:D:327:LYS:CA	1:D:357:MET:HE2	2.14	0.73
1:B:76:GLN:HE22	1:D:6:ILE:H	1.38	0.72
1:C:310:LYS:HG3	4:C:1265:HOH:O	1.90	0.72
1:C:31:VAL:HG11	2:F:6:LEU:HD12	1.73	0.70
1:C:326:LEU:HB3	1:C:357:MET:HE3	1.72	0.70
1:B:6:ILE:H	1:D:76:GLN:HE22	1.39	0.70
1:D:5:LYS:HD2	1:D:7:ILE:CD1	2.22	0.70
1:B:277:GLU:CG	1:B:307:LEU:HD21	2.21	0.70
1:D:5:LYS:HZ1	2:F:23:ARG:NE	1.88	0.69
1:C:33:MET:HE3	2:F:9:ALA:HB1	1.70	0.69
1:C:424:ARG:NH1	1:C:430:GLN:NE2	2.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:THR:HG22	1:D:271:GLU:CB	2.22	0.68
1:B:268:THR:HG22	1:B:271:GLU:CD	2.17	0.68
1:D:5:LYS:HB3	1:D:5:LYS:NZ	2.08	0.68
1:B:5:LYS:HD2	4:D:456:HOH:O	1.93	0.68
1:D:1:SER:OG	1:D:84:LYS:HD2	1.93	0.68
1:C:326:LEU:HD23	1:C:357:MET:CE	2.22	0.68
1:C:302:TYR:O	1:C:306:VAL:CG2	2.30	0.68
1:B:202:ASN:ND2	1:B:204:ALA:H	1.91	0.67
1:C:323:THR:CA	1:C:357:MET:HE1	2.20	0.67
1:C:176:LYS:HE2	1:C:176:LYS:HA	1.75	0.67
1:C:323:THR:HG22	1:C:357:MET:HE2	1.76	0.67
1:D:5:LYS:CD	1:D:7:ILE:CD1	2.72	0.67
1:C:323:THR:HA	1:C:357:MET:CE	2.21	0.67
1:A:1:SER:OG	1:A:84:LYS:HE3	1.96	0.66
1:C:294:GLU:C	1:C:294:GLU:CD	2.64	0.66
1:B:399:SER:HA	1:B:402:VAL:HG22	1.77	0.66
1:B:264:ASN:ND2	1:B:264:ASN:O	2.29	0.65
1:C:318:LEU:HD12	1:C:318:LEU:C	2.21	0.65
1:C:263:GLY:O	1:C:265:LYS:N	2.30	0.65
2:E:4:MET:HE2	2:E:15:LEU:HD22	1.78	0.65
1:C:91:LYS:HE3	4:C:902:HOH:O	1.96	0.64
1:D:268:THR:HG22	1:D:271:GLU:CG	2.28	0.64
1:C:252:TYR:CD1	1:C:257:TYR:CE1	2.86	0.64
1:B:310:LYS:HB2	1:B:311:ILE:HD12	1.79	0.63
1:A:306:VAL:HG12	1:A:307:LEU:HD13	1.80	0.63
1:D:5:LYS:NZ	1:D:5:LYS:CB	2.61	0.63
1:C:326:LEU:HB3	1:C:357:MET:CE	2.29	0.62
1:C:263:GLY:C	1:C:265:LYS:N	2.58	0.61
1:D:259:LEU:HB3	1:D:262:GLU:HB2	1.83	0.61
1:A:5:LYS:HE2	1:A:7:ILE:HD11	1.83	0.61
1:C:318:LEU:HD12	1:C:318:LEU:O	2.01	0.60
1:B:6:ILE:H	1:D:76:GLN:NE2	1.99	0.60
1:C:259:LEU:HD11	1:C:272:PHE:HE1	1.66	0.60
1:B:235:GLU:HG3	1:B:238:LYS:HB3	1.84	0.59
1:A:265:LYS:HD2	1:A:267:PHE:CZ	2.36	0.59
1:D:252:TYR:HD1	1:D:257:TYR:CE1	2.21	0.58
1:C:424:ARG:HH11	1:C:430:GLN:HE21	1.49	0.58
1:B:260:ALA:O	1:B:262:GLU:N	2.37	0.58
4:C:436:HOH:O	1:D:402:VAL:HG23	2.03	0.58
1:D:268:THR:HG23	1:D:271:GLU:N	2.17	0.58
1:A:151:ASN:ND2	1:A:210:GLY:HA3	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:THR:HG22	1:D:271:GLU:CD	2.28	0.57
1:A:345:ILE:HG12	1:A:350:GLU:HB3	1.86	0.57
1:C:263:GLY:C	1:C:265:LYS:H	2.12	0.57
1:D:268:THR:CG2	1:D:271:GLU:H	2.14	0.57
1:C:23:GLU:OE1	1:C:33:MET:HE2	2.03	0.57
1:A:345:ILE:HD13	4:A:509:HOH:O	2.05	0.57
1:D:251:PHE:O	1:D:257:TYR:HA	2.05	0.57
1:C:257:TYR:O	1:C:267:PHE:HB2	2.04	0.56
1:C:33:MET:CE	2:F:9:ALA:CB	2.42	0.56
1:D:265:LYS:HG2	1:D:267:PHE:CE1	2.40	0.56
2:F:8:VAL:HG12	4:F:899:HOH:O	2.05	0.56
1:B:76:GLN:NE2	1:D:6:ILE:H	2.05	0.56
1:B:317:ASP:CG	4:B:1062:HOH:O	2.48	0.55
1:C:46:GLU:O	1:C:48:LEU:HD13	2.06	0.55
1:B:5:LYS:NZ	4:B:1228:HOH:O	2.39	0.55
1:C:91:LYS:HA	1:C:91:LYS:HZ3	1.72	0.55
2:E:10:ALA:HA	4:E:1233:HOH:O	2.07	0.54
1:D:251:PHE:HB2	1:D:258:VAL:O	2.08	0.54
1:B:202:ASN:HD21	1:B:204:ALA:HB3	1.72	0.54
1:C:91:LYS:CE	4:C:902:HOH:O	2.55	0.54
1:D:355:ILE:HG22	1:D:359:LYS:HD2	1.89	0.54
1:B:244:MET:HE2	1:B:246:CYS:SG	2.48	0.54
1:D:152:ILE:HG23	1:D:153:ILE:HG12	1.90	0.54
1:D:190:HIS:HD2	4:D:479:HOH:O	1.91	0.54
1:B:150:MET:HE1	1:B:185:GLY:HA3	1.89	0.53
1:B:145:MET:HE2	1:B:178:VAL:HG11	1.90	0.53
1:C:91:LYS:NZ	1:C:91:LYS:CB	2.61	0.53
1:B:262:GLU:C	1:B:264:ASN:H	2.14	0.53
1:D:5:LYS:HD3	4:D:750:HOH:O	2.07	0.53
1:B:251:PHE:HB2	1:B:258:VAL:O	2.09	0.53
2:F:3:PRO:HG2	2:F:22:ILE:HD13	1.91	0.53
1:C:326:LEU:CG	1:C:357:MET:HE3	2.39	0.53
1:B:267:PHE:N	1:B:267:PHE:CD1	2.76	0.53
1:B:268:THR:CG2	1:B:271:GLU:H	2.10	0.53
1:C:23:GLU:OE2	1:C:25:HIS:HE1	1.92	0.53
1:D:7:ILE:N	1:D:7:ILE:HD13	2.24	0.52
1:C:310:LYS:CG	4:C:1265:HOH:O	2.52	0.52
1:B:101:ASN:H	1:B:101:ASN:HD22	1.58	0.52
1:C:202:ASN:HD21	1:C:204:ALA:HB3	1.75	0.52
1:B:164:ASP:OD2	1:B:261:GLY:HA3	2.09	0.51
1:D:424:ARG:HD2	4:D:653:HOH:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:ARG:O	2:E:26:ILE:HD13	2.10	0.51
1:D:252:TYR:CE1	1:D:257:TYR:CZ	2.97	0.51
1:C:251:PHE:N	1:C:251:PHE:CD2	2.78	0.51
1:A:339:LEU:HD23	1:A:341:LYS:HE3	1.92	0.51
1:C:167:GLU:HG2	1:C:245:ASP:HB3	1.93	0.50
2:E:22:ILE:CG2	2:E:26:ILE:HD11	2.42	0.50
1:B:263:GLY:O	1:B:264:ASN:CB	2.52	0.50
1:C:326:LEU:CB	1:C:357:MET:HE3	2.40	0.50
1:D:399:SER:HA	1:D:402:VAL:CG2	2.37	0.50
1:B:162:ASN:ND2	1:B:261:GLY:HA2	2.26	0.50
1:C:76:GLN:NE2	4:C:579:HOH:O	2.45	0.50
1:C:245:ASP:HA	1:C:289:GLU:HB3	1.94	0.50
2:F:10:ALA:HA	4:F:511:HOH:O	2.12	0.50
1:C:268:THR:H	1:C:271:GLU:HB2	1.76	0.49
1:B:179:LYS:NZ	4:B:778:HOH:O	2.43	0.49
1:B:294:GLU:HB3	1:B:318:LEU:HA	1.94	0.49
1:C:101:ASN:HD22	1:C:101:ASN:H	1.60	0.49
1:D:252:TYR:HD1	1:D:257:TYR:CD1	2.30	0.49
1:C:259:LEU:O	1:C:260:ALA:C	2.55	0.49
1:C:294:GLU:OE2	1:C:294:GLU:O	2.30	0.49
1:A:430:GLN:C	4:A:1166:HOH:O	2.56	0.49
1:D:5:LYS:HZ1	2:F:23:ARG:HD3	1.67	0.49
4:A:540:HOH:O	2:E:8:VAL:HB	2.13	0.48
1:B:260:ALA:C	1:B:262:GLU:N	2.71	0.48
1:A:190:HIS:HD2	4:A:446:HOH:O	1.96	0.48
1:B:139:THR:HB	1:B:142:LYS:HD2	1.94	0.48
1:B:249:SER:HB3	4:B:764:HOH:O	2.12	0.48
1:A:148:PRO:HG2	1:A:150:MET:HE3	1.96	0.48
2:E:23:ARG:HA	4:E:419:HOH:O	2.13	0.48
1:D:294:GLU:OE2	1:D:317:ASP:OD1	2.32	0.48
1:B:162:ASN:HD22	1:B:261:GLY:HA2	1.79	0.48
1:C:248:ALA:HA	1:C:251:PHE:CZ	2.48	0.48
1:C:268:THR:O	1:C:269:SER:C	2.57	0.48
2:E:24:TYR:HA	2:E:25:PRO:C	2.39	0.48
1:A:375:GLU:O	2:E:19:LYS:NZ	2.46	0.48
1:D:202:ASN:HD22	1:D:203:THR:H	1.62	0.48
1:C:253:LYS:O	1:C:254:ASP:C	2.57	0.47
1:D:252:TYR:HB2	1:D:257:TYR:CD1	2.48	0.47
1:B:268:THR:O	1:B:269:SER:C	2.53	0.47
1:D:215:LEU:HD13	1:D:221:ALA:HA	1.95	0.47
1:C:33:MET:HE1	2:F:9:ALA:HB3	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:LEU:HG	1:D:338:ILE:HD12	1.95	0.47
1:A:3:ILE:HA	1:A:26:LEU:HD12	1.96	0.47
1:D:152:ILE:HG12	1:D:192:LEU:CD2	2.44	0.47
1:D:259:LEU:HD22	1:D:267:PHE:CE1	2.49	0.47
1:D:7:ILE:CD1	1:D:7:ILE:N	2.77	0.47
1:D:300:PHE:HB3	1:D:334:ILE:HG23	1.96	0.47
1:B:145:MET:HG2	1:B:419:ALA:O	2.15	0.47
1:B:300:PHE:HB3	1:B:334:ILE:HG23	1.96	0.47
1:C:31:VAL:CG1	2:F:6:LEU:HD12	2.42	0.47
1:B:300:PHE:CE2	1:B:318:LEU:HD13	2.50	0.47
1:D:152:ILE:CB	4:D:737:HOH:O	2.61	0.47
1:D:9:ARG:HG3	1:D:11:ILE:HG23	1.97	0.46
1:B:199:LYS:HD2	1:B:201:MET:HE2	1.96	0.46
1:B:424:ARG:HD2	4:B:744:HOH:O	2.14	0.46
1:B:151:ASN:ND2	1:B:210:GLY:HA3	2.30	0.46
1:D:41:SER:O	4:D:557:HOH:O	2.20	0.46
1:B:202:ASN:HD21	1:B:204:ALA:CB	2.29	0.46
1:C:237:GLY:O	1:C:424:ARG:NH2	2.49	0.46
1:D:152:ILE:CG2	1:D:153:ILE:N	2.78	0.46
1:A:167:GLU:HG2	1:A:245:ASP:HB3	1.97	0.46
1:C:263:GLY:O	1:C:264:ASN:C	2.57	0.46
1:B:264:ASN:O	1:B:265:LYS:C	2.57	0.46
1:B:172:PRO:HG2	1:B:181:ALA:HB1	1.98	0.46
1:D:152:ILE:HG21	1:D:225:ILE:HG12	1.98	0.46
1:C:84:LYS:HE2	1:C:125:LYS:HG3	1.98	0.45
1:D:259:LEU:HD22	1:D:267:PHE:CD1	2.51	0.45
1:A:151:ASN:HD22	1:A:210:GLY:HA3	1.81	0.45
1:A:300:PHE:HB3	1:A:334:ILE:HG23	1.98	0.45
1:B:4:VAL:HG11	2:E:27:VAL:HG11	1.99	0.45
1:B:345:ILE:HG12	1:B:350:GLU:HB3	1.98	0.45
1:D:5:LYS:HZ2	2:F:23:ARG:NE	2.13	0.45
1:D:152:ILE:HG22	1:D:168:PHE:O	2.16	0.45
1:D:5:LYS:NZ	2:F:23:ARG:HD3	2.29	0.45
1:A:259:LEU:HD11	1:A:272:PHE:HE1	1.81	0.45
1:D:202:ASN:HD22	1:D:203:THR:N	2.15	0.45
1:A:245:ASP:HA	1:A:289:GLU:HB3	1.98	0.45
1:C:268:THR:O	1:C:271:GLU:N	2.49	0.45
1:B:262:GLU:C	1:B:264:ASN:N	2.72	0.45
1:C:310:LYS:HB2	4:C:1265:HOH:O	2.16	0.45
1:D:46:GLU:CD	1:D:344:GLN:HG2	2.42	0.45
1:C:256:LYS:HB3	1:C:256:LYS:HE3	1.53	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:THR:HG22	1:C:357:MET:CE	2.45	0.45
1:A:237:GLY:O	1:A:424:ARG:NH1	2.46	0.45
1:D:317:ASP:CG	4:D:490:HOH:O	2.60	0.44
1:A:84:LYS:HE2	1:A:125:LYS:CG	2.47	0.44
1:B:202:ASN:HD22	1:B:204:ALA:H	1.63	0.44
1:A:84:LYS:HE2	1:A:125:LYS:HG3	1.98	0.44
1:B:260:ALA:C	1:B:262:GLU:H	2.24	0.44
1:C:291:GLY:O	1:C:292:LEU:HD13	2.17	0.44
1:D:152:ILE:CG1	4:D:737:HOH:O	2.47	0.44
1:A:345:ILE:CG1	1:A:350:GLU:HB3	2.48	0.44
1:C:292:LEU:HD13	1:C:303:GLN:HE22	1.83	0.44
1:D:327:LYS:N	1:D:357:MET:HE1	2.32	0.44
1:A:101:ASN:HD22	1:A:101:ASN:H	1.64	0.44
1:C:252:TYR:HD1	1:C:257:TYR:CE1	2.31	0.44
1:D:327:LYS:N	1:D:357:MET:CE	2.81	0.43
1:B:197:LYS:HB3	1:B:197:LYS:HE3	1.73	0.43
1:B:5:LYS:HZ3	2:E:23:ARG:HG3	1.76	0.43
1:D:2:LYS:HG2	4:D:1029:HOH:O	2.18	0.43
1:D:259:LEU:CD2	1:D:267:PHE:CE1	3.02	0.43
1:A:164:ASP:OD2	1:A:259:LEU:HB3	2.19	0.43
1:D:151:ASN:O	1:D:395:SER:HB2	2.19	0.43
1:C:1:SER:OG	1:C:84:LYS:HE3	2.18	0.43
2:F:19:LYS:HE3	4:F:106:HOH:O	2.18	0.43
1:C:91:LYS:HZ2	1:C:91:LYS:HG3	1.16	0.43
1:C:92:ILE:O	1:C:96:LEU:HB2	2.18	0.43
1:A:249:SER:HB2	1:A:293:ASP:OD1	2.18	0.43
1:C:259:LEU:HD11	1:C:272:PHE:CE1	2.49	0.42
1:C:292:LEU:HD13	1:C:303:GLN:NE2	2.34	0.42
1:C:297:TRP:N	1:C:297:TRP:CD1	2.85	0.42
1:D:196:LEU:HD23	1:D:201:MET:HE3	2.01	0.42
1:C:57:ARG:NH2	1:C:64:THR:HG23	2.34	0.42
1:B:260:ALA:O	1:B:261:GLY:C	2.60	0.42
1:C:84:LYS:HE2	1:C:125:LYS:CG	2.50	0.42
4:C:436:HOH:O	1:D:402:VAL:CG2	2.64	0.42
1:D:145:MET:HG2	1:D:419:ALA:O	2.19	0.42
1:D:171:GLN:HE22	1:D:286:VAL:CG2	2.33	0.42
1:D:398:ARG:HH11	1:D:398:ARG:HD2	1.67	0.42
1:B:26:LEU:HD11	1:B:83:ALA:HB2	2.01	0.42
1:C:101:ASN:H	1:C:101:ASN:ND2	2.17	0.42
1:A:422:ASN:O	1:A:425:LYS:HD2	2.20	0.42
1:B:274:HIS:HA	1:B:277:GLU:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ASP:HA	1:D:289:GLU:HB3	2.02	0.42
2:E:4:MET:HG2	2:E:4:MET:O	2.20	0.42
1:B:294:GLU:H	1:B:294:GLU:HG3	1.50	0.41
1:B:272:PHE:O	1:B:275:PHE:HB3	2.21	0.41
1:A:215:LEU:HD13	1:A:221:ALA:HA	2.02	0.41
1:B:304:THR:O	1:B:308:GLY:HA3	2.20	0.41
1:D:152:ILE:HG23	1:D:153:ILE:N	2.35	0.41
1:A:339:LEU:HD12	1:A:339:LEU:HA	1.90	0.41
1:D:252:TYR:CD1	1:D:257:TYR:CD1	3.05	0.41
1:C:9:ARG:HG3	1:C:11:ILE:HG23	2.02	0.41
1:D:178:VAL:HG12	1:D:412:GLU:CD	2.46	0.41
1:A:96:LEU:HD13	1:A:105:PHE:CZ	2.56	0.41
1:D:40:ALA:H	1:D:371:SER:HB2	1.85	0.41
1:A:199:LYS:HB3	1:A:199:LYS:HE3	1.94	0.41
1:A:290:ASP:OD2	1:A:316:ASP:HB3	2.21	0.41
1:B:294:GLU:HG3	4:B:764:HOH:O	2.20	0.41
1:A:313:LEU:O	1:A:335:ALA:HB1	2.20	0.40
4:A:435:HOH:O	1:B:402:VAL:HG23	2.19	0.40
1:B:316:ASP:HB2	1:B:339:LEU:HD22	2.02	0.40
1:D:410:ARG:HB3	2:F:10:ALA:HB2	2.02	0.40
1:C:384:VAL:HG11	1:C:411:ILE:HG21	2.03	0.40
1:B:213:PRO:HG2	1:B:215:LEU:HG	2.04	0.40
1:B:91:LYS:NZ	1:B:95:ASP:OD2	2.41	0.40
1:B:10:GLU:HG3	1:B:63:VAL:HG22	2.03	0.40
1:C:215:LEU:HD13	1:C:221:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/432 (99%)	415 (97%)	12 (3%)	2 (0%)	24 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	428/432 (99%)	415 (97%)	10 (2%)	3 (1%)	18	10
1	C	428/432 (99%)	407 (95%)	18 (4%)	3 (1%)	18	10
1	D	429/432 (99%)	417 (97%)	11 (3%)	1 (0%)	43	36
2	E	26/28 (93%)	26 (100%)	0	0	100	100
2	F	23/28 (82%)	23 (100%)	0	0	100	100
All	All	1763/1784 (99%)	1703 (97%)	51 (3%)	9 (0%)	24	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	ASN
1	B	261	GLY
1	B	398	ARG
1	C	248	ALA
1	A	335	ALA
1	A	398	ARG
1	B	335	ALA
1	C	398	ARG
1	D	398	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/326 (99%)	312 (96%)	12 (4%)	30	22
1	B	321/326 (98%)	294 (92%)	27 (8%)	10	4
1	C	324/326 (99%)	296 (91%)	28 (9%)	10	4
1	D	317/326 (97%)	302 (95%)	15 (5%)	23	15
2	E	23/23 (100%)	22 (96%)	1 (4%)	26	18
2	F	20/23 (87%)	19 (95%)	1 (5%)	22	14
All	All	1329/1350 (98%)	1245 (94%)	84 (6%)	16	8

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	26	LEU
1	A	96	LEU
1	A	101	ASN
1	A	142	LYS
1	A	238	LYS
1	A	253	LYS
1	A	265	LYS
1	A	307	LEU
1	A	342	PHE
1	A	400	ASP
1	A	425	LYS
1	B	2	LYS
1	B	26	LEU
1	B	48	LEU
1	B	101	ASN
1	B	111	LEU
1	B	152	ILE
1	B	157	GLU
1	B	162	ASN
1	B	197	LYS
1	B	202	ASN
1	B	214	ASN
1	B	253	LYS
1	B	259	LEU
1	B	273	THR
1	B	277	GLU
1	B	294	GLU
1	B	310	LYS
1	B	311	ILE
1	B	317	ASP
1	B	326	LEU
1	B	327	LYS
1	B	342	PHE
1	B	359	LYS
1	B	400	ASP
1	B	418	LYS
1	B	424	ARG
1	B	425	LYS
1	C	26	LEU
1	C	41	SER
1	C	42	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	48	LEU
1	C	56	SER
1	C	57	ARG
1	C	91	LYS
1	C	96	LEU
1	C	101	ASN
1	C	150	MET
1	C	157	GLU
1	C	176	LYS
1	C	238	LYS
1	C	254	ASP
1	C	256	LYS
1	C	259	LEU
1	C	270	GLU
1	C	278	GLU
1	C	292	LEU
1	C	294	GLU
1	C	306	VAL
1	C	307	LEU
1	C	309	ASP
1	C	318	LEU
1	C	342	PHE
1	C	400	ASP
1	C	418	LYS
1	C	428	LYS
1	D	5	LYS
1	D	7	ILE
1	D	48	LEU
1	D	101	ASN
1	D	111	LEU
1	D	154	ASN
1	D	236	LEU
1	D	259	LEU
1	D	270	GLU
1	D	305	LYS
1	D	326	LEU
1	D	342	PHE
1	D	343	ASN
1	D	400	ASP
1	D	401	ARG
2	E	8	VAL
2	F	1	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	151	ASN
1	A	154	ASN
1	A	190	HIS
1	A	264	ASN
1	A	303	GLN
1	A	430	GLN
1	B	76	GLN
1	B	101	ASN
1	B	137	ASN
1	B	151	ASN
1	B	154	ASN
1	B	162	ASN
1	B	190	HIS
1	B	202	ASN
1	B	303	GLN
1	C	25	HIS
1	C	76	GLN
1	C	101	ASN
1	C	151	ASN
1	C	154	ASN
1	C	166	GLN
1	C	171	GLN
1	C	202	ASN
1	C	274	HIS
1	C	282	GLN
1	C	303	GLN
1	C	322	ASN
1	C	344	GLN
1	C	430	GLN
1	D	76	GLN
1	D	101	ASN
1	D	171	GLN
1	D	190	HIS
1	D	202	ASN
1	D	274	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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	430/432 (99%)	-0.42	2 (0%) 87 89	8, 16, 29, 37	1 (0%)
1	B	430/432 (99%)	0.18	27 (6%) 26 27	10, 22, 50, 68	0
1	C	430/432 (99%)	0.33	49 (11%) 10 10	11, 23, 57, 69	0
1	D	431/432 (99%)	-0.02	17 (3%) 43 46	10, 21, 39, 54	0
2	E	28/28 (100%)	0.74	2 (7%) 22 23	14, 21, 31, 36	0
2	F	25/28 (89%)	1.61	7 (28%) 1 1	20, 26, 31, 41	0
All	All	1774/1784 (99%)	0.05	104 (5%) 28 30	8, 20, 47, 69	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	257	TYR	7.0
1	D	162	ASN	6.3
2	F	25	PRO	5.6
1	C	258	VAL	5.4
1	D	258	VAL	5.1
1	D	431	ALA	4.9
1	B	264	ASN	4.9
1	C	266	ALA	4.8
1	C	257	TYR	4.4
1	B	263	GLY	4.4
1	D	317	ASP	4.1
1	D	159	ALA	4.0
2	E	1	GLN	4.0
1	C	260	ALA	4.0
1	C	259	LEU	3.9
1	B	297	TRP	3.9
1	C	267	PHE	3.9
1	B	142	LYS	3.7
1	C	268	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	273	THR	3.5
1	B	266	ALA	3.4
1	B	265	LYS	3.4
1	D	160	ASP	3.3
1	C	302	TYR	3.3
1	C	307	LEU	3.3
1	C	275	PHE	3.3
1	C	300	PHE	3.2
1	C	263	GLY	3.2
1	D	157	GLU	3.2
1	C	254	ASP	3.1
1	C	160	ASP	3.1
1	C	297	TRP	3.1
1	C	298	ASP	3.0
1	C	317	ASP	3.0
1	C	255	GLY	3.0
1	D	261	GLY	3.0
1	D	158	HIS	2.9
1	D	45	ARG	2.9
1	C	247	ALA	2.9
2	F	22	ILE	2.9
1	C	253	LYS	2.8
1	C	272	PHE	2.8
1	B	162	ASN	2.8
2	F	24	TYR	2.7
1	D	268	THR	2.7
1	B	301	ALA	2.7
1	C	299	GLY	2.7
2	F	15	LEU	2.7
1	C	40	ALA	2.6
1	C	248	ALA	2.6
2	F	23	ARG	2.6
1	C	291	GLY	2.6
1	C	306	VAL	2.6
1	C	318	LEU	2.5
1	C	326	LEU	2.5
1	C	252	TYR	2.5
2	F	11	ALA	2.5
1	C	256	LYS	2.4
1	B	306	VAL	2.4
1	B	269	SER	2.4
1	C	269	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	251	PHE	2.4
1	A	100	GLU	2.4
1	D	56	SER	2.4
1	B	259	LEU	2.4
1	B	302	TYR	2.4
1	B	309	ASP	2.4
2	E	16	ALA	2.4
1	C	100	GLU	2.4
1	C	270	GLU	2.4
2	F	5	PRO	2.4
1	C	44	SER	2.3
1	C	42	THR	2.3
1	C	304	THR	2.3
1	C	276	LEU	2.3
1	B	267	PHE	2.3
1	C	278	GLU	2.3
1	C	328	GLU	2.3
1	B	276	LEU	2.3
1	C	265	LYS	2.2
1	C	301	ALA	2.2
1	C	325	ILE	2.2
1	C	162	ASN	2.2
1	D	41	SER	2.2
1	B	274	HIS	2.2
1	C	273	THR	2.2
1	B	253	LYS	2.2
1	B	298	ASP	2.1
1	B	255	GLY	2.1
1	B	38	SER	2.1
1	D	42	THR	2.1
1	A	309	ASP	2.1
1	B	254	ASP	2.1
1	B	280	THR	2.1
1	B	331	GLU	2.1
1	C	333	GLY	2.1
1	C	334	ILE	2.0
1	B	257	TYR	2.0
1	B	258	VAL	2.0
1	C	292	LEU	2.0
1	D	260	ALA	2.0
1	D	249	SER	2.0
1	B	261	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	261	GLY	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(\AA^2)	Q<0.9
3	MG	A	1431	1/1	0.95	0.07	25,25,25,25	0
3	MG	C	1431	1/1	0.96	0.06	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.