



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:19 PM EDT

PDB ID : 3OWO / pdb_00003owo
Title : Structures of iron-dependent alcohol dehydrogenase 2 from *Zymomonas mobilis* ZM4 with and without NAD cofactor
Authors : Moon, J.H.; Lee, H.J.; Song, J.M.; Park, S.Y.; Park, M.Y.; Park, H.M.; Sun, J.; Park, J.H.; Kim, J.S.
Deposited on : 2010-09-20
Resolution : 2.07 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

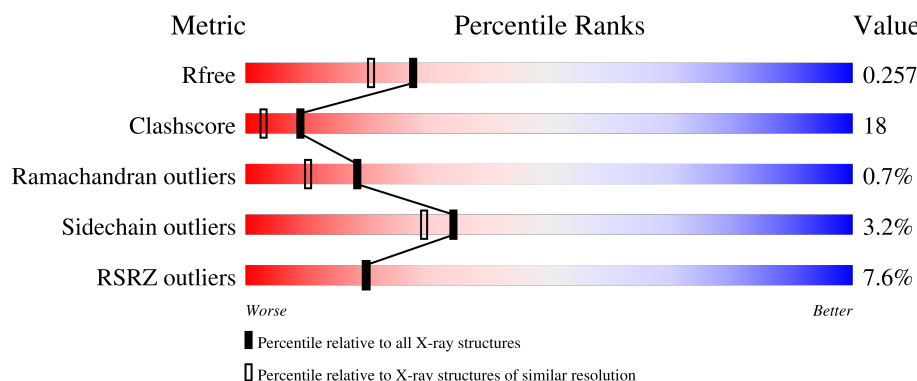
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	383	7% 68% 29% .
1	B	383	4% 70% 26% .
1	C	383	15% 63% 35% .
1	D	383	5% 70% 26% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FE2	B	384	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11939 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 Alcohol dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2798	1759	474	543	22			
1	B	382	Total	C	N	O	S	0	0	0
			2798	1759	474	543	22			
1	C	382	Total	C	N	O	S	0	0	0
			2798	1759	474	543	22			
1	D	381	Total	C	N	O	S	0	0	0
			2793	1756	473	542	22			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

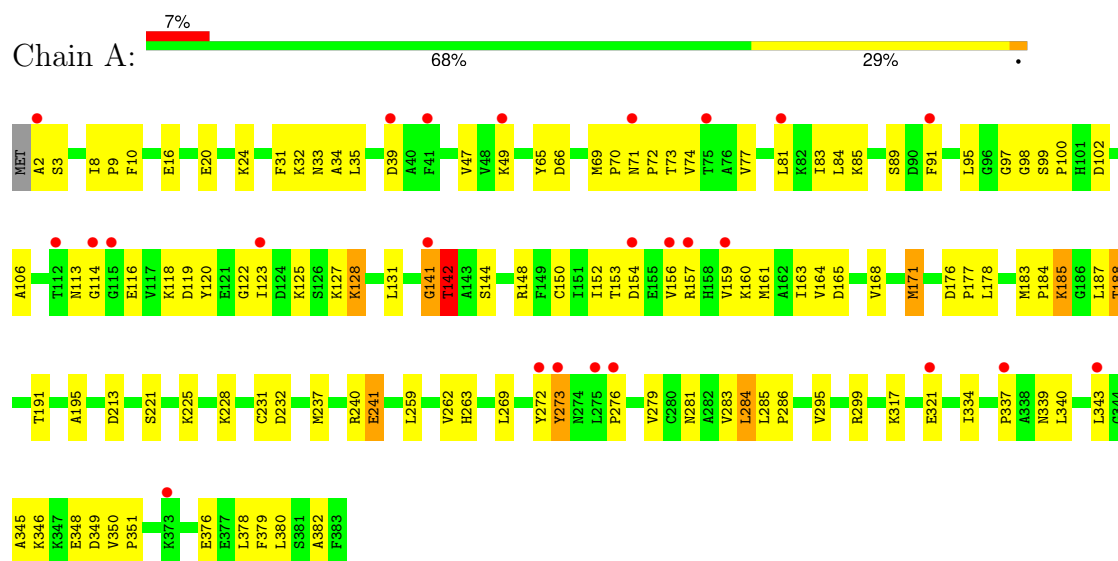
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		
3	B	227	Total	O	0	0
			227	227		
3	C	117	Total	O	0	0
			117	117		
3	D	193	Total	O	0	0
			193	193		

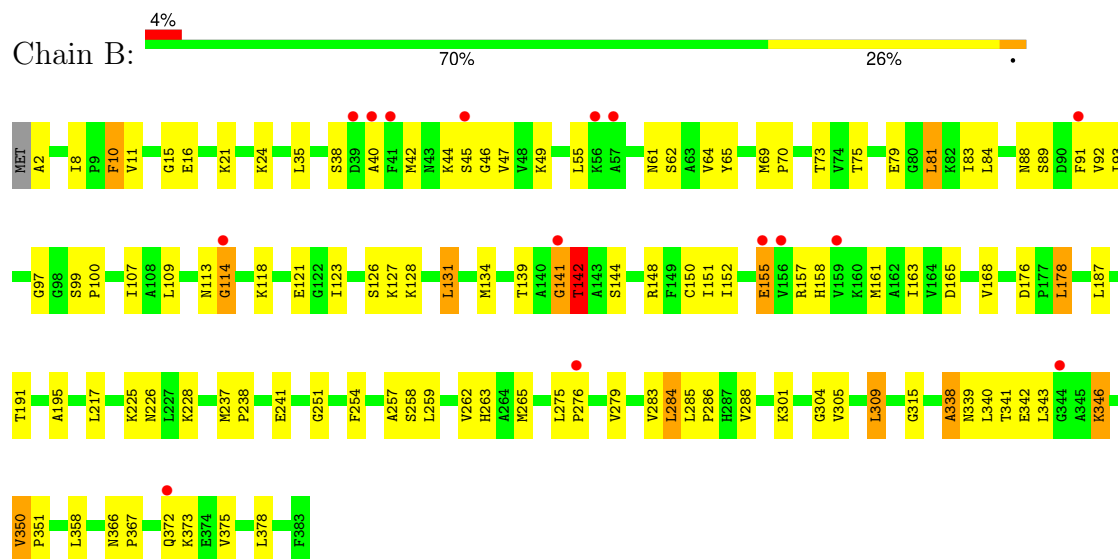
3 Residue-property plots [i](#)

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.

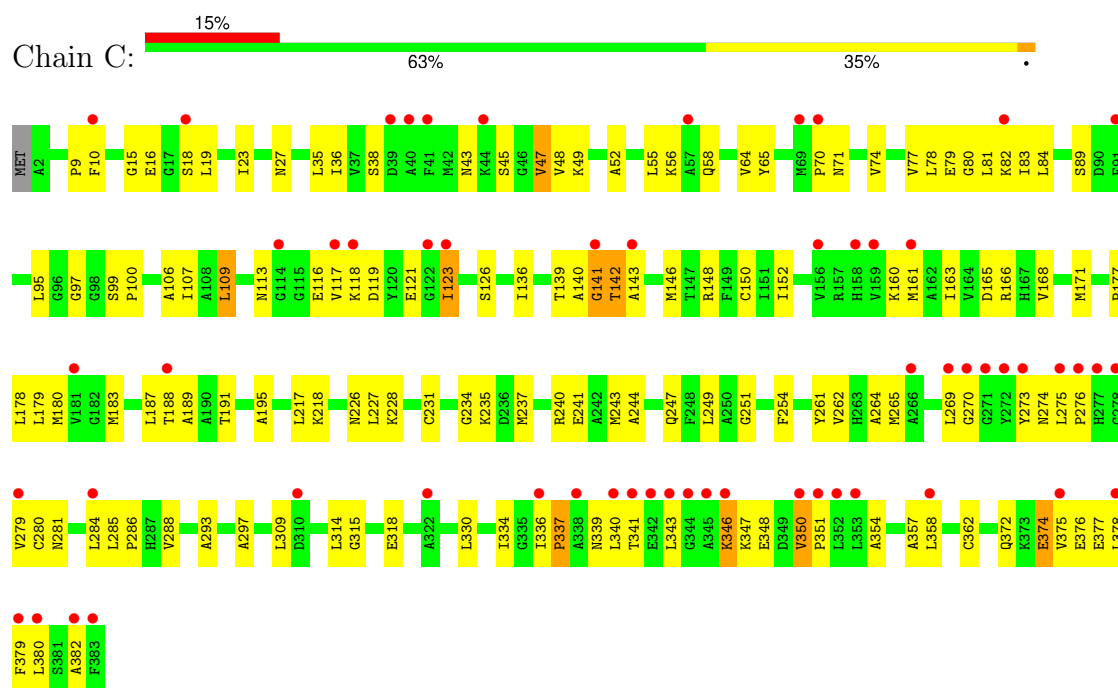
• Molecule 1: Alcohol dehydrogenase 2



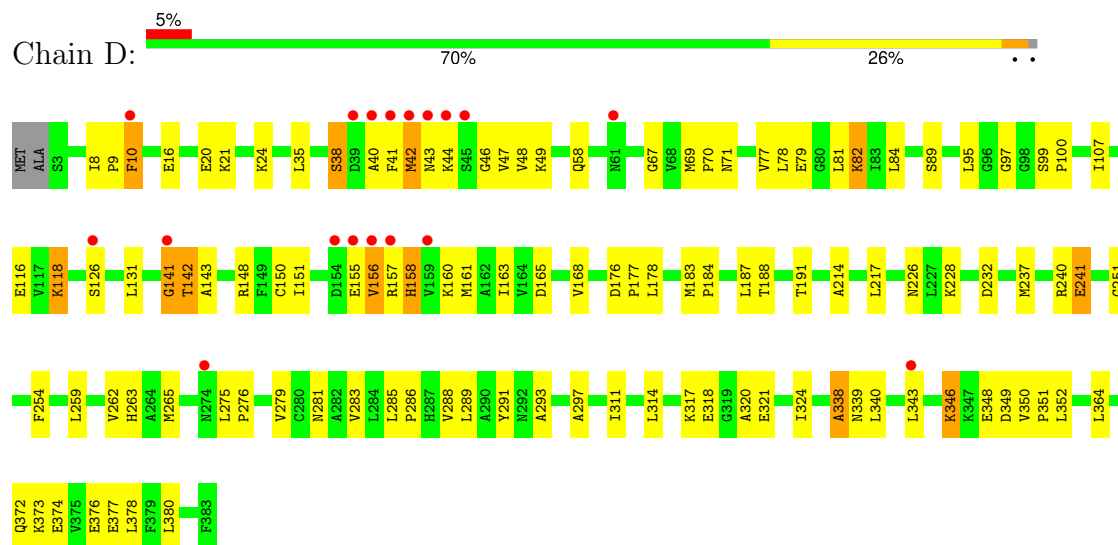
• Molecule 1: Alcohol dehydrogenase 2



• Molecule 1: Alcohol dehydrogenase 2



• Molecule 1: Alcohol dehydrogenase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.92Å 87.51Å 124.71Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07 50.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.07) 97.2 (50.00-2.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.253 0.206 , 0.257	Depositor DCC
R_{free} test set	7848 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11939	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1290e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2842	0.87	3/3851 (0.1%)
1	B	0.39	0/2842	0.89	9/3851 (0.2%)
1	C	0.35	0/2842	0.86	5/3851 (0.1%)
1	D	0.37	0/2837	0.90	10/3844 (0.3%)
All	All	0.37	0/11363	0.88	27/15397 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	THR	N-CA-C	7.95	120.02	111.36
1	B	131	LEU	N-CA-C	-7.04	100.71	109.64
1	D	148	ARG	N-CA-C	-6.43	105.01	112.92
1	B	142	THR	N-CA-C	6.42	119.23	111.40
1	A	142	THR	N-CA-C	6.26	119.39	111.69
1	D	38	SER	N-CA-C	5.79	117.58	108.96
1	D	155	GLU	N-CA-C	-5.68	105.07	112.23
1	D	338	ALA	N-CA-C	5.51	118.05	111.71
1	B	350	VAL	CB-CA-C	-5.50	108.47	113.70
1	B	338	ALA	N-CA-C	5.43	119.01	112.38
1	A	98	GLY	N-CA-C	5.42	119.45	112.83
1	A	131	LEU	N-CA-C	-5.42	102.76	109.64
1	C	142	THR	N-CA-C	5.32	117.89	111.40
1	D	364	LEU	N-CA-C	5.29	117.05	111.28
1	B	226	ASN	N-CA-C	5.28	120.59	114.04
1	B	315	GLY	N-CA-C	-5.25	104.48	112.51
1	B	38	SER	N-CA-C	5.24	115.46	108.38
1	B	123	ILE	N-CA-C	5.24	115.40	107.80
1	C	350	VAL	CB-CA-C	-5.18	108.78	113.70
1	B	64	VAL	N-CA-C	5.17	115.93	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	GLY	N-CA-C	-5.17	106.64	112.33
1	C	226	ASN	N-CA-C	5.09	119.95	113.18
1	D	71	ASN	CA-C-N	5.09	125.37	119.93
1	D	71	ASN	C-N-CA	5.09	125.37	119.93
1	D	226	ASN	N-CA-C	5.07	121.59	110.80
1	D	131	LEU	N-CA-C	-5.06	102.81	109.84
1	C	38	SER	N-CA-C	5.00	114.75	108.45

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	2798	0	2820	110	0
1	B	2798	0	2820	83	0
1	C	2798	0	2820	131	0
1	D	2793	0	2815	105	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	211	0	0	14	0
3	B	227	0	0	9	0
3	C	117	0	0	8	0
3	D	193	0	0	4	0
All	All	11939	0	11275	413	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 18.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:H	1:A:118:LYS:HD2	1.07	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HG	1:C:89:SER:HB2	1.42	1.01
1:D:24:LYS:HA	1:D:58:GLN:HE21	1.26	1.00
1:C:150:CYS:HB3	1:C:163:ILE:HB	1.48	0.94
1:A:106:ALA:HB2	1:A:152:ILE:HD11	1.53	0.89
1:B:142:THR:HG22	1:B:144:SER:H	1.37	0.87
1:D:183:MET:HB3	1:D:188:THR:HG22	1.57	0.87
1:C:35:LEU:HD22	1:C:84:LEU:HB2	1.57	0.86
1:A:118:LYS:HD2	1:A:118:LYS:N	1.90	0.85
1:A:183:MET:HB3	1:A:188:THR:HG22	1.57	0.85
1:A:340:LEU:HA	1:A:343:LEU:HD23	1.60	0.84
1:A:142:THR:HG22	1:A:144:SER:H	1.42	0.84
1:C:123:ILE:HD13	1:C:123:ILE:H	1.42	0.84
1:C:106:ALA:HB2	1:C:152:ILE:HD11	1.59	0.83
1:C:276:PRO:HB2	1:C:279:VAL:HG22	1.59	0.83
1:D:24:LYS:HA	1:D:58:GLN:NE2	1.93	0.82
1:A:99:SER:HB2	1:A:100:PRO:HD3	1.61	0.82
1:B:141:GLY:HA2	1:B:195:ALA:HB2	1.59	0.81
1:D:21:LYS:HA	1:D:24:LYS:HE3	1.62	0.81
1:A:276:PRO:HB2	1:A:279:VAL:HG22	1.62	0.80
1:A:262:VAL:HG12	1:A:281:ASN:HD22	1.46	0.80
1:A:49:LYS:HG3	3:A:537:HOH:O	1.81	0.80
1:D:79:GLU:HA	1:D:82:LYS:HD3	1.62	0.79
1:C:265:MET:HE1	1:C:378:LEU:HD22	1.65	0.78
1:C:79:GLU:HA	1:C:82:LYS:HE2	1.64	0.78
1:A:185:LYS:HE3	1:A:231:CYS:HB3	1.66	0.77
1:D:372:GLN:O	1:D:376:GLU:HG3	1.83	0.77
1:B:99:SER:HB2	1:B:100:PRO:HD3	1.68	0.76
1:D:118:LYS:H	1:D:118:LYS:HD3	1.50	0.75
1:C:165:ASP:O	1:C:168:VAL:HG22	1.86	0.74
1:D:42:MET:HE2	1:D:47:VAL:HG21	1.68	0.74
1:A:3:SER:H	1:B:15:GLY:HA3	1.52	0.74
1:D:99:SER:HB2	1:D:100:PRO:HD3	1.70	0.74
1:C:77:VAL:O	1:C:81:LEU:HD13	1.89	0.73
1:C:52:ALA:O	1:C:56:LYS:HG2	1.89	0.73
1:B:44:LYS:HZ3	1:C:275:LEU:HD23	1.53	0.73
1:B:16:GLU:HG3	1:B:178:LEU:HD13	1.70	0.72
1:B:142:THR:CG2	1:B:144:SER:H	2.02	0.72
1:C:81:LEU:HD12	1:C:107:ILE:HG23	1.72	0.71
1:D:16:GLU:HG3	1:D:178:LEU:HD11	1.72	0.71
1:D:283:VAL:HG21	1:D:343:LEU:HD21	1.72	0.70
1:C:106:ALA:CB	1:C:152:ILE:HD11	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:THR:HG22	1:C:240:ARG:HH12	1.57	0.69
1:D:262:VAL:HG12	1:D:281:ASN:HD22	1.57	0.69
1:B:285:LEU:HB3	1:B:286:PRO:HD3	1.75	0.69
1:D:184:PRO:O	1:D:188:THR:HG23	1.92	0.69
1:A:141:GLY:HA2	1:A:195:ALA:HB2	1.73	0.69
1:D:84:LEU:HG	1:D:89:SER:HB2	1.73	0.69
1:A:184:PRO:O	1:A:188:THR:HG23	1.91	0.69
1:C:262:VAL:HG12	1:C:281:ASN:ND2	2.08	0.69
1:A:16:GLU:HG3	1:A:178:LEU:HD21	1.75	0.69
1:A:272:TYR:HB3	3:A:445:HOH:O	1.93	0.69
1:D:275:LEU:HD13	1:D:343:LEU:HD12	1.74	0.69
1:A:118:LYS:H	1:A:118:LYS:CD	1.92	0.68
1:D:81:LEU:HD22	1:D:107:ILE:HG23	1.75	0.68
1:D:177:PRO:HG3	1:D:241:GLU:HG2	1.76	0.68
1:D:41:PHE:HA	1:D:44:LYS:HD2	1.75	0.67
1:B:142:THR:HB	3:B:429:HOH:O	1.93	0.67
1:B:265:MET:HE1	1:B:378:LEU:HD22	1.77	0.66
1:D:16:GLU:CG	1:D:178:LEU:HD11	2.24	0.66
1:B:276:PRO:HB2	1:B:279:VAL:HG22	1.76	0.66
1:B:118:LYS:CB	1:B:161:MET:HE1	2.26	0.66
1:B:141:GLY:HA3	1:B:191:THR:O	1.95	0.66
1:C:346:LYS:HB3	1:C:346:LYS:HZ2	1.60	0.66
1:D:42:MET:HE3	1:D:42:MET:HA	1.76	0.66
1:B:88:ASN:HB2	3:B:628:HOH:O	1.95	0.66
1:B:44:LYS:NZ	1:C:276:PRO:HD3	2.10	0.66
1:C:16:GLU:HG2	1:C:178:LEU:HD13	1.78	0.66
1:B:69:MET:HB3	1:B:70:PRO:HD2	1.78	0.65
1:B:155:GLU:CD	1:B:155:GLU:H	2.05	0.65
1:C:47:VAL:HG12	1:C:95:LEU:HD21	1.79	0.65
1:C:99:SER:HB2	1:C:100:PRO:HD3	1.77	0.65
1:A:150:CYS:HB3	1:A:163:ILE:HB	1.78	0.65
1:C:285:LEU:HB3	1:C:286:PRO:HD3	1.79	0.65
1:A:123:ILE:HG12	3:A:434:HOH:O	1.95	0.65
1:A:285:LEU:HB3	1:A:286:PRO:HD3	1.78	0.64
1:D:40:ALA:HA	1:D:67:GLY:HA2	1.79	0.64
1:D:276:PRO:HB2	1:D:279:VAL:HG22	1.79	0.64
1:B:372:GLN:HB3	3:B:484:HOH:O	1.98	0.64
1:C:314:LEU:HB3	1:C:318:GLU:HG3	1.80	0.64
1:A:122:GLY:HA3	1:A:125:LYS:NZ	2.13	0.64
1:A:171:MET:HG2	3:B:389:HOH:O	1.98	0.64
1:C:350:VAL:HG21	1:C:380:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:GLU:HG3	3:C:437:HOH:O	1.96	0.64
1:A:8:ILE:O	1:B:10:PHE:HA	1.97	0.64
1:D:77:VAL:O	1:D:81:LEU:HD23	1.97	0.64
1:A:141:GLY:HA3	1:A:191:THR:O	1.98	0.63
1:A:2:ALA:HB1	3:A:403:HOH:O	1.98	0.62
1:C:118:LYS:HG3	3:C:553:HOH:O	1.99	0.62
1:D:118:LYS:H	1:D:118:LYS:CD	2.12	0.62
1:B:358:LEU:HD21	1:B:375:VAL:HG21	1.81	0.62
1:B:127:LYS:O	1:B:128:LYS:HD2	2.00	0.62
1:B:165:ASP:O	1:B:168:VAL:HG22	1.99	0.62
1:A:32:LYS:HG3	3:A:498:HOH:O	2.00	0.62
1:B:118:LYS:HB2	1:B:161:MET:HE1	1.82	0.62
1:D:373:LYS:O	1:D:377:GLU:HG3	1.99	0.62
1:A:34:ALA:HB2	1:A:91:PHE:CE1	2.35	0.62
1:A:84:LEU:HG	1:A:89:SER:HB2	1.81	0.62
1:C:350:VAL:HB	1:C:351:PRO:HD3	1.80	0.62
1:D:285:LEU:HB3	1:D:286:PRO:HD3	1.82	0.62
1:B:44:LYS:HZ1	1:C:276:PRO:HD3	1.65	0.62
1:C:9:PRO:HA	1:D:10:PHE:CE1	2.34	0.62
1:A:142:THR:CG2	1:A:144:SER:H	2.10	0.61
1:B:73:THR:HB	1:B:155:GLU:HG3	1.80	0.61
1:A:317:LYS:O	1:A:321:GLU:HG2	2.00	0.61
1:A:20:GLU:HG3	3:A:513:HOH:O	2.01	0.61
1:A:47:VAL:HG12	1:A:95:LEU:HD21	1.83	0.61
1:B:81:LEU:HD13	1:B:107:ILE:HG23	1.81	0.61
1:A:142:THR:HB	3:A:491:HOH:O	2.00	0.61
1:C:97:GLY:O	1:C:100:PRO:HD2	2.00	0.61
1:C:375:VAL:O	1:C:379:PHE:HB2	2.00	0.61
1:C:141:GLY:HA2	1:C:195:ALA:HB2	1.82	0.61
1:D:126:SER:HB3	1:D:165:ASP:OD1	2.01	0.61
1:A:16:GLU:CG	1:A:178:LEU:HD21	2.31	0.60
1:B:44:LYS:HD3	1:C:275:LEU:HD23	1.83	0.60
1:B:283:VAL:HG11	1:B:343:LEU:HD21	1.82	0.60
1:A:74:VAL:HG11	1:A:118:LYS:NZ	2.16	0.60
1:A:128:LYS:HD2	1:A:128:LYS:N	2.17	0.59
1:C:15:GLY:O	1:C:18:SER:HB2	2.02	0.59
1:A:106:ALA:CB	1:A:152:ILE:HD11	2.29	0.59
1:C:347:LYS:HB3	1:C:347:LYS:NZ	2.16	0.59
1:D:38:SER:OG	1:D:42:MET:HB3	2.02	0.59
1:C:118:LYS:HG2	1:C:161:MET:SD	2.42	0.59
1:D:78:LEU:O	1:D:82:LYS:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HG	1:B:89:SER:HB2	1.85	0.59
1:C:27:ASN:HB2	1:C:58:GLN:OE1	2.02	0.59
1:D:118:LYS:HD3	1:D:118:LYS:N	2.17	0.59
1:A:153:THR:OG1	1:A:160:LYS:HG2	2.02	0.59
1:D:317:LYS:O	1:D:321:GLU:HG2	2.02	0.59
1:A:65:TYR:HB2	1:A:83:ILE:HD12	1.85	0.59
1:D:350:VAL:HG21	1:D:380:LEU:HD21	1.84	0.59
1:D:82:LYS:NZ	1:D:82:LYS:HB3	2.18	0.59
1:B:42:MET:HE2	1:B:42:MET:HA	1.84	0.59
1:D:346:LYS:HB3	1:D:346:LYS:HZ2	1.68	0.58
1:A:262:VAL:HG12	1:A:281:ASN:ND2	2.18	0.58
1:B:275:LEU:HD13	1:B:343:LEU:HD12	1.85	0.58
1:B:44:LYS:HD3	1:C:275:LEU:CD2	2.33	0.58
1:A:122:GLY:HA3	1:A:125:LYS:HZ3	1.67	0.57
1:B:75:THR:O	1:B:79:GLU:HG3	2.04	0.57
1:D:291:TYR:HB2	1:D:378:LEU:HD21	1.86	0.57
1:D:320:ALA:O	1:D:324:ILE:HG12	2.04	0.57
1:C:340:LEU:HA	1:C:343:LEU:HD23	1.85	0.57
1:D:69:MET:HB3	1:D:70:PRO:HD2	1.85	0.57
1:A:283:VAL:HG21	1:A:343:LEU:HD21	1.87	0.57
1:B:372:GLN:HG3	3:B:445:HOH:O	2.04	0.57
1:D:346:LYS:HB2	1:D:349:ASP:OD1	2.05	0.57
1:C:269:LEU:HB3	1:C:275:LEU:HD12	1.87	0.57
1:A:176:ASP:OD2	1:A:178:LEU:HD23	2.04	0.57
1:A:346:LYS:HB3	1:A:348:GLU:OE1	2.05	0.57
1:D:97:GLY:O	1:D:100:PRO:HD2	2.05	0.56
1:D:165:ASP:O	1:D:168:VAL:HG22	2.04	0.56
1:A:74:VAL:HG11	1:A:118:LYS:HZ1	1.68	0.56
1:C:74:VAL:O	1:C:78:LEU:HG	2.06	0.56
1:C:118:LYS:HA	1:C:161:MET:HE1	1.87	0.56
1:B:284:LEU:HD13	1:B:340:LEU:HD21	1.87	0.56
1:A:32:LYS:HE3	3:A:498:HOH:O	2.06	0.56
1:A:283:VAL:CG2	1:A:337:PRO:HG2	2.36	0.56
1:A:106:ALA:HB2	1:A:152:ILE:CD1	2.31	0.56
1:C:117:VAL:CG1	1:C:152:ILE:HD12	2.36	0.56
1:A:346:LYS:HB2	1:A:349:ASP:OD1	2.05	0.56
1:B:127:LYS:C	1:B:128:LYS:HD2	2.31	0.56
1:A:183:MET:HG2	1:A:187:LEU:HD23	1.88	0.55
1:C:354:ALA:HB3	1:C:372:GLN:HE22	1.71	0.55
1:A:118:LYS:HG3	1:A:161:MET:SD	2.47	0.55
1:B:10:PHE:CD2	1:B:11:VAL:HG23	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:O	1:A:71:ASN:HB3	2.07	0.54
1:D:350:VAL:HG21	1:D:380:LEU:CD2	2.37	0.54
1:B:21:LYS:HA	1:B:24:LYS:HG2	1.90	0.54
1:A:185:LYS:HE2	1:A:334:ILE:O	2.07	0.54
1:A:188:THR:CG2	1:A:240:ARG:HH12	2.20	0.54
1:C:10:PHE:HA	1:D:8:ILE:O	2.08	0.54
1:D:188:THR:CG2	1:D:240:ARG:HH12	2.21	0.54
1:C:189:ALA:HB1	1:C:334:ILE:HD12	1.88	0.54
1:C:262:VAL:HG12	1:C:281:ASN:HD22	1.71	0.54
1:D:352:LEU:C	1:D:352:LEU:HD23	2.33	0.53
1:B:176:ASP:OD2	1:B:178:LEU:HB2	2.07	0.53
1:D:70:PRO:HA	1:D:99:SER:OG	2.08	0.53
1:C:117:VAL:HG13	1:C:152:ILE:HD12	1.91	0.53
1:D:118:LYS:HG3	1:D:161:MET:SD	2.48	0.53
1:C:19:LEU:CD1	1:C:136:ILE:HD13	2.38	0.53
1:B:346:LYS:HZ2	1:B:346:LYS:HB3	1.74	0.53
1:C:118:LYS:CB	1:C:161:MET:HE1	2.39	0.53
1:C:188:THR:CG2	1:C:240:ARG:HH12	2.22	0.53
1:C:77:VAL:HG21	1:C:152:ILE:HD13	1.89	0.53
1:C:9:PRO:HA	1:D:10:PHE:HE1	1.74	0.53
1:B:225:LYS:HE3	3:B:469:HOH:O	2.09	0.53
1:C:362:CYS:SG	3:C:442:HOH:O	2.59	0.52
1:D:21:LYS:HA	1:D:24:LYS:CE	2.36	0.52
1:A:269:LEU:O	1:A:273:TYR:HB2	2.09	0.52
1:C:70:PRO:O	1:C:71:ASN:HB2	2.09	0.52
1:B:339:ASN:O	1:B:343:LEU:HD23	2.10	0.52
1:C:171:MET:HA	1:D:10:PHE:HZ	1.74	0.52
1:D:35:LEU:HD22	1:D:84:LEU:HB2	1.91	0.52
1:A:228:LYS:HE3	1:A:232:ASP:OD2	2.10	0.52
1:C:351:PRO:HA	1:C:376:GLU:OE2	2.11	0.51
1:D:43:ASN:CG	1:D:48:VAL:HG11	2.35	0.51
1:A:77:VAL:O	1:A:81:LEU:HB2	2.10	0.51
1:A:177:PRO:HG2	1:A:237:MET:HE1	1.93	0.51
1:C:65:TYR:HB2	1:C:83:ILE:HD12	1.92	0.51
1:A:116:GLU:HB2	1:A:119:ASP:OD1	2.10	0.51
1:A:165:ASP:O	1:A:168:VAL:HG22	2.09	0.51
1:C:346:LYS:HB3	1:C:346:LYS:NZ	2.24	0.51
1:B:237:MET:HB2	1:B:238:PRO:HD3	1.93	0.51
1:C:109:LEU:HD21	1:C:126:SER:CB	2.41	0.50
1:C:123:ILE:HD13	1:C:123:ILE:N	2.19	0.50
1:B:150:CYS:SG	1:B:152:ILE:HD13	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:PRO:HG3	1:C:241:GLU:CD	2.37	0.50
1:D:318:GLU:HG3	3:D:425:HOH:O	2.10	0.50
1:C:293:ALA:O	1:C:297:ALA:HB2	2.11	0.50
1:B:251:GLY:HA2	1:B:254:PHE:CD1	2.46	0.50
1:C:141:GLY:HA3	1:C:191:THR:O	2.11	0.50
1:A:154:ASP:HB2	3:A:522:HOH:O	2.11	0.50
1:C:16:GLU:OE1	1:C:237:MET:HE2	2.11	0.50
1:C:177:PRO:HG3	1:C:241:GLU:HG2	1.93	0.50
1:C:227:LEU:HD13	1:C:243:MET:HE2	1.94	0.50
1:B:97:GLY:O	1:B:100:PRO:HD2	2.12	0.50
1:C:126:SER:OG	1:C:165:ASP:OD1	2.27	0.50
1:D:346:LYS:HB3	1:D:346:LYS:NZ	2.27	0.50
1:A:85:LYS:HD3	3:A:487:HOH:O	2.10	0.50
1:D:40:ALA:O	1:D:44:LYS:HG3	2.11	0.50
1:D:339:ASN:O	1:D:343:LEU:HD23	2.12	0.49
1:D:348:GLU:HG3	3:D:693:HOH:O	2.12	0.49
1:C:139:THR:HB	1:C:191:THR:HG21	1.93	0.49
1:C:347:LYS:HB3	1:C:347:LYS:HZ3	1.77	0.49
1:D:40:ALA:CA	1:D:67:GLY:HA2	2.42	0.49
1:A:284:LEU:HD13	1:A:340:LEU:HD21	1.92	0.49
1:D:340:LEU:HA	1:D:343:LEU:HB2	1.95	0.49
1:A:295:VAL:HA	3:A:463:HOH:O	2.13	0.49
1:B:21:LYS:O	1:B:24:LYS:HG3	2.13	0.49
1:A:34:ALA:HB2	1:A:91:PHE:CZ	2.48	0.49
1:B:228:LYS:HB2	3:B:400:HOH:O	2.13	0.49
1:B:121:GLU:OE1	1:B:161:MET:HE2	2.13	0.48
1:B:259:LEU:HD13	1:B:263:HIS:CG	2.47	0.48
1:D:151:ILE:HG21	1:D:160:LYS:HD3	1.94	0.48
1:C:265:MET:HE1	1:C:378:LEU:CD2	2.41	0.48
1:D:42:MET:HE2	1:D:47:VAL:CG2	2.41	0.48
1:B:150:CYS:HB3	1:B:163:ILE:HB	1.96	0.48
1:B:339:ASN:OD1	1:B:341:THR:HB	2.13	0.48
1:C:81:LEU:HD11	1:C:107:ILE:HA	1.95	0.48
1:D:265:MET:HE1	1:D:378:LEU:HB3	1.94	0.48
1:A:379:PHE:O	1:A:382:ALA:HB3	2.14	0.48
1:B:346:LYS:HB3	1:B:346:LYS:NZ	2.27	0.48
1:C:336:ILE:HG23	1:C:337:PRO:HD2	1.94	0.48
1:D:279:VAL:O	1:D:283:VAL:HG23	2.14	0.48
1:D:157:ARG:O	1:D:158:HIS:CB	2.60	0.48
1:C:261:TYR:HA	1:C:264:ALA:HB3	1.95	0.48
1:D:374:GLU:HA	1:D:377:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:C	1:B:84:LEU:HD23	2.39	0.48
1:C:339:ASN:C	1:C:341:THR:H	2.22	0.48
1:D:84:LEU:C	1:D:84:LEU:HD23	2.38	0.48
1:D:237:MET:O	1:D:241:GLU:HB2	2.12	0.48
1:B:46:GLY:HA2	1:B:49:LYS:NZ	2.28	0.48
1:C:270:GLY:O	1:C:274:ASN:HA	2.14	0.48
1:B:2:ALA:N	3:B:450:HOH:O	2.46	0.47
1:A:8:ILE:HG13	1:A:9:PRO:HD2	1.96	0.47
1:C:244:ALA:O	1:C:247:GLN:HG3	2.14	0.47
1:A:185:LYS:O	1:A:185:LYS:HD3	2.15	0.47
1:A:350:VAL:HB	1:A:351:PRO:HD3	1.97	0.47
1:C:183:MET:HE3	1:C:240:ARG:NH1	2.28	0.47
1:C:330:LEU:O	1:C:334:ILE:HG12	2.14	0.47
1:A:123:ILE:HA	1:A:164:VAL:O	2.14	0.47
1:C:309:LEU:N	1:C:309:LEU:HD12	2.30	0.47
1:A:127:LYS:HB2	1:A:128:LYS:HD2	1.97	0.47
1:A:142:THR:HG23	1:A:144:SER:OG	2.15	0.47
1:A:350:VAL:HG12	1:A:376:GLU:HG2	1.96	0.47
1:B:61:ASN:ND2	1:B:62:SER:H	2.12	0.47
1:D:43:ASN:HA	1:D:48:VAL:CG1	2.45	0.47
1:D:81:LEU:HD21	1:D:107:ILE:HA	1.97	0.47
1:D:293:ALA:O	1:D:297:ALA:HB2	2.14	0.47
1:A:185:LYS:HD3	1:A:185:LYS:C	2.40	0.47
1:C:140:ALA:HB2	1:C:180:MET:CE	2.45	0.47
1:B:151:ILE:C	1:B:152:ILE:HD12	2.40	0.47
1:D:79:GLU:HA	1:D:82:LYS:CD	2.41	0.47
1:A:32:LYS:O	1:A:32:LYS:HD3	2.15	0.47
1:B:65:TYR:HB2	1:B:83:ILE:HD12	1.96	0.46
1:D:42:MET:HG2	1:D:95:LEU:HG	1.97	0.46
1:A:84:LEU:HD23	1:A:84:LEU:C	2.41	0.46
1:C:118:LYS:CA	1:C:161:MET:HE1	2.46	0.46
1:C:49:LYS:HG3	3:C:587:HOH:O	2.14	0.46
1:C:189:ALA:HB2	1:C:231:CYS:SG	2.56	0.46
1:C:284:LEU:O	1:C:288:VAL:HG23	2.15	0.46
1:A:177:PRO:CG	1:A:237:MET:HE1	2.45	0.46
1:B:92:VAL:HG23	1:B:131:LEU:HD23	1.98	0.46
1:C:378:LEU:C	1:C:378:LEU:HD23	2.41	0.46
1:A:157:ARG:O	1:A:159:VAL:HG23	2.16	0.46
1:A:221:SER:O	1:A:225:LYS:HG3	2.15	0.46
1:C:116:GLU:HB2	1:C:119:ASP:OD1	2.15	0.46
1:C:279:VAL:HG23	1:C:280:CYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:LEU:HB3	1:D:324:ILE:CD1	2.46	0.46
1:D:350:VAL:HB	1:D:351:PRO:HD3	1.98	0.46
1:B:358:LEU:HD12	1:B:372:GLN:HG2	1.97	0.46
1:D:262:VAL:HG22	1:D:288:VAL:HB	1.98	0.46
1:C:183:MET:HG2	1:C:187:LEU:HD23	1.98	0.45
1:A:35:LEU:HD22	1:A:84:LEU:HB2	1.98	0.45
1:C:43:ASN:HA	1:C:48:VAL:CG2	2.47	0.45
1:C:380:LEU:C	1:C:382:ALA:H	2.24	0.45
1:C:123:ILE:HG12	1:C:123:ILE:O	2.16	0.45
1:A:114:GLY:N	1:A:120:TYR:OH	2.50	0.45
1:B:350:VAL:HB	1:B:351:PRO:HD3	1.97	0.45
1:C:10:PHE:CE2	1:D:10:PHE:CD2	3.05	0.45
1:D:46:GLY:HA2	3:D:465:HOH:O	2.17	0.45
1:D:48:VAL:HG13	1:D:49:LYS:N	2.31	0.45
1:A:97:GLY:O	1:A:100:PRO:HD2	2.15	0.45
1:C:140:ALA:HB3	3:C:468:HOH:O	2.16	0.45
1:C:218:LYS:HG2	1:D:214:ALA:HB2	1.98	0.45
1:C:264:ALA:O	1:C:357:ALA:HA	2.17	0.45
1:D:141:GLY:HA3	1:D:191:THR:HB	1.99	0.45
1:B:40:ALA:O	1:B:44:LYS:HG3	2.17	0.45
1:B:301:LYS:O	1:B:305:VAL:HG23	2.17	0.45
1:C:80:GLY:HA3	1:C:107:ILE:HD13	1.98	0.45
1:A:24:LYS:HE3	3:A:483:HOH:O	2.17	0.45
1:A:123:ILE:N	1:A:125:LYS:HZ3	2.14	0.45
1:D:289:LEU:HB2	1:D:324:ILE:HD12	1.99	0.45
1:D:351:PRO:HA	1:D:376:GLU:OE2	2.16	0.45
1:A:259:LEU:HD13	1:A:263:HIS:CG	2.52	0.44
1:C:71:ASN:HD22	1:C:160:LYS:HE2	1.82	0.44
1:C:235:LYS:HD2	1:C:235:LYS:N	2.32	0.44
1:A:24:LYS:CE	3:A:483:HOH:O	2.66	0.44
1:B:262:VAL:HG22	1:B:288:VAL:HB	2.00	0.44
1:B:366:ASN:CG	1:B:367:PRO:HD2	2.42	0.44
1:C:218:LYS:HG3	1:C:249:LEU:HD13	2.00	0.44
1:A:113:ASN:HB3	1:A:120:TYR:OH	2.17	0.44
1:C:10:PHE:CE1	1:D:9:PRO:HA	2.52	0.44
1:C:374:GLU:C	1:C:376:GLU:N	2.74	0.44
1:D:126:SER:CB	1:D:165:ASP:OD1	2.65	0.44
1:D:142:THR:O	1:D:143:ALA:HB3	2.18	0.44
1:D:259:LEU:HD13	1:D:263:HIS:CG	2.53	0.44
1:B:113:ASN:O	1:B:114:GLY:O	2.36	0.44
1:C:358:LEU:CG	1:C:375:VAL:HG21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:HA	1:A:153:THR:O	2.18	0.44
1:C:109:LEU:HD23	1:C:113:ASN:ND2	2.33	0.44
1:D:176:ASP:OD2	1:D:178:LEU:HD13	2.18	0.43
1:A:77:VAL:HG21	1:A:152:ILE:HD13	1.99	0.43
1:C:378:LEU:HD23	1:C:378:LEU:O	2.18	0.43
1:C:15:GLY:C	1:C:177:PRO:HD2	2.42	0.43
1:C:234:GLY:C	1:C:235:LYS:HD2	2.43	0.43
1:A:16:GLU:HA	1:A:178:LEU:HD23	2.00	0.43
1:A:177:PRO:HG3	1:A:241:GLU:HG2	2.00	0.43
1:C:140:ALA:HB2	1:C:180:MET:HE2	2.00	0.43
1:A:10:PHE:HA	1:B:8:ILE:O	2.18	0.43
1:C:43:ASN:C	1:C:45:SER:H	2.27	0.43
1:C:380:LEU:C	1:C:382:ALA:N	2.76	0.43
1:D:338:ALA:HB1	3:D:436:HOH:O	2.17	0.43
1:A:154:ASP:OD1	1:A:154:ASP:O	2.37	0.43
1:B:157:ARG:O	1:B:158:HIS:HB2	2.19	0.43
1:A:31:PHE:HB3	1:A:91:PHE:CD1	2.54	0.43
1:D:348:GLU:H	1:D:348:GLU:CD	2.27	0.43
1:B:45:SER:OG	1:B:47:VAL:HG23	2.19	0.42
1:C:84:LEU:HD23	1:C:84:LEU:C	2.44	0.42
1:D:263:HIS:HA	1:D:281:ASN:HD21	1.84	0.42
1:A:127:LYS:C	1:A:128:LYS:HD2	2.45	0.42
1:D:352:LEU:HD23	1:D:352:LEU:O	2.19	0.42
1:A:340:LEU:CA	1:A:343:LEU:HD23	2.41	0.42
1:D:116:GLU:HB3	1:D:118:LYS:HE3	2.01	0.42
1:A:188:THR:HG21	3:A:409:HOH:O	2.18	0.42
1:C:109:LEU:HD23	1:C:113:ASN:HD22	1.85	0.42
1:C:146:MET:SD	1:C:146:MET:C	3.03	0.42
1:C:358:LEU:HG	1:C:375:VAL:HG21	2.01	0.42
1:D:43:ASN:HA	1:D:48:VAL:HG12	2.01	0.42
1:A:69:MET:HB3	1:A:70:PRO:HD2	2.01	0.42
1:B:338:ALA:HB3	1:B:342:GLU:OE2	2.19	0.42
1:A:350:VAL:HG21	1:A:380:LEU:CD2	2.50	0.42
1:C:377:GLU:O	1:C:380:LEU:HB2	2.20	0.42
1:D:24:LYS:CA	1:D:58:GLN:HE21	2.13	0.42
1:A:32:LYS:HD2	1:A:33:ASN:ND2	2.35	0.42
1:D:157:ARG:O	1:D:158:HIS:HB3	2.19	0.42
1:A:346:LYS:HB3	1:A:348:GLU:CD	2.44	0.42
1:D:150:CYS:HB3	1:D:163:ILE:HB	2.02	0.42
1:C:36:ILE:HB	1:C:64:VAL:HG22	2.01	0.42
1:C:188:THR:HG21	3:C:477:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:PRO:HB2	1:C:279:VAL:CG2	2.41	0.42
1:D:289:LEU:CB	1:D:324:ILE:HD12	2.49	0.42
1:D:311:ILE:HB	1:D:314:LEU:HD12	2.02	0.42
1:A:273:TYR:CZ	1:A:345:ALA:HA	2.55	0.41
1:D:251:GLY:HA2	1:D:254:PHE:CD1	2.55	0.41
1:C:228:LYS:HG3	3:C:469:HOH:O	2.20	0.41
1:D:20:GLU:C	1:D:24:LYS:HE2	2.45	0.41
1:B:358:LEU:CD2	1:B:375:VAL:HG21	2.46	0.41
1:C:23:ILE:HG23	1:C:55:LEU:HD23	2.02	0.41
1:C:228:LYS:HE2	1:C:330:LEU:HD13	2.02	0.41
1:D:254:PHE:HB2	1:D:259:LEU:CD2	2.50	0.41
1:A:276:PRO:HB2	1:A:279:VAL:CG2	2.43	0.41
1:C:49:LYS:HG3	3:C:494:HOH:O	2.20	0.41
1:C:358:LEU:HD21	1:C:375:VAL:HG21	2.02	0.41
1:A:72:PRO:HG2	1:A:102:ASP:HB2	2.02	0.41
1:B:91:PHE:CD2	1:B:92:VAL:N	2.89	0.41
1:C:109:LEU:HD21	1:C:126:SER:HB3	2.03	0.41
1:C:121:GLU:HB2	1:C:161:MET:HE2	2.01	0.41
1:B:178:LEU:HD12	1:B:178:LEU:HA	1.95	0.41
1:A:2:ALA:N	1:B:241:GLU:OE2	2.54	0.41
1:A:123:ILE:H	1:A:125:LYS:NZ	2.18	0.41
1:A:213:ASP:OD1	1:A:299:ARG:NH2	2.53	0.41
1:B:88:ASN:ND2	3:B:675:HOH:O	2.54	0.41
1:C:379:PHE:O	1:C:382:ALA:HB3	2.19	0.41
1:D:156:VAL:O	1:D:157:ARG:C	2.63	0.41
1:B:93:ILE:HA	1:B:134:MET:O	2.22	0.41
1:B:257:ALA:O	1:B:258:SER:HB3	2.21	0.41
1:A:84:LEU:HD23	1:A:84:LEU:O	2.20	0.40
1:C:372:GLN:C	1:C:374:GLU:H	2.29	0.40
1:D:16:GLU:CD	1:D:178:LEU:HD11	2.46	0.40
1:B:109:LEU:HD11	1:B:126:SER:CB	2.52	0.40
1:C:269:LEU:HA	1:C:273:TYR:HD2	1.86	0.40
1:C:142:THR:O	1:C:143:ALA:HB3	2.21	0.40
1:C:251:GLY:HA2	1:C:254:PHE:CE1	2.56	0.40
1:A:339:ASN:HB2	1:A:382:ALA:O	2.21	0.40
1:D:82:LYS:HB3	1:D:82:LYS:HZ3	1.85	0.40
1:D:228:LYS:HE3	1:D:232:ASP:OD2	2.20	0.40
1:A:39:ASP:O	1:A:66:ASP:HB2	2.21	0.40
1:B:35:LEU:HD22	1:B:84:LEU:HB2	2.04	0.40
1:B:139:THR:HB	1:B:191:THR:HG21	2.04	0.40
1:B:304:GLY:CA	1:B:309:LEU:HD22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:HB2	1:B:373:LYS:HE3	1.80	0.40
1:C:123:ILE:H	1:C:123:ILE:CD1	2.22	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	380/383 (99%)	362 (95%)	15 (4%)	3 (1%)	16	8
1	B	380/383 (99%)	363 (96%)	15 (4%)	2 (0%)	24	17
1	C	380/383 (99%)	353 (93%)	24 (6%)	3 (1%)	16	8
1	D	379/383 (99%)	358 (94%)	18 (5%)	3 (1%)	16	8
All	All	1519/1532 (99%)	1436 (94%)	72 (5%)	11 (1%)	18	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	GLY
1	A	156	VAL
1	D	158	HIS
1	C	337	PRO
1	D	141	GLY
1	A	141	GLY
1	D	156	VAL
1	A	273	TYR
1	B	141	GLY
1	C	141	GLY
1	C	47	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/295 (100%)	285 (97%)	9 (3%)	35	30
1	B	294/295 (100%)	282 (96%)	12 (4%)	27	21
1	C	294/295 (100%)	285 (97%)	9 (3%)	35	30
1	D	294/295 (100%)	286 (97%)	8 (3%)	39	35
All	All	1176/1180 (100%)	1138 (97%)	38 (3%)	34	29

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LYS
1	A	142	THR
1	A	148	ARG
1	A	171	MET
1	A	185	LYS
1	A	188	THR
1	A	241	GLU
1	A	284	LEU
1	A	378	LEU
1	B	10	PHE
1	B	55	LEU
1	B	81	LEU
1	B	142	THR
1	B	148	ARG
1	B	155	GLU
1	B	178	LEU
1	B	187	LEU
1	B	217	LEU
1	B	284	LEU
1	B	309	LEU
1	B	346	LYS
1	C	109	LEU
1	C	123	ILE
1	C	148	ARG

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Mol	Chain	Res	Type
1	C	166	ARG
1	C	179	LEU
1	C	217	LEU
1	C	346	LYS
1	C	348	GLU
1	C	374	GLU
1	D	10	PHE
1	D	42	MET
1	D	82	LYS
1	D	118	LYS
1	D	187	LEU
1	D	217	LEU
1	D	241	GLU
1	D	346	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	88	ASN
1	A	137	ASN
1	A	175	ASN
1	A	281	ASN
1	A	356	HIS
1	B	33	ASN
1	B	58	GLN
1	B	61	ASN
1	B	281	ASN
1	B	372	GLN
1	C	71	ASN
1	C	158	HIS
1	C	281	ASN
1	C	287	HIS
1	C	356	HIS
1	C	372	GLN
1	D	43	ASN
1	D	50	GLN
1	D	71	ASN
1	D	88	ASN
1	D	281	ASN
1	D	356	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	382/383 (99%)	0.28	25 (6%)	25	24	11, 26, 55, 80	0
1	B	382/383 (99%)	0.16	15 (3%)	43	44	9, 24, 50, 73	0
1	C	382/383 (99%)	0.97	58 (15%)	5	5	13, 39, 73, 90	0
1	D	381/383 (99%)	0.28	18 (4%)	36	36	9, 26, 50, 88	0
All	All	1527/1532 (99%)	0.42	116 (7%)	20	20	9, 28, 64, 90	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	PHE	5.9
1	D	41	PHE	5.8
1	D	42	MET	5.7
1	B	141	GLY	5.5
1	D	40	ALA	5.0
1	C	272	TYR	5.0
1	C	340	LEU	5.0
1	D	159	VAL	4.9
1	C	41	PHE	4.7
1	A	272	TYR	4.6
1	C	159	VAL	4.4
1	B	41	PHE	4.3
1	C	375	VAL	4.3
1	C	379	PHE	4.3
1	D	44	LYS	4.3
1	C	345	ALA	4.2
1	D	156	VAL	4.2
1	C	343	LEU	4.1
1	A	2	ALA	4.0
1	A	114	GLY	4.0
1	D	39	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	378	LEU	3.9
1	C	383	PHE	3.9
1	A	41	PHE	3.8
1	B	114	GLY	3.8
1	C	380	LEU	3.7
1	A	115	GLY	3.6
1	C	352	LEU	3.6
1	C	350	VAL	3.5
1	C	156	VAL	3.5
1	D	154	ASP	3.4
1	D	343	LEU	3.4
1	C	338	ALA	3.3
1	C	271	GLY	3.2
1	D	157	ARG	3.2
1	B	39	ASP	3.2
1	C	39	ASP	3.2
1	C	276	PRO	3.2
1	A	273	TYR	3.2
1	A	159	VAL	3.1
1	C	284	LEU	3.1
1	A	141	GLY	3.1
1	D	141	GLY	3.1
1	C	341	THR	3.1
1	C	270	GLY	3.0
1	C	382	ALA	3.0
1	C	91	PHE	3.0
1	C	118	LYS	2.9
1	A	154	ASP	2.9
1	C	273	TYR	2.9
1	B	45	SER	2.9
1	D	61	ASN	2.9
1	B	40	ALA	2.9
1	B	156	VAL	2.9
1	A	39	ASP	2.8
1	A	343	LEU	2.8
1	C	161	MET	2.8
1	C	123	ILE	2.8
1	A	71	ASN	2.8
1	B	155	GLU	2.8
1	C	40	ALA	2.7
1	C	117	VAL	2.7
1	C	358	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	276	PRO	2.7
1	C	141	GLY	2.7
1	A	156	VAL	2.6
1	D	45	SER	2.6
1	C	344	GLY	2.6
1	D	155	GLU	2.6
1	D	126	SER	2.6
1	C	181	VAL	2.6
1	C	143	ALA	2.5
1	C	342	GLU	2.5
1	D	10	PHE	2.5
1	C	158	HIS	2.5
1	B	159	VAL	2.5
1	C	188	THR	2.4
1	A	276	PRO	2.4
1	A	275	LEU	2.4
1	C	346	LYS	2.4
1	C	277	HIS	2.4
1	C	10	PHE	2.4
1	D	274	ASN	2.4
1	B	372	GLN	2.4
1	C	310	ASP	2.4
1	C	351	PRO	2.4
1	C	353	LEU	2.4
1	C	278	GLY	2.3
1	C	279	VAL	2.3
1	A	321	GLU	2.3
1	A	157	ARG	2.3
1	C	69	MET	2.3
1	D	43	ASN	2.3
1	C	44	LYS	2.3
1	C	275	LEU	2.3
1	C	322	ALA	2.2
1	A	81	LEU	2.2
1	C	70	PRO	2.2
1	B	57	ALA	2.2
1	C	57	ALA	2.2
1	C	266	ALA	2.2
1	A	373	LYS	2.2
1	A	91	PHE	2.1
1	A	112	THR	2.1
1	C	336	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	56	LYS	2.1
1	A	75	THR	2.1
1	A	123	ILE	2.1
1	C	18	SER	2.1
1	A	337	PRO	2.0
1	A	49	LYS	2.0
1	B	344	GLY	2.0
1	C	269	LEU	2.0
1	C	82	LYS	2.0
1	C	114	GLY	2.0
1	C	122	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(Å ²)	Q<0.9
2	FE2	B	384	1/1	0.77	0.41	105,105,105,105	0
2	FE2	C	384	1/1	0.98	0.03	33,33,33,33	0
2	FE2	A	384	1/1	1.00	0.02	23,23,23,23	0
2	FE2	D	384	1/1	1.00	0.05	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.