Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 08:53 PM EDT

PDB ID	:	3OWO
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 (i) 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 (1)) were used in the production of this report:

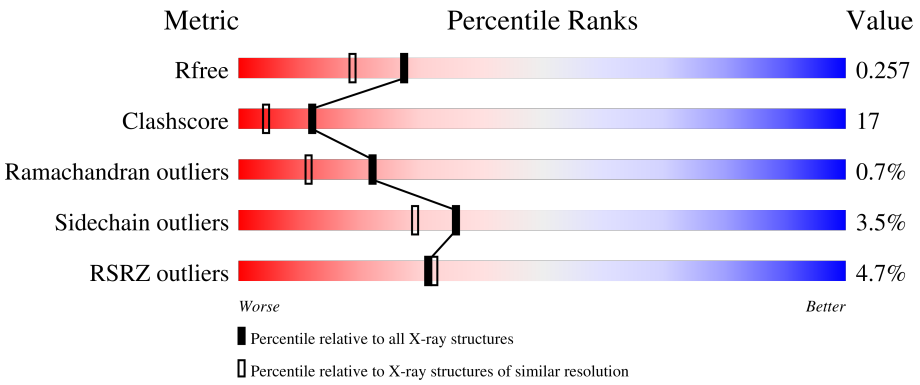
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.07 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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (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 <=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	3% 69% 28% •
1	B	383	2% 73% 24% •
1	C	383	11% 65% 32% •
1	D	383	3% 72% 25% • •

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 (i)

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
			Total	C	N	O	S			
1	A	382	2798	1759	474	543	22	0	0	0
1	B	382	2798	1759	474	543	22	0	0	0
1	C	382	2798	1759	474	543	22	0	0	0
1	D	381	2793	1756	473	542	22	0	0	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 3 is water.

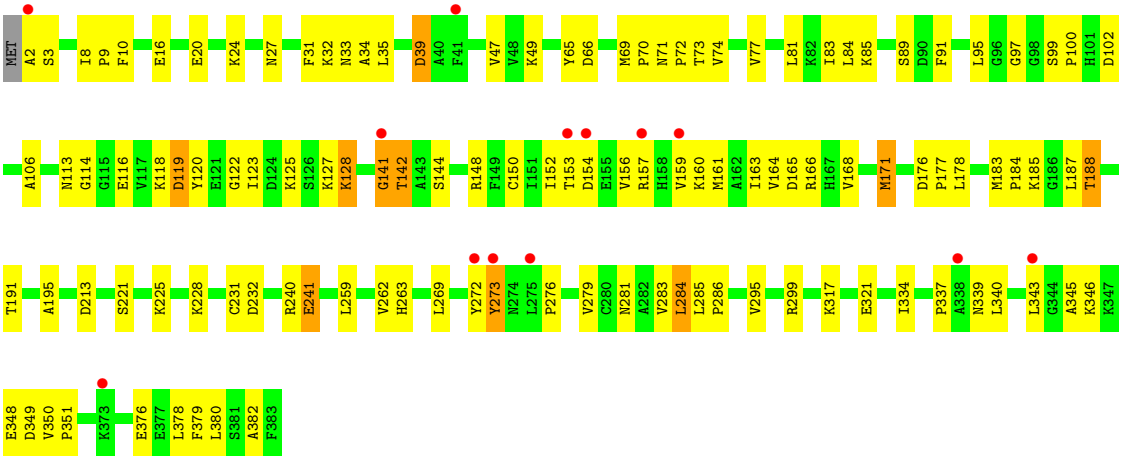
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	211	211	211	0	0
3	B	227	227	227	0	0
3	C	117	117	117	0	0
3	D	193	193	193	0	0

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.

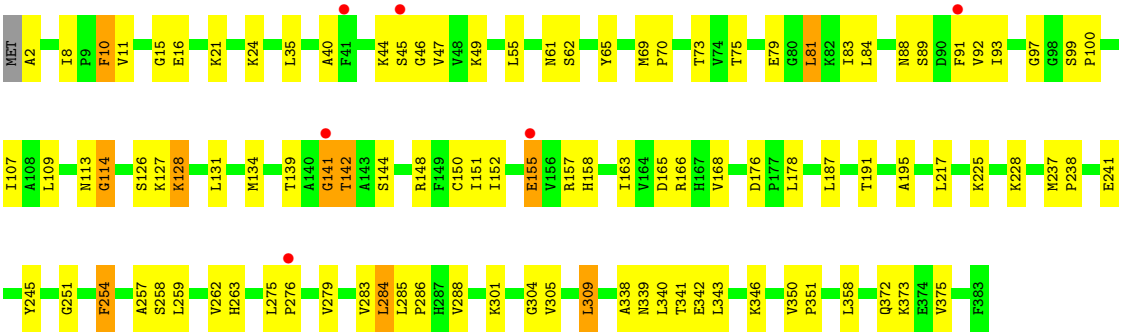
- Molecule 1: Alcohol dehydrogenase 2

Chain A:



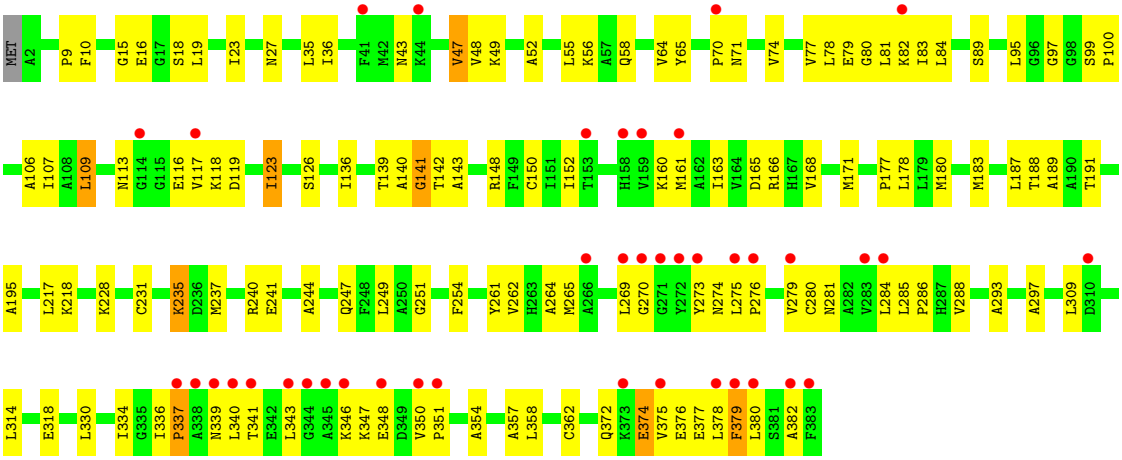
- Molecule 1: Alcohol dehydrogenase 2

Chain B:



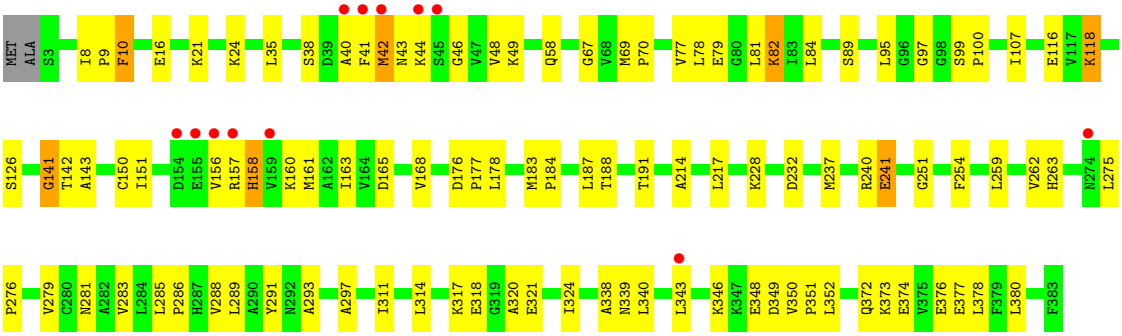
- Molecule 1: Alcohol dehydrogenase 2

Chain C:



- Molecule 1: Alcohol dehydrogenase 2

Chain D:



4 Data and refinement statistics (i)

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 49.88 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.07) 97.1 (49.88-2.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [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)	0.32 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.30	0/2842	0.55	0/3851
1	B	0.31	0/2842	0.57	0/3851
1	C	0.28	0/2842	0.53	0/3851
1	D	0.30	0/2837	0.57	0/3844
All	All	0.30	0/11363	0.56	0/15397

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2798	0	2820	107	0
1	B	2798	0	2820	79	0
1	C	2798	0	2820	117	0
1	D	2793	0	2815	97	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	227	0	0	9	0
3	C	117	0	0	8	0
3	D	193	0	0	5	0
All	All	11939	0	11275	383	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 17.

All (383) 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
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: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:A:3:SER:H	1:B:15:GLY:HA3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.54	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
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: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:141:GLY:HA3	1:B:191:THR:O	1.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:155:GLU:CD	1:B:155:GLU:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:44:LYS:HZ3	1:C:276:PRO:HD3	1.69	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: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: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:16:GLU:OE1	1:C:237:MET:HE2	2.08	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:A:122:GLY:HA3	1:A:125:LYS:HZ3	1.72	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: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:C:346:LYS:NZ	1:C:346:LYS:HB3	2.24	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:A:77:VAL:O	1:A:81:LEU:HB2	2.10	0.51
1:B:127:LYS:C	1:B:128:LYS:HD2	2.31	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:B:46:GLY:HA2	1:B:49:LYS:HZ2	1.75	0.51
1:C:346:LYS:HB3	1:C:346:LYS:HZ2	1.75	0.51
1:A:165:ASP:O	1:A:168:VAL:HG22	2.09	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: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:177:PRO:HG3	1:C:241:GLU:HG2	1.93	0.50
1:B:97:GLY:O	1:B:100:PRO:HD2	2.12	0.50
1:D:346:LYS:NZ	1:D:346:LYS:HB3	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:2:ALA:N	1:B:245:TYR:HH	2.10	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: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:D:352:LEU:C	1:D:352:LEU:HD23	2.33	0.48
1:C:265:MET:HE1	1:C:378:LEU:HD22	1.95	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: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
1:D:42:MET:HE1	3:D:484:HOH:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:140:ALA:HB2	1:C:180:MET:CE	2.45	0.47
1:C:140:ALA:HB2	1:C:180:MET:HE2	1.97	0.47
1:D:43:ASN:CG	1:D:48:VAL:HG11	2.35	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: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:B:92:VAL:HG23	1:B:131:LEU:HD23	1.98	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:118:LYS:HA	1:C:161:MET:HE2	1.98	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
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:C:177:PRO:HG3	1:C:241:GLU:CD	2.37	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:A:123:ILE:N	1:A:125:LYS:HZ3	2.14	0.45
1:C:43:ASN:HA	1:C:48:VAL:CG2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:126:SER:CB	1:D:165:ASP:OD1	2.65	0.44
1:C:265:MET:CE	1:C:378:LEU:HD22	2.47	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
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:D:84:LEU:C	1:D:84:LEU:HD23	2.38	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:B:84:LEU:C	1:B:84:LEU:HD23	2.39	0.43
1:C:339:ASN:C	1:C:341:THR:H	2.22	0.43
1:A:10:PHE:HA	1:B:8:ILE:O	2.18	0.43
1:D:338:ALA:HB1	3:D:436:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:45:SER:OG	1:B:47:VAL:HG23	2.19	0.42
1:D:263:HIS:HA	1:D:281:ASN:HD21	1.84	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: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:A:185:LYS:HD3	1:A:185:LYS:C	2.40	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:B:346:LYS:HB3	1:B:346:LYS:HZ2	1.84	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: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
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:84:LEU:HD23	1:A:84:LEU:C	2.41	0.41
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:B:151:ILE:C	1:B:152:ILE:HD12	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LEU:HD21	1:C:126:SER:HB3	2.03	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:82:LYS:HB3	1:D:82:LYS:HZ2	1.86	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:C:378:LEU:HD23	1:C:378:LEU:C	2.41	0.41
1:C:380:LEU:C	1:C:382:ALA:H	2.24	0.41
1:A:84:LEU:HD23	1:A:84:LEU:O	2.20	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: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
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%)	19 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	380/383 (99%)	363 (96%)	15 (4%)	2 (0%)	29	19
1	C	380/383 (99%)	353 (93%)	24 (6%)	3 (1%)	19	9
1	D	379/383 (99%)	358 (94%)	18 (5%)	3 (1%)	19	9
All	All	1519/1532 (99%)	1436 (94%)	72 (5%)	11 (1%)	22	11

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 (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	294/295 (100%)	282 (96%)	12 (4%)	30	23
1	B	294/295 (100%)	281 (96%)	13 (4%)	28	21
1	C	294/295 (100%)	285 (97%)	9 (3%)	40	34
1	D	294/295 (100%)	287 (98%)	7 (2%)	49	43
All	All	1176/1180 (100%)	1135 (96%)	41 (4%)	36	29

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	39	ASP
1	A	119	ASP
1	A	128	LYS
1	A	142	THR
1	A	148	ARG
1	A	166	ARG
1	A	171	MET
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	128	LYS
1	B	142	THR
1	B	148	ARG
1	B	155	GLU
1	B	166	ARG
1	B	187	LEU
1	B	217	LEU
1	B	254	PHE
1	B	284	LEU
1	B	309	LEU
1	C	109	LEU
1	C	123	ILE
1	C	148	ARG
1	C	166	ARG
1	C	217	LEU
1	C	235	LYS
1	C	348	GLU
1	C	374	GLU
1	C	379	PHE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	274	ASN
1	A	281	ASN
1	A	356	HIS
1	B	61	ASN
1	B	281	ASN
1	B	372	GLN
1	C	61	ASN
1	C	71	ASN
1	C	281	ASN
1	C	287	HIS
1	C	372	GLN
1	D	43	ASN
1	D	50	GLN
1	D	88	ASN
1	D	281	ASN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.04	13 (3%) 45 47	11, 26, 55, 80	0
1	B	382/383 (99%)	-0.11	6 (1%) 72 73	9, 24, 50, 73	0
1	C	382/383 (99%)	0.65	41 (10%) 6 5	13, 39, 73, 90	0
1	D	381/383 (99%)	0.01	12 (3%) 49 52	9, 26, 50, 88	0
All	All	1527/1532 (99%)	0.13	72 (4%) 31 32	9, 28, 64, 90	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	PHE	13.0
1	C	272	TYR	10.6
1	C	340	LEU	8.9
1	A	272	TYR	8.7
1	C	343	LEU	7.1
1	C	375	VAL	7.1
1	D	44	LYS	6.6
1	C	346	LYS	6.6
1	D	159	VAL	6.2
1	D	42	MET	6.1
1	C	338	ALA	5.6
1	D	40	ALA	5.4
1	C	341	THR	5.4
1	C	159	VAL	5.1
1	C	271	GLY	5.1
1	B	41	PHE	5.0
1	C	344	GLY	5.0
1	C	378	LEU	4.9
1	C	350	VAL	4.9
1	C	41	PHE	4.8
1	C	379	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	383	PHE	4.8
1	C	380	LEU	4.7
1	B	141	GLY	4.6
1	C	283	VAL	4.4
1	C	382	ALA	4.1
1	C	276	PRO	4.0
1	C	345	ALA	4.0
1	A	159	VAL	3.9
1	C	273	TYR	3.8
1	C	270	GLY	3.8
1	D	45	SER	3.7
1	A	343	LEU	3.6
1	B	91	PHE	3.6
1	D	157	ARG	3.4
1	D	156	VAL	3.3
1	D	274	ASN	3.2
1	A	2	ALA	3.1
1	C	275	LEU	3.1
1	B	276	PRO	3.1
1	A	273	TYR	3.1
1	D	154	ASP	3.0
1	D	343	LEU	3.0
1	C	279	VAL	3.0
1	C	117	VAL	2.9
1	D	155	GLU	2.9
1	C	284	LEU	2.8
1	C	44	LYS	2.8
1	B	155	GLU	2.8
1	C	351	PRO	2.7
1	A	275	LEU	2.7
1	C	158	HIS	2.7
1	C	114	GLY	2.6
1	A	373	LYS	2.5
1	A	41	PHE	2.5
1	A	157	ARG	2.5
1	C	269	LEU	2.5
1	A	154	ASP	2.3
1	C	310	ASP	2.3
1	B	45	SER	2.3
1	C	161	MET	2.3
1	C	348	GLU	2.2
1	C	373	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	338	ALA	2.1
1	C	70	PRO	2.1
1	C	82	LYS	2.1
1	C	337	PRO	2.1
1	C	339	ASN	2.1
1	C	153	THR	2.1
1	C	266	ALA	2.1
1	A	141	GLY	2.0
1	A	153	THR	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 monosaccharides 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	0.10	0.58	105,105,105,105	0
2	FE2	A	384	1/1	0.98	0.09	23,23,23,23	0
2	FE2	C	384	1/1	0.98	0.07	33,33,33,33	0
2	FE2	D	384	1/1	1.00	0.11	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.