



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:20 PM GMT

PDB ID : 2CFY
Title : CRYSTAL STRUCTURE OF HUMAN THIOREDOXIN REDUCTASE 1
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Deposited on : 2006-02-26
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

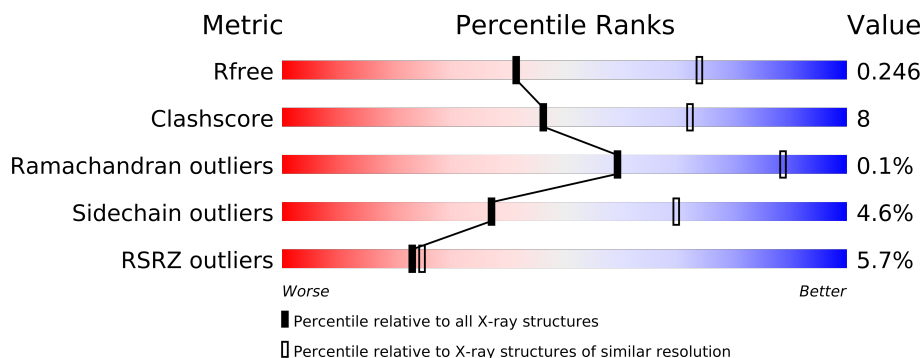
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	521	
1	B	521	
1	C	521	
1	D	521	
1	E	521	
1	F	521	

2 Entry composition i

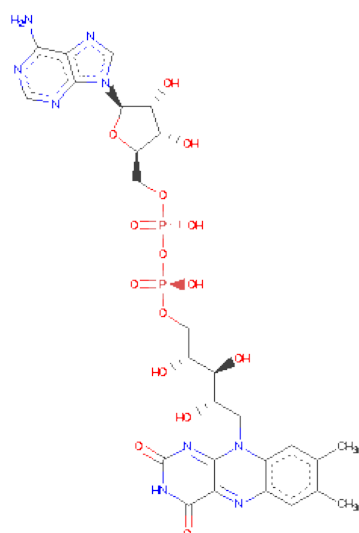
There are 3 unique types of molecules in this entry. The entry contains 22479 atoms, of which 0 are hydrogen and 0 are deuterium.

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 THIOREDOXIN REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3687	2354	619	695	19			
1	B	484	Total	C	N	O	S	0	1	0
			3698	2363	619	697	19			
1	C	484	Total	C	N	O	S	0	0	0
			3702	2360	624	699	19			
1	D	484	Total	C	N	O	S	0	0	0
			3692	2356	618	699	19			
1	E	484	Total	C	N	O	S	0	0	0
			3576	2282	593	682	19			
1	F	484	Total	C	N	O	S	0	0	0
			3624	2314	602	689	19			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			33	14	5	12	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

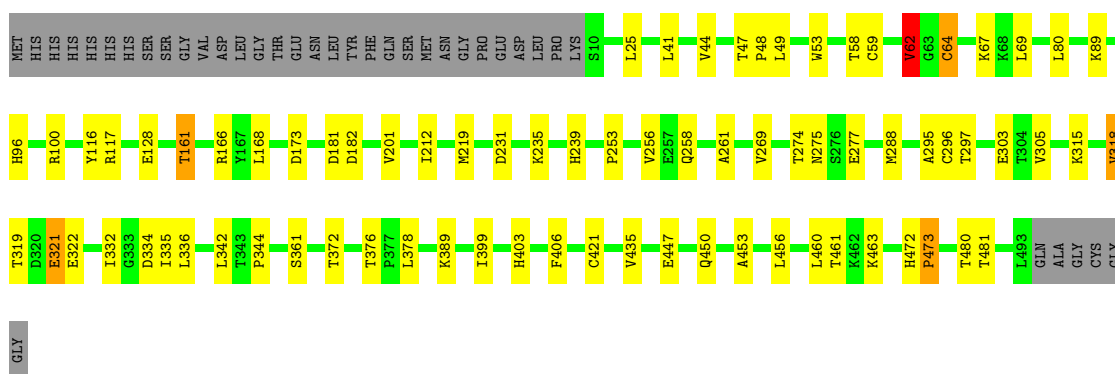
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	53	Total	O	0	0
			53	53		
3	C	57	Total	O	0	0
			57	57		
3	D	59	Total	O	0	0
			59	59		
3	E	1	Total	O	0	0
			1	1		
3	F	6	Total	O	0	0
			6	6		

3 Residue-property plots

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

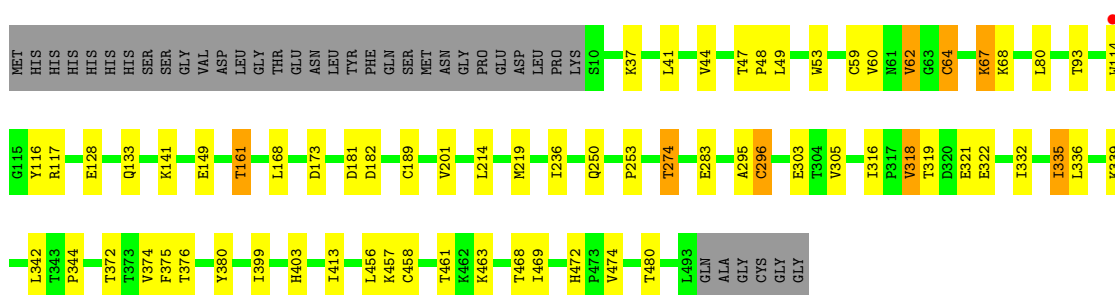
• Molecule 1: THIOREDOXIN REDUCTASE 1

Chain A:



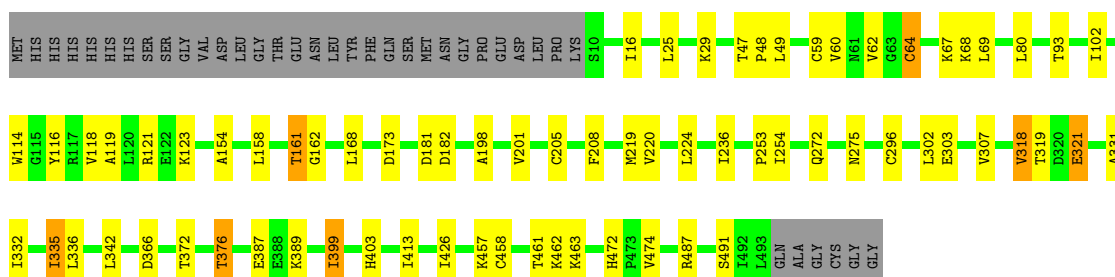
• Molecule 1: THIOREDOXIN REDUCTASE 1

Chain B:



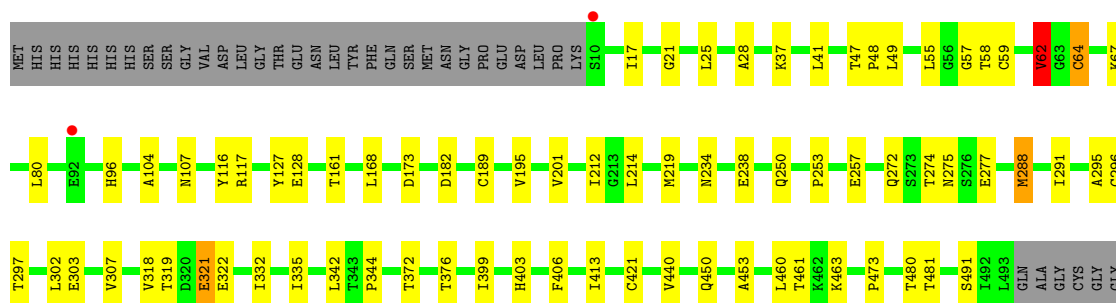
• Molecule 1: THIOREDOXIN REDUCTASE 1

Chain C:



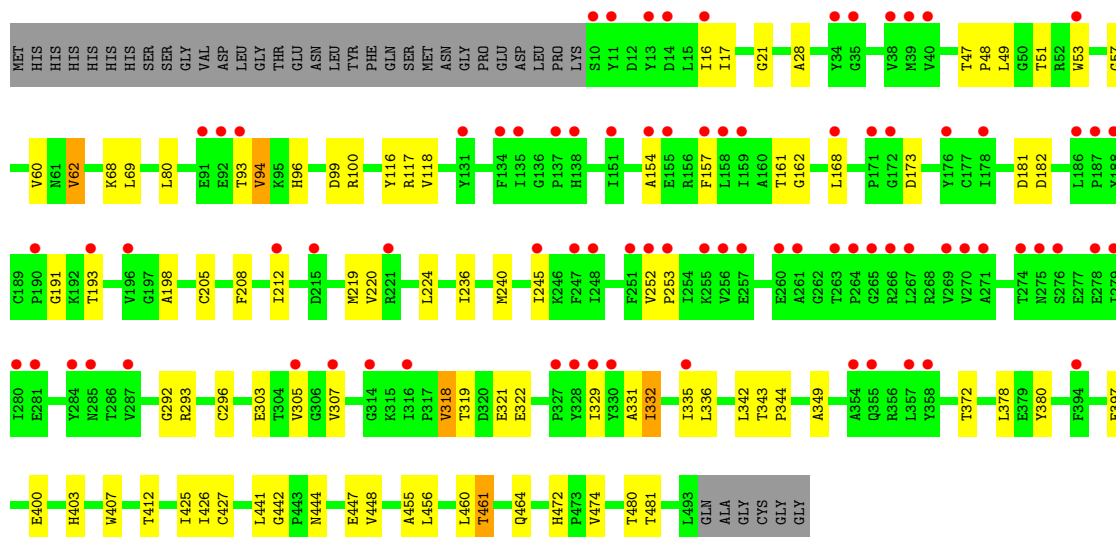
• Molecule 1: THIOREDOXIN REDUCTASE 1

Chain D:



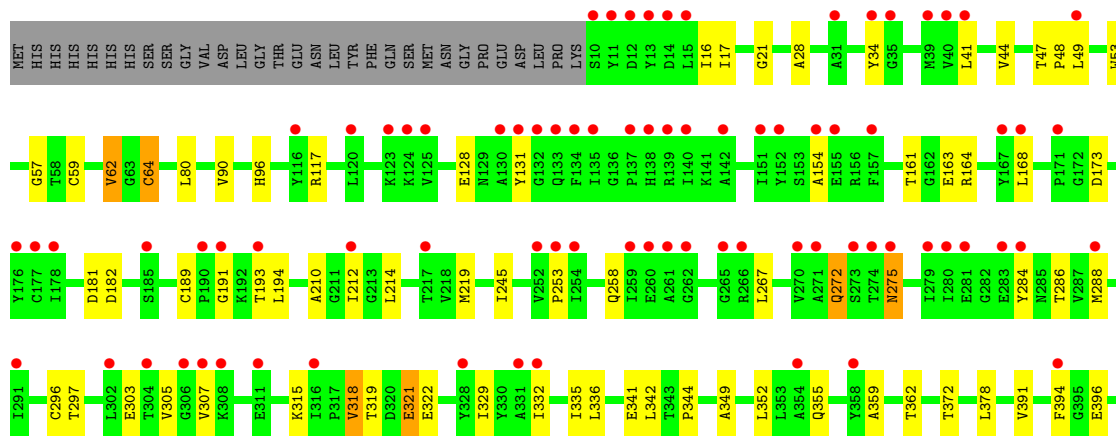
• Molecule 1: THIOREDOXIN REDUCTASE 1

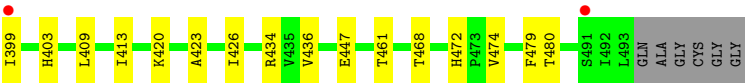
Chain E:



• Molecule 1: THIOREDOXIN REDUCTASE 1

Chain F:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.76Å 149.65Å 146.79Å 90.00° 91.96° 90.00°	Depositor
Resolution (Å)	149.07 – 2.70 47.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (149.07-2.70) 95.0 (47.23-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.248 0.204 , 0.246	Depositor DCC
R_{free} test set	5025 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 13.3	EDS
Estimated twinning fraction	0.001 for -h,-l,-k 0.000 for -h,l,k 0.036 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 100946 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22479	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.58	0/3761	0.66	1/5104 (0.0%)
1	B	0.58	1/3777 (0.0%)	0.63	0/5128
1	C	0.59	0/3776	0.66	0/5123
1	D	0.57	0/3766	0.63	0/5110
1	E	0.44	0/3649	0.54	0/4973
1	F	0.43	0/3698	0.55	0/5034
All	All	0.54	1/22427 (0.0%)	0.61	1/30472 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	CYS	CB-SG	-5.68	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3687	0	3635	62	0
1	B	3698	0	3638	55	0
1	C	3702	0	3655	61	0
1	D	3692	0	3644	57	0
1	E	3576	0	3397	76	0
1	F	3624	0	3509	75	0
2	A	53	0	31	3	0
2	B	53	0	31	5	0
2	C	53	0	31	3	0
2	D	53	0	31	2	0
2	E	33	0	18	2	0
2	F	27	0	11	2	0
3	A	52	0	0	1	0
3	B	53	0	0	0	0
3	C	57	0	0	1	0
3	D	59	0	0	0	0
3	E	1	0	0	0	0
3	F	6	0	0	0	0
All	All	22479	0	21631	357	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (357) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:342:LEU:HD11	1:E:372:THR:HG22	1.45	0.95
1:A:480:THR:HG21	3:A:2050:HOH:O	1.67	0.93
1:D:47:THR:HG22	1:D:49:LEU:H	1.34	0.93
1:F:332:ILE:HD11	1:F:349:ALA:CB	1.99	0.92
1:F:59:CYS:HG	1:F:64:CYS:HG	0.92	0.91
1:A:47:THR:HG22	1:A:49:LEU:H	1.35	0.91
1:E:332:ILE:HD11	1:E:349:ALA:HB1	1.51	0.90
1:C:342:LEU:HD11	1:C:372:THR:HG22	1.55	0.87
1:B:47:THR:HG22	1:B:49:LEU:H	1.43	0.84
1:D:168:LEU:HD23	1:D:291:ILE:HD13	1.58	0.83
1:C:47:THR:HG22	1:C:49:LEU:H	1.42	0.82
1:C:80:LEU:HD23	1:D:80:LEU:CD2	2.08	0.82
1:E:161:THR:HG22	1:E:296:CYS:HB2	1.61	0.82
1:F:332:ILE:HD11	1:F:349:ALA:HB1	1.59	0.81
1:F:322:GLU:HG2	1:F:332:ILE:HD13	1.61	0.81
1:F:297:THR:HG23	1:F:335:ILE:HD12	1.63	0.80
1:C:59:CYS:HG	1:C:64:CYS:HG	1.18	0.80
1:F:342:LEU:HD11	1:F:372:THR:HG22	1.64	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.65	0.78
1:C:161:THR:HG21	1:C:296:CYS:O	1.84	0.78
1:D:161:THR:HG22	1:D:335:ILE:HG13	1.66	0.77
1:B:168:LEU:O	1:B:173:ASP:OD2	2.03	0.77
1:C:161:THR:HG23	1:C:296:CYS:HB2	1.66	0.75
1:D:47:THR:HG22	1:D:49:LEU:N	2.01	0.74
1:F:210:ALA:HB2	1:F:245:ILE:HD11	1.70	0.73
1:D:41:LEU:HD23	1:D:128:GLU:HB3	1.71	0.73
1:C:201:VAL:HG22	2:C:600:FAD:HM73	1.71	0.73
1:A:219:MET:HE2	1:A:253:PRO:HD3	1.70	0.73
1:B:59:CYS:HG	1:B:64:CYS:HG	0.72	0.72
1:E:80:LEU:HD22	1:F:80:LEU:HD23	1.69	0.72
1:F:219:MET:HE1	1:F:253:PRO:CD	2.20	0.72
1:C:62:VAL:CG1	1:C:62:VAL:O	2.37	0.72
1:F:62:VAL:CG1	1:F:62:VAL:O	2.38	0.71
1:F:468:THR:O	1:F:480:THR:HG23	1.91	0.71
1:C:80:LEU:HD23	1:D:80:LEU:HD23	1.72	0.70
1:E:161:THR:HG23	2:E:600:FAD:N7A	2.06	0.70
1:D:62:VAL:HG13	1:D:62:VAL:O	1.91	0.70
1:B:62:VAL:O	1:B:62:VAL:CG1	2.39	0.70
1:A:47:THR:HG22	1:A:49:LEU:N	2.06	0.70
1:E:62:VAL:O	1:E:62:VAL:CG1	2.41	0.69
1:A:62:VAL:CG2	1:A:181:ASP:HA	2.23	0.69
1:C:47:THR:HG21	1:C:182:ASP:OD1	1.93	0.69
1:C:62:VAL:HG13	1:C:62:VAL:O	1.92	0.69
1:F:219:MET:HE1	1:F:253:PRO:HD3	1.74	0.68
1:A:219:MET:CE	1:A:253:PRO:HD3	2.24	0.68
1:F:161:THR:HG22	1:F:335:ILE:HG13	1.75	0.68
1:A:161:THR:HG21	1:A:296:CYS:O	1.93	0.67
1:A:212:ILE:HG22	1:A:212:ILE:O	1.93	0.67
1:B:342:LEU:HD11	1:B:372:THR:HG22	1.75	0.67
1:D:47:THR:HG21	1:D:182:ASP:OD1	1.95	0.67
1:B:201:VAL:HG22	2:B:600:FAD:HM73	1.76	0.66
1:C:198:ALA:HB2	1:C:220:VAL:HG13	1.76	0.66
1:B:342:LEU:HD11	1:B:372:THR:CG2	2.24	0.66
1:D:342:LEU:HD11	1:D:372:THR:CG2	2.24	0.66
1:B:374:VAL:HG12	1:B:376:THR:HG23	1.76	0.66
1:B:161:THR:HG21	1:B:296:CYS:O	1.95	0.66
1:A:80:LEU:HD23	1:B:80:LEU:CD2	2.26	0.66
1:A:256:VAL:HG22	1:A:269:VAL:HG22	1.79	0.65
1:C:342:LEU:CD1	1:C:372:THR:HG22	2.26	0.65
1:E:322:GLU:HG2	1:E:332:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:HIS:ND1	1:A:212:ILE:HG23	2.12	0.65
1:F:219:MET:CE	1:F:253:PRO:HD3	2.27	0.65
1:A:161:THR:HG23	1:A:296:CYS:HB2	1.79	0.64
1:F:332:ILE:CD1	1:F:349:ALA:HB1	2.25	0.64
1:F:62:VAL:HG11	1:F:181:ASP:OD1	1.98	0.64
1:B:62:VAL:O	1:B:62:VAL:HG13	1.97	0.64
1:E:378:LEU:HD11	1:E:442:GLY:HA2	1.79	0.64
1:B:468:THR:O	1:B:480:THR:HG23	1.98	0.63
1:F:258:GLN:HA	1:F:267:LEU:HD23	1.81	0.63
1:E:80:LEU:CD2	1:F:80:LEU:HD23	2.28	0.63
1:D:297:THR:HG23	1:D:335:ILE:HD12	1.80	0.62
1:B:161:THR:HG23	1:B:296:CYS:HB2	1.80	0.62
1:D:219:MET:CE	1:D:253:PRO:HG3	2.29	0.62
1:F:342:LEU:HD11	1:F:372:THR:CG2	2.27	0.62
1:D:62:VAL:O	1:D:62:VAL:CG1	2.47	0.62
1:E:305:VAL:HG21	1:E:329:ILE:HD11	1.81	0.62
1:A:201:VAL:HG22	2:A:600:FAD:HM73	1.82	0.62
1:F:342:LEU:CD1	1:F:372:THR:HG22	2.29	0.61
1:E:161:THR:HG23	2:E:600:FAD:C8A	2.30	0.61
1:F:96:HIS:CD2	1:F:212:ILE:HD12	2.35	0.61
1:C:80:LEU:HD23	1:D:80:LEU:HD22	1.80	0.61
1:F:62:VAL:HG13	1:F:62:VAL:O	1.99	0.61
1:E:198:ALA:HB2	1:E:220:VAL:HG13	1.82	0.61
1:A:69:LEU:HD13	1:B:413:ILE:HD11	1.82	0.61
1:D:219:MET:HE1	1:D:253:PRO:HG3	1.83	0.60
1:E:47:THR:HG21	1:E:182:ASP:OD1	2.00	0.60
1:E:47:THR:HG23	1:E:48:PRO:HD2	1.83	0.60
1:C:201:VAL:CG2	2:C:600:FAD:HM73	2.32	0.60
1:E:455:ALA:HB1	1:E:460:LEU:HD22	1.83	0.60
1:D:168:LEU:CD2	1:D:291:ILE:HD13	2.32	0.59
1:F:168:LEU:O	1:F:173:ASP:OD2	2.21	0.59
1:B:201:VAL:HG13	2:B:600:FAD:HM73	1.85	0.59
1:E:47:THR:HG22	1:E:49:LEU:H	1.67	0.59
1:B:161:THR:HG22	1:B:335:ILE:HG13	1.84	0.59
1:C:219:MET:CE	1:C:253:PRO:HG3	2.32	0.59
1:A:64:CYS:SG	2:A:600:FAD:C10	2.90	0.59
1:A:62:VAL:HG22	1:A:181:ASP:HA	1.84	0.59
1:D:480:THR:HG22	1:D:481:THR:HG23	1.85	0.59
1:F:191:GLY:O	1:F:193:THR:HG23	2.03	0.59
1:A:212:ILE:O	1:A:212:ILE:CG2	2.50	0.58
1:B:201:VAL:CG2	2:B:600:FAD:HM73	2.32	0.58
1:A:168:LEU:O	1:A:173:ASP:OD2	2.21	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:47:THR:HG21	1:F:182:ASP:OD1	2.04	0.58
1:A:41:LEU:HD23	1:A:128:GLU:HB3	1.86	0.58
1:D:17:ILE:HD12	1:D:28:ALA:HB2	1.86	0.58
1:D:342:LEU:HD11	1:D:372:THR:HG22	1.87	0.57
1:D:295:ALA:HB1	1:D:335:ILE:CD1	2.34	0.57
1:D:201:VAL:HG22	2:D:600:FAD:HM73	1.87	0.57
1:F:161:THR:HG21	1:F:296:CYS:O	2.04	0.57
1:F:210:ALA:HB2	1:F:245:ILE:CD1	2.35	0.57
1:C:219:MET:CE	1:C:253:PRO:HD3	2.35	0.57
1:C:342:LEU:HD11	1:C:372:THR:CG2	2.30	0.57
1:E:212:ILE:O	1:E:212:ILE:HG22	2.02	0.57
1:E:191:GLY:O	1:E:193:THR:HG23	2.05	0.57
1:A:219:MET:CE	1:A:253:PRO:CD	2.82	0.56
1:E:342:LEU:CD1	1:E:372:THR:HG22	2.27	0.56
1:A:161:THR:HG22	1:A:335:ILE:HG13	1.86	0.56
1:C:219:MET:CE	1:C:253:PRO:CD	2.83	0.56
1:A:47:THR:HG21	1:A:182:ASP:OD1	2.04	0.56
1:D:55:LEU:HD13	1:D:127:TYR:CE1	2.41	0.56
1:C:16:ILE:HG13	1:C:154:ALA:HB2	1.86	0.56
1:E:53:TRP:CZ3	1:E:62:VAL:HG21	2.41	0.56
1:D:195:VAL:HG22	1:D:288:MET:HE2	1.86	0.56
1:F:315:LYS:NZ	1:F:341:GLU:OE2	2.39	0.56
1:F:394:PHE:HB2	1:F:399:ILE:HD11	1.87	0.55
1:B:250:GLN:HB3	1:B:274:THR:HG22	1.89	0.55
1:F:219:MET:HE1	1:F:253:PRO:N	2.21	0.55
1:D:96:HIS:ND1	1:D:212:ILE:HG23	2.22	0.55
1:C:47:THR:HG22	1:C:49:LEU:N	2.19	0.55
1:B:318:VAL:HG13	1:B:319:THR:O	2.06	0.55
1:A:480:THR:HG22	1:A:481:THR:HG23	1.89	0.54
1:D:47:THR:HG23	1:D:48:PRO:HD2	1.89	0.54
1:B:161:THR:HG22	1:B:335:ILE:CG1	2.37	0.54
1:E:318:VAL:HG13	1:E:319:THR:O	2.07	0.54
1:F:305:VAL:HG13	1:F:307:VAL:HG23	1.89	0.54
1:E:461:THR:HG22	1:E:464:GLN:H	1.73	0.54
1:F:332:ILE:HD11	1:F:349:ALA:HB3	1.88	0.54
1:A:47:THR:HG23	1:A:48:PRO:HD2	1.89	0.54
1:B:316:ILE:HD12	1:B:335:ILE:CG2	2.37	0.54
1:F:275:ASN:OD1	1:F:275:ASN:N	2.39	0.54
1:B:62:VAL:HG11	1:B:181:ASP:OD1	2.08	0.53
1:E:80:LEU:HD22	1:F:80:LEU:CD2	2.36	0.53
1:D:219:MET:HE3	1:D:253:PRO:HD3	1.90	0.53
1:C:161:THR:CG2	1:C:296:CYS:O	2.54	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:25:LEU:HD13	1:A:116:TYR:CD1	2.43	0.53
1:F:96:HIS:CG	1:F:212:ILE:HD12	2.43	0.53
1:C:461:THR:HG22	1:C:463:LYS:N	2.24	0.53
1:B:201:VAL:CG1	2:B:600:FAD:HM73	2.39	0.53
1:E:472:HIS:HB2	1:F:344:PRO:HG3	1.90	0.53
1:E:474:VAL:HG13	1:F:447:GLU:CD	2.29	0.53
1:E:305:VAL:HG13	1:E:307:VAL:HG23	1.89	0.52
1:B:47:THR:HG21	1:B:182:ASP:OD1	2.09	0.52
1:D:58:THR:HG23	1:D:62:VAL:HG12	1.91	0.52
1:A:62:VAL:HG21	1:A:181:ASP:HA	1.90	0.52
1:B:322:GLU:HG2	1:B:332:ILE:HG22	1.92	0.52
1:C:69:LEU:HD22	1:D:413:ILE:HD12	1.92	0.52
1:E:332:ILE:HD11	1:E:349:ALA:CB	2.31	0.52
1:D:161:THR:HG21	1:D:296:CYS:O	2.09	0.52
1:B:295:ALA:HB1	1:B:335:ILE:HD12	1.92	0.52
1:F:332:ILE:CD1	1:F:349:ALA:CB	2.80	0.51
1:F:210:ALA:CB	1:F:245:ILE:HD11	2.38	0.51
1:C:168:LEU:O	1:C:173:ASP:OD2	2.28	0.51
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.93	0.51
1:C:219:MET:HE1	1:C:253:PRO:HG3	1.93	0.51
1:D:322:GLU:HG2	1:D:332:ILE:HG22	1.93	0.51
1:E:480:THR:HG22	1:E:481:THR:HG23	1.92	0.51
1:B:47:THR:HG23	1:B:48:PRO:HD2	1.92	0.51
1:B:374:VAL:CG1	1:B:376:THR:HG23	2.41	0.51
1:A:461:THR:HG22	1:A:463:LYS:N	2.26	0.50
1:E:344:PRO:HG3	1:F:472:HIS:HB2	1.93	0.50
1:A:322:GLU:HG2	1:A:332:ILE:HG22	1.93	0.50
1:A:342:LEU:HD11	1:A:372:THR:CG2	2.41	0.50
1:D:234:ASN:O	1:D:238:GLU:HG3	2.11	0.50
1:E:16:ILE:CD1	1:E:154:ALA:HB2	2.42	0.50
1:B:316:ILE:HD12	1:B:335:ILE:HG21	1.94	0.50
1:E:62:VAL:O	1:E:62:VAL:HG12	2.12	0.49
1:F:47:THR:HG21	1:F:182:ASP:OD2	2.12	0.49
1:A:295:ALA:HB1	1:A:335:ILE:CD1	2.41	0.49
1:E:96:HIS:CE1	1:E:212:ILE:HD12	2.47	0.49
1:F:305:VAL:HG21	1:F:329:ILE:HD11	1.93	0.49
1:E:17:ILE:HD12	1:E:28:ALA:HB2	1.94	0.49
1:B:336:LEU:HD23	1:B:339:LYS:HG3	1.94	0.49
1:A:318:VAL:HG13	1:A:319:THR:O	2.13	0.49
1:A:435:VAL:O	1:A:456:LEU:HD22	2.13	0.49
1:F:17:ILE:HD12	1:F:28:ALA:HB2	1.94	0.49
1:C:318:VAL:HG13	1:C:319:THR:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:16:ILE:HD12	1:E:154:ALA:HB2	1.94	0.49
1:E:94:VAL:HG11	1:F:90:VAL:HG22	1.94	0.49
1:C:161:THR:HG22	1:C:335:ILE:HG12	1.95	0.49
1:F:47:THR:HG22	1:F:49:LEU:H	1.77	0.49
1:E:162:GLY:N	1:E:335:ILE:HD11	2.28	0.49
1:F:194:LEU:HD13	1:F:284:TYR:CZ	2.48	0.49
1:E:205:CYS:HA	1:E:208:PHE:CE2	2.47	0.48
1:E:425:ILE:HD12	1:E:427:CYS:SG	2.53	0.48
1:C:60:VAL:HG21	1:C:116:TYR:HE2	1.78	0.48
1:C:413:ILE:HD13	1:D:104:ALA:HB1	1.94	0.48
1:D:302:LEU:HD22	1:D:307:VAL:HB	1.96	0.48
1:C:47:THR:HG23	1:C:48:PRO:HD2	1.94	0.48
1:A:59:CYS:CB	1:A:64:CYS:HG	2.26	0.48
1:B:342:LEU:CD1	1:B:372:THR:HG22	2.43	0.48
1:E:318:VAL:HG22	1:E:322:GLU:C	2.34	0.48
1:E:62:VAL:HG11	1:E:181:ASP:OD1	2.14	0.48
1:A:406:PHE:CZ	1:A:421:CYS:HB3	2.48	0.48
1:C:62:VAL:HG11	1:C:181:ASP:OD1	2.14	0.48
1:E:62:VAL:O	1:E:62:VAL:HG13	2.12	0.48
1:C:68:LYS:HE2	3:C:2007:HOH:O	2.14	0.48
1:A:297:THR:HG23	1:A:335:ILE:HD12	1.95	0.48
1:E:461:THR:HG22	1:E:464:GLN:HG3	1.96	0.48
1:F:193:THR:HG22	1:F:286:THR:HB	1.96	0.48
1:F:391:VAL:HG13	1:F:396:GLU:CA	2.43	0.48
1:F:434:ARG:HH11	1:F:461:THR:HG22	1.79	0.48
1:E:236:ILE:HD11	1:E:380:TYR:HB2	1.96	0.47
1:E:426:ILE:HD12	1:E:426:ILE:N	2.29	0.47
1:A:319:THR:C	1:A:321:GLU:H	2.18	0.47
1:C:162:GLY:O	1:C:335:ILE:HD11	2.15	0.47
1:E:96:HIS:ND1	1:E:212:ILE:HG23	2.30	0.47
1:E:69:LEU:HD22	1:F:413:ILE:HD12	1.97	0.47
1:E:331:ALA:C	1:E:336:LEU:HD11	2.34	0.47
1:D:440:VAL:O	1:D:440:VAL:HG13	2.14	0.47
1:D:25:LEU:HD13	1:D:116:TYR:CD1	2.49	0.47
1:C:366:ASP:OD2	1:C:457:LYS:HE3	2.15	0.47
1:E:219:MET:CE	1:E:253:PRO:HD3	2.44	0.47
1:C:219:MET:HE2	1:C:253:PRO:HG3	1.97	0.47
1:B:114[B]:TRP:CD1	1:C:114:TRP:CD1	3.02	0.47
1:C:205:CYS:HA	1:C:208:PHE:CE2	2.50	0.47
1:D:219:MET:CE	1:D:253:PRO:HD3	2.45	0.47
1:F:212:ILE:O	1:F:212:ILE:CG2	2.62	0.47
1:F:16:ILE:HG13	1:F:154:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:168:LEU:O	1:D:173:ASP:OD2	2.33	0.46
1:E:154:ALA:HB3	1:E:157:PHE:CE1	2.50	0.46
1:F:318:VAL:HG22	1:F:322:GLU:C	2.36	0.46
1:A:44:VAL:HG11	1:A:53:TRP:CE2	2.50	0.46
1:A:258:GLN:OE1	1:A:261:ALA:HB2	2.15	0.46
1:F:34:TYR:CE2	1:F:359:ALA:HB2	2.50	0.46
1:F:164:ARG:HG2	1:F:296:CYS:SG	2.56	0.46
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.50	0.46
1:A:342:LEU:HD11	1:A:372:THR:HG23	1.97	0.46
1:E:60:VAL:HG21	1:E:116:TYR:HE2	1.81	0.46
1:C:458:CYS:SG	1:D:460:LEU:HD12	2.56	0.46
1:B:41:LEU:HD23	1:B:128:GLU:HB2	1.97	0.46
1:A:318:VAL:HG22	1:A:322:GLU:C	2.36	0.46
1:A:450:GLN:O	1:A:453:ALA:HB3	2.16	0.46
1:F:47:THR:HG23	1:F:48:PRO:HD2	1.98	0.46
1:E:461:THR:CG2	1:E:464:GLN:H	2.29	0.46
1:C:413:ILE:HD13	1:D:104:ALA:CB	2.46	0.46
1:E:240:MET:HB3	1:E:245:ILE:HD12	1.98	0.45
1:D:461:THR:HG22	1:D:463:LYS:N	2.30	0.45
1:C:25:LEU:O	1:C:29:LYS:HD3	2.16	0.45
1:C:201:VAL:HG13	2:C:600:FAD:HM73	1.98	0.45
1:D:342:LEU:CD1	1:D:372:THR:HG22	2.46	0.45
1:F:352:LEU:HD23	1:F:355:GLN:NE2	2.30	0.45
1:B:461:THR:HG22	1:B:463:LYS:H	1.82	0.45
1:E:305:VAL:CG2	1:E:329:ILE:HD11	2.47	0.45
1:E:219:MET:HE1	1:E:252:VAL:CA	2.47	0.45
1:C:162:GLY:O	1:C:335:ILE:CD1	2.65	0.45
1:E:460:LEU:HD12	1:E:461:THR:H	1.82	0.45
1:E:219:MET:HE1	1:E:253:PRO:N	2.32	0.45
1:D:319:THR:C	1:D:321:GLU:H	2.20	0.45
1:D:64:CYS:SG	2:D:600:FAD:C10	3.05	0.45
1:F:44:VAL:HG11	1:F:53:TRP:CE2	2.52	0.45
1:E:447:GLU:CD	1:F:474:VAL:HG13	2.38	0.45
1:C:387:GLU:HA	1:C:426:ILE:HD13	1.99	0.44
1:A:344:PRO:HB2	1:B:469:ILE:CG2	2.47	0.44
1:C:59:CYS:CB	1:C:64:CYS:HG	2.30	0.44
1:F:47:THR:HG21	1:F:182:ASP:CG	2.37	0.44
1:F:391:VAL:HG13	1:F:396:GLU:HA	2.00	0.44
1:B:114[A]:TRP:CZ3	1:C:118:VAL:HG21	2.52	0.44
1:B:67:LYS:HZ3	1:B:375:PHE:HD1	1.63	0.44
1:E:305:VAL:HG22	1:E:305:VAL:O	2.18	0.44
1:B:44:VAL:HG11	1:B:53:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:MET:HE2	1:B:253:PRO:HD3	1.99	0.44
1:F:272:GLN:HB3	1:F:272:GLN:HE21	1.61	0.44
1:B:141:LYS:NZ	1:B:149:GLU:OE2	2.45	0.44
1:B:461:THR:HG22	1:B:463:LYS:N	2.32	0.44
1:C:119:ALA:O	1:C:123:LYS:HG3	2.18	0.44
1:C:319:THR:C	1:C:321:GLU:H	2.22	0.44
1:F:41:LEU:HD23	1:F:128:GLU:HB3	1.99	0.44
1:D:250:GLN:HB3	1:D:274:THR:OG1	2.17	0.44
1:E:68:LYS:HG2	1:F:409:LEU:HD23	2.00	0.44
1:B:201:VAL:HG22	2:B:600:FAD:C7M	2.46	0.43
1:A:344:PRO:HG3	1:B:472:HIS:HB2	2.00	0.43
1:D:21:GLY:HA2	1:D:57:GLY:HA3	2.00	0.43
1:E:292:GLY:C	1:E:293:ARG:HG2	2.38	0.43
1:D:189:CYS:SG	1:D:214:LEU:HD21	2.57	0.43
1:A:480:THR:HG22	1:A:481:THR:CG2	2.48	0.43
1:C:219:MET:CE	1:C:253:PRO:CG	2.96	0.43
1:F:319:THR:C	1:F:321:GLU:H	2.22	0.43
1:B:319:THR:C	1:B:321:GLU:H	2.22	0.43
1:A:41:LEU:CD2	1:A:128:GLU:HB3	2.48	0.43
1:E:168:LEU:O	1:E:173:ASP:OD2	2.37	0.43
1:A:59:CYS:SG	1:A:64:CYS:SG	3.06	0.42
1:D:480:THR:HG22	1:D:481:THR:CG2	2.48	0.42
1:C:461:THR:CG2	1:C:462:LYS:N	2.81	0.42
1:C:236:ILE:HG21	1:C:376:THR:HG21	2.00	0.42
1:A:473:PRO:O	1:B:68:LYS:NZ	2.49	0.42
1:B:47:THR:HG22	1:B:49:LEU:N	2.22	0.42
1:D:195:VAL:HG22	1:D:288:MET:CE	2.50	0.42
1:C:472:HIS:HB2	1:D:344:PRO:HG3	2.01	0.42
1:F:219:MET:CE	1:F:253:PRO:CD	2.92	0.42
1:C:254:ILE:HD13	1:C:272:GLN:HB2	2.02	0.42
1:F:423:ALA:HB1	1:F:479:PHE:CE1	2.54	0.42
1:E:322:GLU:HG2	1:E:332:ILE:CD1	2.49	0.42
1:A:219:MET:HE1	1:A:253:PRO:CD	2.50	0.42
1:A:58:THR:HA	1:A:62:VAL:HG12	2.01	0.42
1:B:114[B]:TRP:CZ2	1:B:117:ARG:NH1	2.88	0.42
1:A:96:HIS:CE1	1:A:212:ILE:HD13	2.55	0.42
1:D:59:CYS:CB	1:D:64:CYS:HG	2.32	0.42
1:F:131:TYR:CE1	2:F:600:FAD:N6A	2.88	0.41
1:E:161:THR:HG22	1:E:296:CYS:CB	2.41	0.41
1:B:189:CYS:SG	1:B:214:LEU:HD21	2.60	0.41
1:A:447:GLU:CD	1:B:474:VAL:HG13	2.41	0.41
1:F:426:ILE:HD12	1:F:426:ILE:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:426:ILE:HG22	1:F:436:VAL:HG22	2.01	0.41
1:C:198:ALA:HB1	1:C:224:LEU:HA	2.02	0.41
1:D:219:MET:HE1	1:D:253:PRO:CG	2.49	0.41
1:E:212:ILE:O	1:E:212:ILE:CG2	2.68	0.41
1:C:331:ALA:O	1:C:336:LEU:HD11	2.20	0.41
1:C:335:ILE:HA	1:C:335:ILE:HD12	1.70	0.41
1:E:198:ALA:HB1	1:E:224:LEU:HA	2.03	0.41
1:A:461:THR:HG22	1:A:463:LYS:H	1.85	0.41
1:E:219:MET:HE1	1:E:252:VAL:C	2.41	0.41
1:F:21:GLY:HA2	1:F:57:GLY:HA3	2.02	0.41
1:A:201:VAL:CG2	2:A:600:FAD:HM73	2.50	0.41
1:E:47:THR:CG2	1:E:48:PRO:HD2	2.49	0.41
1:C:219:MET:HE3	1:C:253:PRO:HD3	2.02	0.41
1:C:158:LEU:HD11	1:C:332:ILE:HG23	2.02	0.41
1:E:407:TRP:CZ2	1:E:412:THR:HA	2.56	0.41
1:D:47:THR:CG2	1:D:49:LEU:H	2.18	0.41
1:B:236:ILE:HD11	1:B:380:TYR:HB2	2.03	0.41
1:C:102:ILE:N	1:C:102:ILE:HD13	2.36	0.41
1:C:399:ILE:HD12	1:C:399:ILE:HA	1.86	0.41
1:E:444:ASN:O	1:E:448:VAL:HG23	2.21	0.41
1:E:21:GLY:HA2	1:E:57:GLY:HA3	2.03	0.41
1:F:394:PHE:HB2	1:F:399:ILE:CD1	2.50	0.41
1:E:480:THR:HG22	1:E:481:THR:CG2	2.50	0.41
1:B:60:VAL:HG21	1:B:116:TYR:HE2	1.86	0.41
1:A:239:HIS:CE1	1:A:378:LEU:HB2	2.56	0.41
1:E:303:GLU:CD	1:E:303:GLU:H	2.24	0.41
1:A:231:ASP:O	1:A:235:LYS:HG3	2.20	0.41
1:A:212:ILE:HG21	1:A:212:ILE:HD13	1.81	0.41
1:D:212:ILE:HG22	1:D:212:ILE:O	2.21	0.41
1:F:189:CYS:SG	1:F:214:LEU:HD21	2.60	0.41
1:D:297:THR:CG2	1:D:335:ILE:HD12	2.49	0.40
1:D:450:GLN:O	1:D:453:ALA:HB3	2.21	0.40
1:E:319:THR:C	1:E:321:GLU:H	2.24	0.40
1:A:219:MET:HE1	1:A:253:PRO:N	2.37	0.40
1:E:53:TRP:CH2	1:E:62:VAL:HG21	2.56	0.40
1:F:378:LEU:HA	1:F:378:LEU:HD12	1.85	0.40
1:D:295:ALA:HB1	1:D:335:ILE:HD12	2.01	0.40
1:E:378:LEU:HD23	1:E:441:LEU:HD21	2.03	0.40
1:A:315:LYS:NZ	1:A:334:ASP:O	2.52	0.40
1:B:236:ILE:HG21	1:B:376:THR:HG21	2.03	0.40
1:F:57:GLY:HA2	2:F:600:FAD:O3B	2.21	0.40
1:E:161:THR:HG21	1:E:296:CYS:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:161:THR:CG2	1:A:296:CYS:O	2.67	0.40
1:A:460:LEU:HD12	1:B:458:CYS:SG	2.61	0.40
1:C:302:LEU:HD22	1:C:307:VAL:HB	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	482/521 (92%)	467 (97%)	13 (3%)	2 (0%)	43	76
1	B	483/521 (93%)	468 (97%)	15 (3%)	0	100	100
1	C	482/521 (92%)	466 (97%)	16 (3%)	0	100	100
1	D	482/521 (92%)	464 (96%)	16 (3%)	2 (0%)	43	76
1	E	482/521 (92%)	466 (97%)	16 (3%)	0	100	100
1	F	482/521 (92%)	468 (97%)	14 (3%)	0	100	100
All	All	2893/3126 (92%)	2799 (97%)	90 (3%)	4 (0%)	59	89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	D	62	VAL
1	A	473	PRO
1	D	473	PRO

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	379/428 (89%)	358 (94%)	21 (6%)	30	60
1	B	380/428 (89%)	363 (96%)	17 (4%)	38	70
1	C	383/428 (90%)	366 (96%)	17 (4%)	39	71
1	D	382/428 (89%)	364 (95%)	18 (5%)	36	69
1	E	350/428 (82%)	334 (95%)	16 (5%)	37	70
1	F	367/428 (86%)	353 (96%)	14 (4%)	44	76
All	All	2241/2568 (87%)	2138 (95%)	103 (5%)	37	70

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	64	CYS
1	A	67	LYS
1	A	89	LYS
1	A	100	ARG
1	A	117	ARG
1	A	161	THR
1	A	274	THR
1	A	275	ASN
1	A	277	GLU
1	A	288	MET
1	A	303	GLU
1	A	305	VAL
1	A	318	VAL
1	A	321	GLU
1	A	336	LEU
1	A	361	SER
1	A	376	THR
1	A	389	LYS
1	A	399	ILE
1	A	403	HIS
1	B	37	LYS
1	B	62	VAL
1	B	64	CYS
1	B	67	LYS
1	B	93	THR
1	B	133	GLN
1	B	161	THR
1	B	274	THR
1	B	283	GLU

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Mol	Chain	Res	Type
1	B	303	GLU
1	B	305	VAL
1	B	318	VAL
1	B	335	ILE
1	B	399	ILE
1	B	403	HIS
1	B	456	LEU
1	B	457	LYS
1	C	64	CYS
1	C	67	LYS
1	C	93	THR
1	C	121	ARG
1	C	161	THR
1	C	275	ASN
1	C	303	GLU
1	C	318	VAL
1	C	321	GLU
1	C	335	ILE
1	C	376	THR
1	C	389	LYS
1	C	399	ILE
1	C	403	HIS
1	C	474	VAL
1	C	487	ARG
1	C	491	SER
1	D	37	LYS
1	D	62	VAL
1	D	64	CYS
1	D	67	LYS
1	D	107	ASN
1	D	117	ARG
1	D	257	GLU
1	D	272	GLN
1	D	275	ASN
1	D	277	GLU
1	D	288	MET
1	D	303	GLU
1	D	318	VAL
1	D	321	GLU
1	D	376	THR
1	D	399	ILE
1	D	403	HIS

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Mol	Chain	Res	Type
1	D	491	SER
1	E	51	THR
1	E	62	VAL
1	E	93	THR
1	E	94	VAL
1	E	99	ASP
1	E	100	ARG
1	E	117	ARG
1	E	118	VAL
1	E	318	VAL
1	E	332	ILE
1	E	343	THR
1	E	397	GLU
1	E	400	GLU
1	E	403	HIS
1	E	456	LEU
1	E	461	THR
1	F	62	VAL
1	F	64	CYS
1	F	117	ARG
1	F	163	GLU
1	F	272	GLN
1	F	275	ASN
1	F	288	MET
1	F	303	GLU
1	F	318	VAL
1	F	321	GLU
1	F	336	LEU
1	F	362	THR
1	F	403	HIS
1	F	420	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	C	275	ASN
1	D	85	ASN
1	D	275	ASN
1	E	439	HIS
1	F	272	GLN
1	F	355	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	600	-	58,58,58	1.21	6 (10%)	85,89,89	1.86	17 (20%)
2	FAD	B	600	-	58,58,58	1.24	7 (12%)	85,89,89	1.89	15 (17%)
2	FAD	C	600	-	58,58,58	1.18	5 (8%)	85,89,89	1.86	12 (14%)
2	FAD	D	600	-	58,58,58	1.18	7 (12%)	85,89,89	1.91	14 (16%)
2	FAD	E	600	-	34,35,58	1.00	2 (5%)	51,53,89	1.87	7 (13%)
2	FAD	F	600	-	29,29,58	1.17	3 (10%)	45,45,89	2.31	10 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	-	-	0/34/50/50	0/1/6/6
2	FAD	B	600	-	-	0/34/50/50	0/1/6/6
2	FAD	C	600	-	-	0/34/50/50	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	600	-	-	0/34/50/50	0/1/6/6
2	FAD	E	600	-	-	0/26/42/50	0/1/3/6
2	FAD	F	600	-	-	0/16/32/50	0/1/3/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	FAD	C1'-N10	3.91	1.52	1.48
2	F	600	FAD	P-O5'	3.34	1.62	1.50
2	A	600	FAD	C1'-N10	3.34	1.51	1.48
2	C	600	FAD	C2A-N3A	3.29	1.38	1.32
2	B	600	FAD	C1'-N10	3.16	1.51	1.48
2	B	600	FAD	C2A-N3A	3.14	1.38	1.32
2	F	600	FAD	C2A-N3A	3.14	1.38	1.32
2	A	600	FAD	C2A-N3A	3.09	1.38	1.32
2	E	600	FAD	C2A-N3A	3.08	1.38	1.32
2	D	600	FAD	C1'-N10	3.01	1.51	1.48
2	D	600	FAD	C5X-N5	2.99	1.39	1.35
2	B	600	FAD	C5X-N5	2.80	1.39	1.35
2	B	600	FAD	P-O3P	2.78	1.64	1.59
2	C	600	FAD	C2A-N1A	2.76	1.39	1.33
2	A	600	FAD	C10-N1	2.74	1.40	1.35
2	D	600	FAD	C2A-N3A	2.69	1.37	1.32
2	B	600	FAD	C2A-N1A	2.57	1.39	1.33
2	A	600	FAD	C2A-N1A	2.53	1.38	1.33
2	D	600	FAD	P-O3P	2.52	1.64	1.59
2	D	600	FAD	C2A-N1A	2.46	1.38	1.33
2	D	600	FAD	C10-N1	2.44	1.40	1.35
2	E	600	FAD	C2A-N1A	2.44	1.38	1.33
2	A	600	FAD	C5X-N5	2.40	1.39	1.35
2	C	600	FAD	C5X-N5	2.39	1.39	1.35
2	A	600	FAD	P-O3P	2.34	1.64	1.59
2	F	600	FAD	C2A-N1A	2.31	1.38	1.33
2	C	600	FAD	C10-N1	2.20	1.39	1.35
2	B	600	FAD	C10-N1	2.17	1.39	1.35
2	B	600	FAD	C2B-C1B	-2.14	1.50	1.53
2	D	600	FAD	C9A-N10	2.11	1.42	1.38

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	FAD	N3A-C2A-N1A	-11.08	119.44	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	FAD	N3A-C2A-N1A	-10.76	119.71	128.71
2	E	600	FAD	N3A-C2A-N1A	-10.73	119.74	128.71
2	B	600	FAD	N3A-C2A-N1A	-10.72	119.75	128.71
2	D	600	FAD	N3A-C2A-N1A	-10.57	119.87	128.71
2	A	600	FAD	N3A-C2A-N1A	-9.86	120.46	128.71
2	D	600	FAD	C2-N1-C10	6.08	121.10	114.98
2	B	600	FAD	C2-N1-C10	5.78	120.80	114.98
2	A	600	FAD	C2-N1-C10	5.76	120.78	114.98
2	C	600	FAD	C2-N1-C10	5.21	120.23	114.98
2	F	600	FAD	O3B-C3B-C4B	5.10	126.12	111.08
2	D	600	FAD	C2'-C1'-N10	-4.24	106.83	112.45
2	A	600	FAD	C4X-C10-N1	-4.02	118.71	122.73
2	A	600	FAD	N3A-C4A-N9A	3.80	132.30	125.43
2	F	600	FAD	N3A-C4A-N9A	3.74	132.19	125.43
2	E	600	FAD	N3A-C4A-N9A	3.52	131.79	125.43
2	B	600	FAD	C1'-N10-C9A	3.52	122.30	118.87
2	C	600	FAD	C5X-C9A-N10	3.49	120.24	116.80
2	D	600	FAD	C1'-N10-C9A	3.46	122.24	118.87
2	F	600	FAD	O3B-C3B-C2B	3.43	122.98	111.83
2	C	600	FAD	C4A-C5A-N7A	-3.29	106.70	109.52
2	B	600	FAD	C4A-C5A-N7A	-3.29	106.71	109.52
2	A	600	FAD	C4X-N5-C5X	3.28	120.38	116.69
2	C	600	FAD	C4X-N5-C5X	3.28	120.38	116.69
2	D	600	FAD	C4X-N5-C5X	3.28	120.37	116.69
2	D	600	FAD	N3A-C4A-N9A	3.16	131.15	125.43
2	A	600	FAD	C5X-C9A-N10	3.12	119.87	116.80
2	D	600	FAD	C4A-C5A-N7A	-3.10	106.87	109.52
2	B	600	FAD	C4X-N5-C5X	3.09	120.16	116.69
2	F	600	FAD	O4B-C1B-N9A	3.09	111.31	108.44
2	A	600	FAD	O4B-C1B-N9A	3.07	111.29	108.44
2	F	600	FAD	C2B-C3B-C4B	3.01	108.64	102.65
2	B	600	FAD	C2'-C1'-N10	-2.93	108.56	112.45
2	B	600	FAD	O4B-C1B-N9A	2.90	111.14	108.44
2	C	600	FAD	C4X-C10-N1	-2.90	119.83	122.73
2	D	600	FAD	C4X-C10-N1	-2.79	119.94	122.73
2	B	600	FAD	C4X-C10-N1	-2.77	119.96	122.73
2	A	600	FAD	C4-N3-C2	-2.71	119.83	125.39
2	D	600	FAD	C1B-N9A-C4A	-2.67	122.03	126.64
2	B	600	FAD	N3A-C4A-N9A	2.66	130.24	125.43
2	C	600	FAD	N3A-C4A-N9A	2.64	130.19	125.43
2	A	600	FAD	C9A-N10-C10	-2.55	119.26	121.77
2	A	600	FAD	C2'-C1'-N10	-2.55	109.07	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C4A-C5A-N7A	-2.53	107.35	109.52
2	C	600	FAD	C9A-N10-C10	-2.53	119.28	121.77
2	D	600	FAD	N7A-C8A-N9A	-2.53	107.20	114.36
2	C	600	FAD	C1B-N9A-C4A	-2.52	122.28	126.64
2	A	600	FAD	N7A-C8A-N9A	-2.49	107.32	114.36
2	A	600	FAD	P-O3P-PA	-2.45	124.50	131.68
2	B	600	FAD	C4-N3-C2	-2.45	120.37	125.39
2	D	600	FAD	C4-N3-C2	-2.42	120.42	125.39
2	F	600	FAD	C5A-C4A-N3A	-2.42	120.43	125.70
2	C	600	FAD	C2'-C1'-N10	-2.40	109.27	112.45
2	B	600	FAD	O4B-C1B-C2B	-2.38	103.13	106.77
2	C	600	FAD	C4-N3-C2	-2.37	120.52	125.39
2	B	600	FAD	C5X-C9A-N10	2.31	119.08	116.80
2	C	600	FAD	N7A-C8A-N9A	-2.29	107.88	114.36
2	A	600	FAD	C5A-C4A-N3A	-2.28	120.73	125.70
2	E	600	FAD	N7A-C8A-N9A	-2.25	108.00	114.36
2	F	600	FAD	C4A-C5A-N7A	-2.24	107.60	109.52
2	F	600	FAD	C2A-N3A-C4A	2.24	120.39	114.01
2	F	600	FAD	N7A-C8A-N9A	-2.19	108.16	114.36
2	E	600	FAD	C5A-C4A-N3A	-2.18	120.96	125.70
2	A	600	FAD	C8A-N7A-C5A	2.18	110.33	103.58
2	A	600	FAD	C1'-N10-C9A	2.17	120.98	118.87
2	B	600	FAD	N7A-C8A-N9A	-2.13	108.34	114.36
2	D	600	FAD	C8A-N7A-C5A	2.13	110.17	103.58
2	D	600	FAD	P-O3P-PA	-2.12	125.47	131.68
2	A	600	FAD	N1-C10-N10	2.08	121.45	115.97
2	E	600	FAD	O4B-C1B-N9A	2.08	110.38	108.44
2	E	600	FAD	C4A-C5A-N7A	-2.06	107.76	109.52
2	B	600	FAD	C1B-N9A-C4A	-2.06	123.08	126.64
2	E	600	FAD	C2A-N3A-C4A	2.05	119.86	114.01
2	D	600	FAD	C5X-C9A-N10	2.04	118.81	116.80
2	B	600	FAD	C8A-N7A-C5A	2.03	109.86	103.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	484/521 (92%)	-0.04	0 100 100	27, 36, 44, 53	0
1	B	484/521 (92%)	-0.00	1 (0%) 93 96	24, 35, 44, 52	0
1	C	484/521 (92%)	0.00	0 100 100	25, 35, 43, 53	0
1	D	484/521 (92%)	-0.06	2 (0%) 90 93	25, 35, 43, 52	0
1	E	484/521 (92%)	0.85	82 (16%) 2 2	52, 62, 68, 71	0
1	F	484/521 (92%)	0.86	82 (16%) 2 2	50, 62, 67, 71	0
All	All	2904/3126 (92%)	0.27	167 (5%) 23 24	24, 38, 66, 71	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	135	ILE	6.2
1	E	137	PRO	5.3
1	E	280	ILE	5.3
1	E	188	TYR	4.9
1	F	140	ILE	4.8
1	F	328	TYR	4.6
1	E	269	VAL	4.6
1	F	254	ILE	4.5
1	E	274	THR	4.4
1	E	157	PHE	4.3
1	E	10	SER	4.2
1	E	279	ILE	4.2
1	F	284	TYR	4.1
1	F	39	MET	4.1
1	E	354	ALA	4.1
1	F	131	TYR	4.1
1	E	267	LEU	4.1
1	F	253	PRO	4.0
1	F	152	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	168	LEU	4.0
1	F	10	SER	4.0
1	F	137	PRO	3.9
1	E	270	VAL	3.9
1	E	256	VAL	3.9
1	E	187	PRO	3.9
1	E	93	THR	3.8
1	F	275	ASN	3.8
1	E	168	LEU	3.8
1	F	134	PHE	3.8
1	E	134	PHE	3.7
1	F	307	VAL	3.6
1	F	280	ILE	3.6
1	F	358	TYR	3.5
1	E	178	ILE	3.5
1	E	171	PRO	3.5
1	F	15	LEU	3.5
1	E	159	ILE	3.5
1	F	154	ALA	3.5
1	F	316	ILE	3.5
1	E	176	TYR	3.4
1	E	196	VAL	3.3
1	E	263	THR	3.3
1	F	11	TYR	3.3
1	E	135	ILE	3.3
1	E	328	TYR	3.3
1	E	260	GLU	3.3
1	E	284	TYR	3.3
1	F	176	TYR	3.3
1	F	274	THR	3.3
1	F	138	HIS	3.2
1	E	193	THR	3.2
1	E	35	GLY	3.2
1	F	13	TYR	3.2
1	F	14	ASP	3.1
1	F	157	PHE	3.1
1	E	358	TYR	3.1
1	E	261	ALA	3.0
1	E	287	VAL	3.0
1	E	131	TYR	3.0
1	F	261	ALA	3.0
1	E	186	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	252	VAL	3.0
1	F	354	ALA	2.9
1	F	178	ILE	2.9
1	F	281	GLU	2.9
1	F	304	THR	2.9
1	F	266	ARG	2.9
1	F	306	GLY	2.9
1	B	114[A]	TRP	2.9
1	E	264	PRO	2.8
1	F	279	ILE	2.8
1	E	275	ASN	2.8
1	E	305	VAL	2.8
1	F	34	TYR	2.8
1	E	38	VAL	2.8
1	E	252	VAL	2.8
1	F	132	GLY	2.7
1	E	327	PRO	2.7
1	D	92	GLU	2.7
1	F	12	ASP	2.7
1	F	31	ALA	2.7
1	F	151	ILE	2.7
1	E	11	TYR	2.7
1	F	191	GLY	2.7
1	F	142	ALA	2.7
1	E	357	LEU	2.7
1	E	266	ARG	2.7
1	E	16	ILE	2.7
1	F	265	GLY	2.7
1	E	39	MET	2.6
1	E	285	ASN	2.6
1	F	185	SER	2.6
1	E	253	PRO	2.6
1	E	158	LEU	2.6
1	F	116	TYR	2.6
1	F	40	VAL	2.6
1	E	172	GLY	2.5
1	E	155	GLU	2.5
1	E	14	ASP	2.5
1	E	281	GLU	2.5
1	F	291	ILE	2.5
1	F	130	ALA	2.5
1	F	270	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	221	ARG	2.5
1	F	120	LEU	2.5
1	E	247	PHE	2.5
1	E	154	ALA	2.4
1	F	288	MET	2.4
1	E	255	LYS	2.4
1	F	35	GLY	2.4
1	E	13	TYR	2.4
1	F	139	ARG	2.4
1	E	276	SER	2.4
1	E	245	ILE	2.3
1	E	248	ILE	2.3
1	E	355	GLN	2.3
1	F	167	TYR	2.3
1	E	151	ILE	2.3
1	F	308	LYS	2.3
1	E	335	ILE	2.3
1	E	190	PRO	2.3
1	E	314	GLY	2.3
1	F	41	LEU	2.3
1	F	259	ILE	2.3
1	F	155	GLU	2.3
1	F	311	GLU	2.3
1	F	190	PRO	2.3
1	F	124	LYS	2.3
1	E	316	ILE	2.2
1	E	251	PHE	2.2
1	E	330	TYR	2.2
1	F	193	THR	2.2
1	F	217	THR	2.2
1	F	49	LEU	2.2
1	E	265	GLY	2.2
1	D	10	SER	2.2
1	F	283	GLU	2.2
1	E	394	PHE	2.2
1	E	138	HIS	2.2
1	F	177	CYS	2.2
1	E	92	GLU	2.2
1	F	262	GLY	2.2
1	E	257	GLU	2.2
1	F	260	GLU	2.2
1	F	394	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	123	LYS	2.2
1	F	273	SER	2.2
1	F	331	ALA	2.1
1	F	332	ILE	2.1
1	E	91	GLU	2.1
1	F	302	LEU	2.1
1	E	307	VAL	2.1
1	E	329	ILE	2.1
1	E	34	TYR	2.1
1	F	491	SER	2.1
1	F	212	ILE	2.1
1	E	53	TRP	2.1
1	E	40	VAL	2.1
1	E	215	ASP	2.0
1	E	278	GLU	2.0
1	F	399	ILE	2.0
1	E	212	ILE	2.0
1	F	133	GLN	2.0
1	E	271	ALA	2.0
1	F	171	PRO	2.0
1	F	271	ALA	2.0
1	F	125	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	A	600	53/53	0.19	0.48	34,55,75,75	0
2	FAD	B	600	53/53	0.19	0.22	27,53,75,75	0
2	FAD	C	600	53/53	0.18	0.17	32,51,71,71	0
2	FAD	D	600	53/53	0.18	0.11	32,55,77,77	0
2	FAD	F	600	27/53	0.18	-0.46	73,76,77,78	0
2	FAD	E	600	33/53	0.14	-0.81	77,78,82,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.