Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:55 AM GMT

PDB ID	:	3QFB
Title	:	Crystal structure of the human thioredoxin reductase-thioredoxin complex
Authors	:	Fritz-Wolf, K.; Kehr, S.; Stumpf, M.; Rahlfs, S.; Becker, K.
Deposited on	:	2011-01-21
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

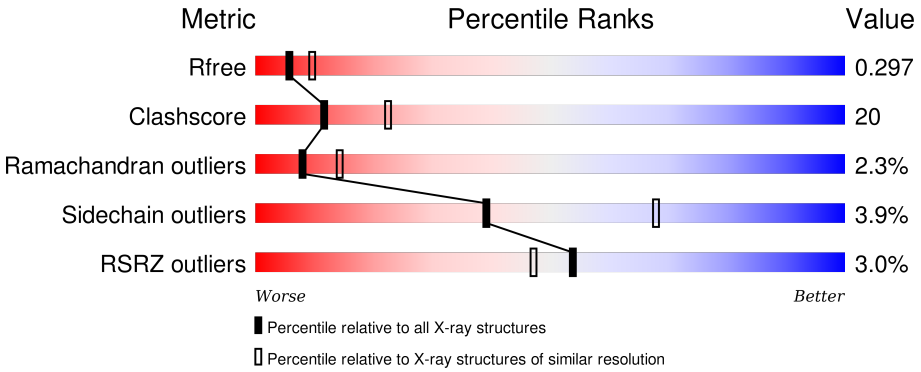
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	519	63% 31% • 5%
1	B	519	3% 58% 35% • 5%
2	C	116	6% 41% 45% • 9%
2	D	116	10% 46% 42% • 9%

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
4	GOL	A	801	-	X	-	X
4	GOL	A	802	-	X	-	-
4	GOL	A	804	-	X	-	X
4	GOL	A	806	-	X	-	X
4	GOL	B	807	-	X	-	X
4	GOL	B	808	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9621 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 Thioredoxin reductase 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3816	2423	651	722	20			
1	B	491	Total	C	N	O	S	0	0	0
			3784	2403	647	714	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q16881
A	-18	GLY	-	EXPRESSION TAG	UNP Q16881
A	-17	SER	-	EXPRESSION TAG	UNP Q16881
A	-16	SER	-	EXPRESSION TAG	UNP Q16881
A	-15	HIS	-	EXPRESSION TAG	UNP Q16881
A	-14	HIS	-	EXPRESSION TAG	UNP Q16881
A	-13	HIS	-	EXPRESSION TAG	UNP Q16881
A	-12	HIS	-	EXPRESSION TAG	UNP Q16881
A	-11	HIS	-	EXPRESSION TAG	UNP Q16881
A	-10	HIS	-	EXPRESSION TAG	UNP Q16881
A	-9	SER	-	EXPRESSION TAG	UNP Q16881
A	-8	SER	-	EXPRESSION TAG	UNP Q16881
A	-7	GLY	-	EXPRESSION TAG	UNP Q16881
A	-6	LEU	-	EXPRESSION TAG	UNP Q16881
A	-5	VAL	-	EXPRESSION TAG	UNP Q16881
A	-4	PRO	-	EXPRESSION TAG	UNP Q16881
A	-3	ARG	-	EXPRESSION TAG	UNP Q16881
A	-2	GLY	-	EXPRESSION TAG	UNP Q16881
A	-1	SER	-	EXPRESSION TAG	UNP Q16881
A	0	HIS	-	EXPRESSION TAG	UNP Q16881
A	497	SER	CYS	ENGINEERED MUTATION	UNP Q16881
A	498	CYS	U	SEE REMARK 999	UNP Q16881
B	-19	MET	-	EXPRESSION TAG	UNP Q16881
B	-18	GLY	-	EXPRESSION TAG	UNP Q16881
B	-17	SER	-	EXPRESSION TAG	UNP Q16881

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP Q16881
B	-15	HIS	-	EXPRESSION TAG	UNP Q16881
B	-14	HIS	-	EXPRESSION TAG	UNP Q16881
B	-13	HIS	-	EXPRESSION TAG	UNP Q16881
B	-12	HIS	-	EXPRESSION TAG	UNP Q16881
B	-11	HIS	-	EXPRESSION TAG	UNP Q16881
B	-10	HIS	-	EXPRESSION TAG	UNP Q16881
B	-9	SER	-	EXPRESSION TAG	UNP Q16881
B	-8	SER	-	EXPRESSION TAG	UNP Q16881
B	-7	GLY	-	EXPRESSION TAG	UNP Q16881
B	-6	LEU	-	EXPRESSION TAG	UNP Q16881
B	-5	VAL	-	EXPRESSION TAG	UNP Q16881
B	-4	PRO	-	EXPRESSION TAG	UNP Q16881
B	-3	ARG	-	EXPRESSION TAG	UNP Q16881
B	-2	GLY	-	EXPRESSION TAG	UNP Q16881
B	-1	SER	-	EXPRESSION TAG	UNP Q16881
B	0	HIS	-	EXPRESSION TAG	UNP Q16881
B	497	SER	CYS	ENGINEERED MUTATION	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP Q16881

- Molecule 2 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	105	Total	C	N	O	S	0	0	0
			819	523	128	163	5			
2	D	105	Total	C	N	O	S	0	0	0
			819	523	128	163	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	EXPRESSION TAG	UNP P10599
C	-9	ARG	-	EXPRESSION TAG	UNP P10599
C	-8	GLY	-	EXPRESSION TAG	UNP P10599
C	-7	SER	-	EXPRESSION TAG	UNP P10599
C	-6	HIS	-	EXPRESSION TAG	UNP P10599
C	-5	HIS	-	EXPRESSION TAG	UNP P10599
C	-4	HIS	-	EXPRESSION TAG	UNP P10599
C	-3	HIS	-	EXPRESSION TAG	UNP P10599
C	-2	HIS	-	EXPRESSION TAG	UNP P10599
C	-1	HIS	-	EXPRESSION TAG	UNP P10599
C	0	GLY	-	EXPRESSION TAG	UNP P10599

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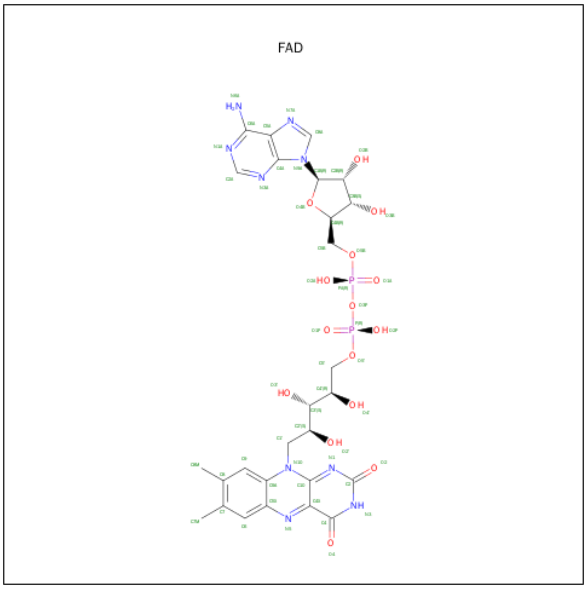
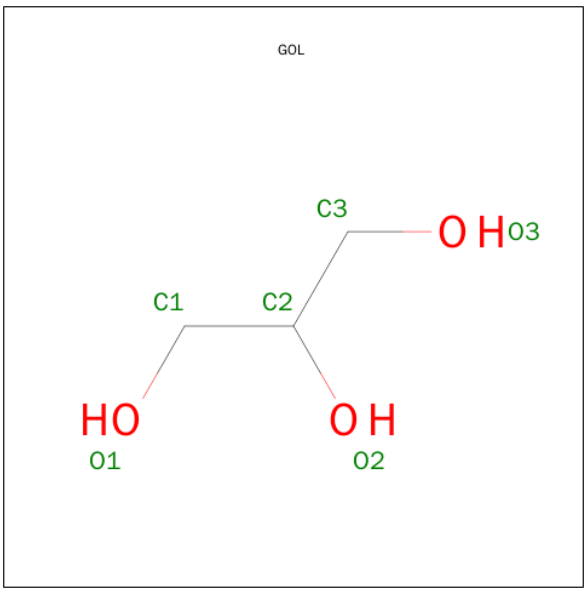
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	-	EXPRESSION TAG	UNP P10599
C	35	SER	CYS	ENGINEERED MUTATION	UNP P10599
C	73	SER	CYS	ENGINEERED MUTATION	UNP P10599
D	-10	MET	-	EXPRESSION TAG	UNP P10599
D	-9	ARG	-	EXPRESSION TAG	UNP P10599
D	-8	GLY	-	EXPRESSION TAG	UNP P10599
D	-7	SER	-	EXPRESSION TAG	UNP P10599
D	-6	HIS	-	EXPRESSION TAG	UNP P10599
D	-5	HIS	-	EXPRESSION TAG	UNP P10599
D	-4	HIS	-	EXPRESSION TAG	UNP P10599
D	-3	HIS	-	EXPRESSION TAG	UNP P10599
D	-2	HIS	-	EXPRESSION TAG	UNP P10599
D	-1	HIS	-	EXPRESSION TAG	UNP P10599
D	0	GLY	-	EXPRESSION TAG	UNP P10599
D	1	SER	-	EXPRESSION TAG	UNP P10599
D	35	SER	CYS	ENGINEERED MUTATION	UNP P10599
D	73	SER	CYS	ENGINEERED MUTATION	UNP P10599

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

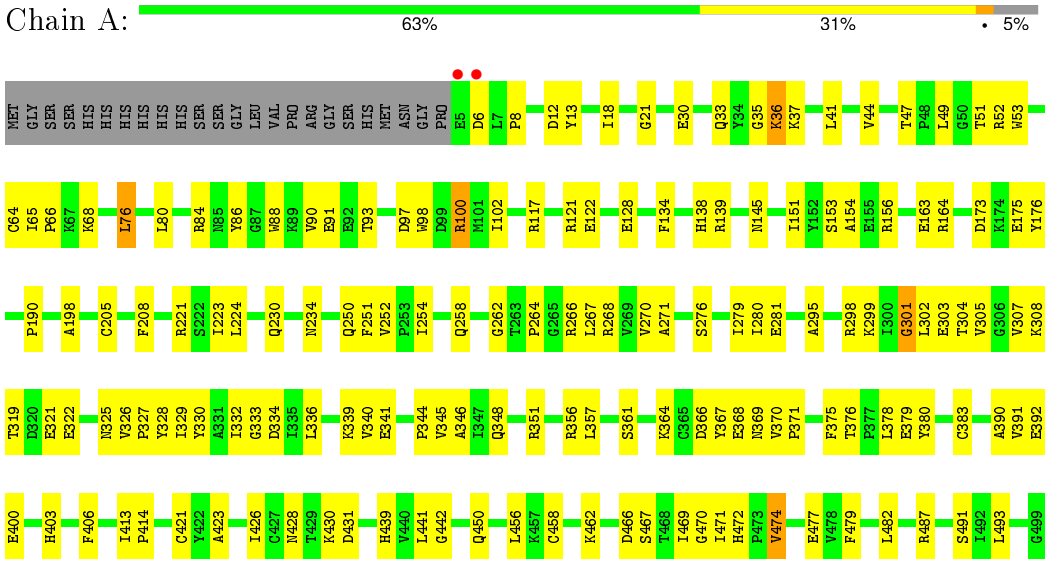
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	123	Total O 123 123	0	0
5	B	94	Total O 94 94	0	0
5	C	13	Total O 13 13	0	0
5	D	11	Total O 11 11	0	0

3 Residue-property plots (i)

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.

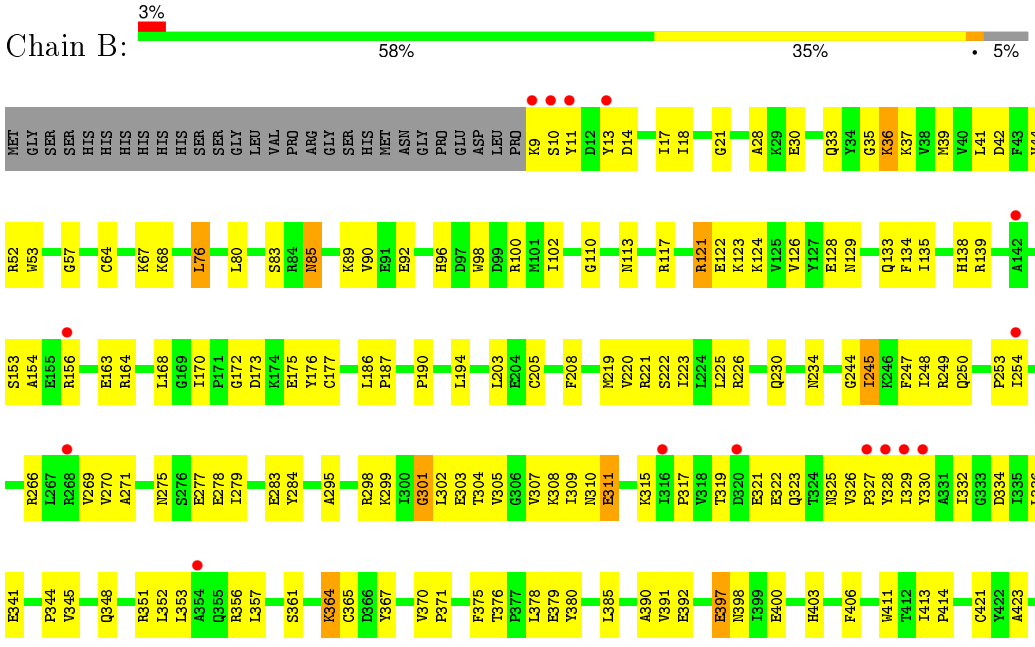
- Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain A:

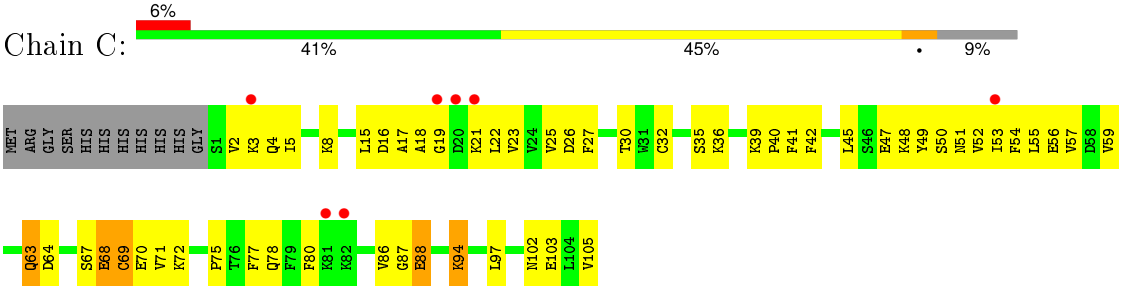


- Molecule 1: Thioredoxin reductase 1, cytoplasmic

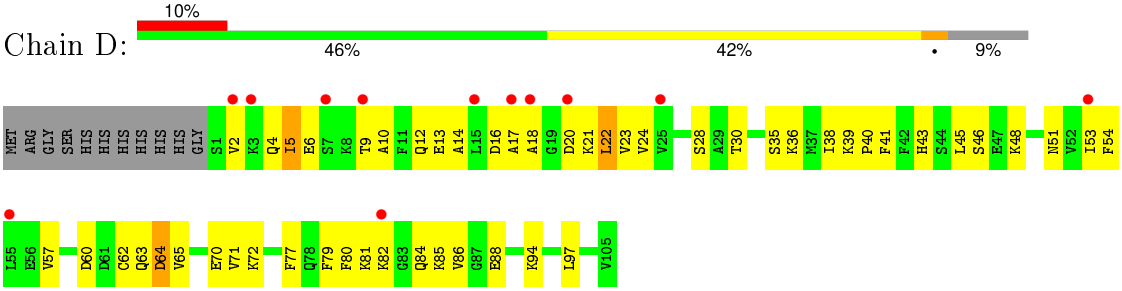
Chain B:



• Molecule 2: Thioredoxin



• Molecule 2: Thioredoxin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.27Å 121.70Å 73.89Å 90.00° 95.33° 90.00°	Depositor
Resolution (Å)	49.07 – 2.60 49.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.07-2.60) 90.0 (49.07-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.235 , 0.297 0.235 , 0.297	Depositor DCC
R_{free} test set	2318 reflections (6.00%)	DCC
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.4	EDS
Estimated twinning fraction	0.166 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 283630 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.40	0/3891	0.64	2/5268 (0.0%)
1	B	0.40	0/3858	0.64	1/5222 (0.0%)
2	C	0.41	0/834	0.57	0/1120
2	D	0.39	0/834	0.54	0/1120
All	All	0.40	0/9417	0.62	3/12730 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	CYS	CA-CB-SG	5.84	124.52	114.00
1	B	64	CYS	CA-CB-SG	5.27	123.48	114.00
1	A	59	CYS	CA-CB-SG	5.05	123.08	114.00

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	3816	0	3820	138	0
1	B	3784	0	3792	168	0
2	C	819	0	806	61	0
2	D	819	0	806	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	53	0	31	2	0
3	B	53	0	31	1	0
4	A	24	0	16	2	0
4	B	12	0	8	0	0
5	A	123	0	0	8	0
5	B	94	0	0	11	0
5	C	13	0	0	0	0
5	D	11	0	0	1	0
All	All	9621	0	9310	379	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 20.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASN:N	1:B:85:ASN:HD22	1.55	1.02
2:C:18:ALA:HB2	2:C:53:ILE:HD12	1.41	1.00
1:A:121:ARG:CZ	2:C:67:SER:HA	1.92	1.00
1:B:85:ASN:H	1:B:85:ASN:HD22	0.93	0.92
1:B:85:ASN:H	1:B:85:ASN:ND2	1.67	0.90
2:C:102:ASN:O	2:C:105:VAL:HG23	1.73	0.89
1:B:245:ILE:H	1:B:245:ILE:HD12	1.38	0.88
1:B:223:ILE:HD11	1:B:226:ARG:HG3	1.57	0.85
2:C:70:GLU:HG3	2:C:72:LYS:HE2	1.58	0.85
2:C:15:LEU:HD23	2:C:23:VAL:HG11	1.58	0.84
2:D:81:LYS:HE2	2:D:86:VAL:HG11	1.59	0.83
1:A:428:ASN:HD22	1:A:431:ASP:HB2	1.44	0.82
1:A:221:ARG:NH1	1:A:252:VAL:HG21	1.95	0.82
1:A:428:ASN:ND2	1:A:431:ASP:HB2	1.95	0.81
1:A:134:PHE:HB2	1:A:301:GLY:O	1.79	0.81
1:B:85:ASN:OD1	1:B:414:PRO:HA	1.82	0.79
2:C:39:LYS:HE2	2:C:56:GLU:OE2	1.84	0.78
1:B:398:ASN:ND2	1:B:430:LYS:HB2	1.98	0.78
2:C:86:VAL:HG23	2:C:87:GLY:H	1.50	0.77
1:B:398:ASN:HD22	1:B:430:LYS:HB2	1.49	0.77
1:B:307:VAL:HG21	1:B:329:ILE:HG21	1.65	0.77
1:B:254:ILE:HD11	1:B:270:VAL:HG12	1.68	0.76
1:A:308:LYS:HG2	1:A:325:ASN:OD1	1.86	0.76
1:A:450:GLN:HE22	1:B:471:ILE:H	1.34	0.75
2:C:18:ALA:CB	2:C:53:ILE:HD12	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:HG21	1:A:329:ILE:HG21	1.68	0.74
1:B:308:LYS:HG2	1:B:325:ASN:OD1	1.87	0.74
2:D:41:PHE:CE2	2:D:94:LYS:HD3	2.23	0.73
1:B:156:ARG:HD3	1:B:330:TYR:HE2	1.54	0.73
1:B:340:VAL:HG13	1:B:345:VAL:HG21	1.68	0.73
1:B:220:VAL:HB	1:B:249:ARG:HD2	1.72	0.71
1:A:156:ARG:HD3	1:A:330:TYR:HE2	1.54	0.71
2:D:5:ILE:HG12	2:D:57:VAL:HG22	1.73	0.70
1:A:398:ASN:ND2	1:A:430:LYS:HB2	2.05	0.70
1:A:13:TYR:O	1:A:154:ALA:HA	1.91	0.70
1:B:364:LYS:HB3	5:B:578:HOH:O	1.92	0.70
1:B:305:VAL:HG21	1:B:329:ILE:HD11	1.73	0.70
1:A:339:LYS:HD2	1:A:367:TYR:CE2	2.27	0.70
2:C:4:GLN:NE2	2:C:56:GLU:HB3	2.07	0.70
2:C:5:ILE:HD12	2:C:5:ILE:O	1.93	0.69
2:D:85:LYS:NZ	2:D:85:LYS:HB3	2.08	0.68
1:A:305:VAL:HG21	1:A:329:ILE:HD11	1.75	0.68
2:D:39:LYS:HB3	2:D:40:PRO:HD3	1.76	0.68
1:B:406:PHE:CZ	1:B:421:CYS:HB3	2.29	0.68
1:A:471:ILE:H	1:B:450:GLN:HE22	1.41	0.68
1:A:398:ASN:HD22	1:A:430:LYS:HB2	1.58	0.67
1:A:8:PRO:HG3	1:A:139:ARG:CZ	2.24	0.67
2:C:36:LYS:NZ	2:C:36:LYS:HB2	2.10	0.67
2:C:86:VAL:HG23	2:C:87:GLY:N	2.09	0.66
1:A:90:VAL:HG12	1:A:91:GLU:O	1.94	0.66
2:C:3:LYS:HB3	2:C:55:LEU:HD23	1.78	0.66
1:B:303:GLU:OE2	1:B:304:THR:HG23	1.96	0.66
2:C:78:GLN:HG2	2:C:88:GLU:HG3	1.78	0.65
1:B:428:ASN:HD22	1:B:431:ASP:HB3	1.61	0.65
1:A:117:ARG:NH2	2:C:63:GLN:HB3	2.12	0.65
1:B:134:PHE:HB2	1:B:301:GLY:O	1.97	0.64
1:A:221:ARG:HH11	1:A:252:VAL:HG21	1.60	0.64
1:A:406:PHE:CZ	1:A:421:CYS:HB3	2.33	0.64
1:B:339:LYS:HD2	1:B:367:TYR:CE2	2.33	0.64
1:A:303:GLU:OE2	1:A:304:THR:HG23	1.98	0.63
1:B:98:TRP:CZ2	1:B:102:ILE:HD11	2.33	0.63
1:B:176:TYR:CE1	1:B:258:GLN:HB2	2.33	0.62
1:A:450:GLN:NE2	1:B:471:ILE:H	1.97	0.62
2:D:23:VAL:HG22	2:D:53:ILE:HB	1.80	0.62
1:A:469:ILE:HB	1:B:370:VAL:HG13	1.82	0.62
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HB	1:B:266:ARG:O	1.99	0.62
2:D:41:PHE:O	2:D:45:LEU:HB2	2.00	0.61
2:C:36:LYS:HZ2	2:C:36:LYS:HB2	1.65	0.61
1:A:428:ASN:HD22	1:A:431:ASP:CB	2.11	0.61
1:B:317:PRO:HG3	1:B:337:GLU:OE1	2.01	0.61
2:C:26:ASP:HB2	2:C:42:PHE:CZ	2.36	0.61
1:B:340:VAL:HG11	1:B:370:VAL:HG21	1.82	0.61
2:C:71:VAL:O	2:C:72:LYS:HD3	2.00	0.61
2:C:39:LYS:HB3	2:C:40:PRO:HD3	1.81	0.61
2:C:4:GLN:HE22	2:C:56:GLU:HB3	1.66	0.61
2:D:46:SER:HA	2:D:54:PHE:CE1	2.35	0.61
1:B:85:ASN:N	1:B:85:ASN:ND2	2.29	0.60
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.85	0.59
1:B:163:GLU:OE2	1:B:334:ASP:HB3	2.03	0.59
1:A:52:ARG:NH2	5:A:545:HOH:O	2.35	0.59
2:C:77:PHE:O	2:C:88:GLU:HA	2.03	0.59
2:D:14:ALA:C	2:D:16:ASP:H	2.05	0.59
2:D:5:ILE:CG1	2:D:57:VAL:HG22	2.32	0.59
1:A:86:TYR:O	1:B:96:HIS:HE1	1.86	0.59
2:C:22:LEU:HB3	2:C:52:VAL:HG13	1.85	0.58
1:A:450:GLN:HE22	1:B:471:ILE:N	1.99	0.58
2:D:5:ILE:HD12	2:D:5:ILE:C	2.24	0.58
2:C:41:PHE:O	2:C:45:LEU:HB2	2.02	0.58
1:A:268:ARG:HD2	1:A:281:GLU:OE2	2.04	0.58
2:C:5:ILE:HG23	2:C:55:LEU:HD22	1.86	0.58
1:A:339:LYS:HD2	1:A:367:TYR:CD2	2.39	0.58
1:B:315:LYS:NZ	1:B:341:GLU:OE2	2.30	0.57
1:B:39:MET:HG3	1:B:126:VAL:HG12	1.87	0.57
1:B:339:LYS:HD2	1:B:367:TYR:CD2	2.40	0.56
1:A:163:GLU:OE2	1:A:334:ASP:HB3	2.05	0.56
1:A:221:ARG:HD3	5:A:604:HOH:O	2.04	0.56
1:B:322:GLU:HG2	1:B:332:ILE:HG22	1.87	0.56
1:A:41:LEU:HD23	1:A:128:GLU:HB3	1.88	0.56
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.88	0.56
2:C:35:SER:HA	2:C:75:PRO:HG3	1.88	0.56
1:B:44:VAL:HG11	1:B:53:TRP:CE2	2.41	0.55
1:A:450:GLN:HE22	1:B:470:GLY:HA2	1.70	0.55
1:A:117:ARG:HH21	2:C:63:GLN:HB3	1.70	0.55
1:A:470:GLY:HA2	1:B:450:GLN:HE22	1.70	0.55
1:A:366:ASP:HB3	5:A:527:HOH:O	2.07	0.55
1:B:223:ILE:HD11	1:B:226:ARG:CG	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:HG2	1:A:332:ILE:HG22	1.89	0.55
1:B:245:ILE:H	1:B:245:ILE:CD1	2.15	0.54
1:A:12:ASP:HB2	1:A:153:SER:O	2.07	0.54
1:B:428:ASN:HD22	1:B:431:ASP:CB	2.19	0.54
1:B:138:HIS:O	1:B:153:SER:HA	2.08	0.54
2:D:6:GLU:HA	2:D:62:CYS:SG	2.48	0.54
1:B:462:LYS:HE2	1:B:466:ASP:OD1	2.07	0.54
1:A:340:VAL:HG21	1:A:370:VAL:HG21	1.90	0.54
1:B:18:ILE:HD12	1:B:18:ILE:N	2.23	0.54
1:A:471:ILE:H	1:B:450:GLN:NE2	2.04	0.53
1:A:49:LEU:HG	5:A:525:HOH:O	2.08	0.53
1:B:42:ASP:O	1:B:129:ASN:HA	2.07	0.53
2:D:9:THR:O	2:D:13:GLU:HB3	2.08	0.53
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.91	0.53
1:A:462:LYS:HE2	1:A:466:ASP:OD1	2.08	0.53
2:D:23:VAL:HG13	2:D:53:ILE:O	2.08	0.53
1:B:254:ILE:HD11	1:B:270:VAL:CG1	2.38	0.53
1:B:30:GLU:HG3	1:B:351:ARG:HA	1.91	0.53
1:B:474:VAL:O	1:B:477:GLU:HG2	2.09	0.53
2:D:22:LEU:HD12	2:D:80:PHE:O	2.08	0.53
1:A:450:GLN:HE22	1:B:470:GLY:CA	2.22	0.53
2:C:2:VAL:HG22	2:C:54:PHE:HB3	1.90	0.53
1:B:254:ILE:HG12	1:B:270:VAL:O	2.08	0.53
2:C:68:GLU:O	2:C:70:GLU:N	2.42	0.52
1:B:121:ARG:HH11	1:B:121:ARG:CB	2.22	0.52
1:A:482:LEU:HA	5:A:522:HOH:O	2.08	0.52
1:A:18:ILE:HD12	1:A:18:ILE:N	2.24	0.52
1:B:221:ARG:HG2	1:B:222:SER:N	2.24	0.52
2:C:78:GLN:NE2	2:C:88:GLU:OE2	2.39	0.52
1:B:254:ILE:CD1	1:B:270:VAL:HG12	2.37	0.52
1:A:251:PHE:CE2	1:A:280:ILE:HG12	2.45	0.52
1:A:470:GLY:CA	1:B:450:GLN:HE22	2.23	0.52
1:A:474:VAL:O	1:A:477:GLU:HG2	2.10	0.52
1:A:44:VAL:HG11	1:A:53:TRP:CE2	2.45	0.51
2:C:16:ASP:O	2:C:18:ALA:N	2.43	0.51
1:B:340:VAL:CG1	1:B:345:VAL:HG21	2.39	0.51
1:A:30:GLU:HG3	1:A:351:ARG:HA	1.92	0.51
1:B:411:TRP:C	1:B:414:PRO:HD2	2.31	0.51
2:D:81:LYS:O	2:D:81:LYS:HG3	2.11	0.51
1:A:271:ALA:O	1:A:279:ILE:HG23	2.11	0.51
1:A:76:LEU:O	1:A:80:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLN:NE2	5:B:517:HOH:O	2.43	0.51
1:B:298:ARG:HG2	1:B:298:ARG:HH11	1.75	0.51
1:A:471:ILE:N	1:B:450:GLN:HE22	2.07	0.51
1:A:370:VAL:HG13	1:B:469:ILE:HB	1.92	0.51
1:A:121:ARG:NH2	2:C:67:SER:HA	2.26	0.51
1:A:380:TYR:OH	1:A:439:HIS:CD2	2.63	0.51
1:B:9:LYS:C	1:B:11:TYR:H	2.14	0.51
1:B:52:ARG:NH2	5:B:530:HOH:O	2.43	0.51
1:B:89:LYS:HG3	1:B:89:LYS:O	2.09	0.51
1:B:391:VAL:HG23	1:B:392:GLU:N	2.26	0.51
1:A:138:HIS:O	1:A:153:SER:HA	2.11	0.51
1:A:254:ILE:HD11	1:A:270:VAL:HG12	1.92	0.51
2:C:15:LEU:CD2	2:C:23:VAL:HG11	2.35	0.50
1:B:83:SER:OG	1:B:90:VAL:HG21	2.10	0.50
1:B:121:ARG:NH2	2:D:71:VAL:O	2.43	0.50
1:A:254:ILE:HD11	1:A:270:VAL:CG1	2.41	0.50
2:D:70:GLU:HG3	2:D:70:GLU:O	2.10	0.50
2:C:8:LYS:HB3	2:C:64:ASP:OD2	2.10	0.50
1:A:21:GLY:HA2	1:A:57:GLY:HA3	1.92	0.50
1:A:397:GLU:H	1:A:397:GLU:CD	2.15	0.50
1:B:219:MET:SD	1:B:253:PRO:HG3	2.52	0.50
1:B:323:GLN:HG3	5:B:564:HOH:O	2.11	0.50
1:A:186:LEU:HD23	1:A:190:PRO:HG3	1.93	0.50
1:A:121:ARG:NH1	2:C:67:SER:HA	2.27	0.50
1:B:330:TYR:OH	1:B:357:LEU:HD21	2.12	0.50
2:C:16:ASP:C	2:C:18:ALA:H	2.15	0.49
1:A:391:VAL:HG23	1:A:392:GLU:N	2.26	0.49
1:B:334:ASP:OD1	1:B:341:GLU:HB3	2.12	0.49
1:B:21:GLY:HA2	1:B:57:GLY:HA3	1.93	0.49
1:B:76:LEU:O	1:B:80:LEU:HG	2.13	0.49
1:B:329:ILE:C	5:B:564:HOH:O	2.50	0.49
1:A:47:THR:HG23	1:A:51:THR:O	2.11	0.49
1:A:305:VAL:CG2	1:A:329:ILE:HD11	2.42	0.49
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.95	0.49
1:B:302:LEU:O	1:B:305:VAL:HG12	2.12	0.49
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.28	0.49
1:B:380:TYR:OH	1:B:439:HIS:CD2	2.65	0.49
1:B:186:LEU:HD23	1:B:190:PRO:HG3	1.95	0.49
2:C:18:ALA:HB1	2:C:21:LYS:HB2	1.95	0.49
1:A:430:LYS:O	1:A:430:LYS:HG2	2.13	0.49
2:C:5:ILE:HD11	2:C:57:VAL:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:VAL:CG2	2:C:87:GLY:H	2.24	0.48
1:A:151:ILE:HD12	1:A:151:ILE:N	2.28	0.48
3:B:600:FAD:HM83	5:B:504:HOH:O	2.12	0.48
1:B:397:GLU:CD	1:B:397:GLU:H	2.16	0.48
1:A:302:LEU:O	1:A:305:VAL:HG12	2.13	0.48
1:A:493:LEU:N	1:A:493:LEU:HD12	2.27	0.48
1:A:426:ILE:N	1:A:426:ILE:HD12	2.29	0.48
1:A:330:TYR:OH	1:A:357:LEU:HD21	2.14	0.48
1:B:221:ARG:CG	1:B:222:SER:N	2.77	0.48
1:A:477:GLU:HA	1:B:450:GLN:NE2	2.29	0.48
1:A:321:GLU:O	1:A:322:GLU:HB2	2.13	0.48
2:C:5:ILE:HG13	2:C:56:GLU:O	2.13	0.48
1:B:230:GLN:O	1:B:234:ASN:ND2	2.46	0.48
1:B:260:GLU:HG2	1:B:261:ALA:O	2.14	0.48
1:B:406:PHE:CE1	1:B:421:CYS:HB3	2.49	0.47
2:C:36:LYS:NZ	2:C:36:LYS:CB	2.77	0.47
2:C:69:CYS:HB3	2:C:78:GLN:OE1	2.14	0.47
2:C:16:ASP:C	2:C:18:ALA:N	2.67	0.47
1:B:305:VAL:CG2	1:B:329:ILE:HD11	2.41	0.47
1:A:340:VAL:HB	1:A:345:VAL:HG21	1.96	0.47
2:D:85:LYS:HB3	2:D:85:LYS:HZ3	1.80	0.47
1:B:315:LYS:HD2	1:B:336:LEU:O	2.14	0.47
1:B:250:GLN:HB3	1:B:275:ASN:HD21	1.77	0.47
1:A:230:GLN:O	1:A:234:ASN:ND2	2.47	0.47
1:A:266:ARG:O	1:A:267:LEU:HD23	2.13	0.47
1:B:259:ILE:HD12	1:B:283:GLU:HG3	1.96	0.47
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.80	0.47
1:A:477:GLU:HA	1:B:450:GLN:HE21	1.79	0.47
1:B:254:ILE:CG1	1:B:270:VAL:HG12	2.45	0.47
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.95	0.47
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.97	0.47
1:B:33:GLN:NE2	1:B:33:GLN:HA	2.29	0.47
1:B:135:ILE:HG22	5:B:551:HOH:O	2.15	0.47
1:A:450:GLN:NE2	1:B:470:GLY:HA2	2.30	0.47
1:B:319:THR:C	1:B:321:GLU:H	2.18	0.47
1:B:423:ALA:HB1	1:B:479:PHE:CZ	2.50	0.46
1:B:426:ILE:HD12	1:B:426:ILE:N	2.30	0.46
1:B:321:GLU:O	1:B:322:GLU:HB2	2.15	0.46
2:C:49:TYR:C	2:C:51:ASN:H	2.18	0.46
2:D:64:ASP:OD2	2:D:65:VAL:HG23	2.16	0.46
1:B:41:LEU:HD23	1:B:128:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:VAL:HG11	2:C:27:PHE:CZ	2.49	0.46
2:D:28:SER:HB2	2:D:35:SER:OG	2.15	0.46
1:B:203:LEU:HD12	1:B:225:LEU:HD21	1.98	0.46
1:A:97:ASP:OD2	1:A:100:ARG:HB2	2.16	0.46
2:D:85:LYS:HB3	2:D:85:LYS:HZ2	1.80	0.46
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.80	0.46
1:B:173:ASP:HA	1:B:177:CYS:SG	2.56	0.46
1:A:413:ILE:N	1:A:414:PRO:CD	2.79	0.46
2:C:22:LEU:HD12	2:C:80:PHE:O	2.16	0.46
2:C:4:GLN:HA	2:C:4:GLN:HE21	1.81	0.46
1:B:17:ILE:HD12	1:B:28:ALA:HB2	1.98	0.46
1:A:319:THR:C	1:A:321:GLU:H	2.20	0.46
1:B:123:LYS:O	1:B:124:LYS:HB2	2.15	0.46
2:C:5:ILE:HD11	2:C:57:VAL:HG22	1.98	0.46
1:A:68:LYS:HE3	1:A:375:PHE:CE2	2.50	0.46
1:B:151:ILE:HD12	1:B:151:ILE:N	2.30	0.46
1:A:346:ALA:HB2	5:A:601:HOH:O	2.17	0.45
1:B:68:LYS:HE3	1:B:375:PHE:CE2	2.51	0.45
1:A:470:GLY:HA2	1:B:450:GLN:NE2	2.31	0.45
2:D:18:ALA:HB1	2:D:53:ILE:HD12	1.99	0.45
1:A:163:GLU:O	1:A:164:ARG:HD2	2.16	0.45
1:B:413:ILE:N	1:B:414:PRO:CD	2.80	0.45
1:A:423:ALA:HB1	1:A:479:PHE:CZ	2.51	0.45
2:C:87:GLY:O	2:C:88:GLU:HB2	2.16	0.45
1:A:8:PRO:HG3	1:A:139:ARG:NH2	2.31	0.45
1:B:219:MET:SD	1:B:253:PRO:HD3	2.56	0.45
2:D:30:THR:O	2:D:36:LYS:HE2	2.17	0.45
1:A:176:TYR:CE1	1:A:258:GLN:HB2	2.51	0.45
1:B:163:GLU:O	1:B:164:ARG:HD2	2.16	0.45
1:B:247:PHE:O	1:B:248:ILE:HG13	2.17	0.45
2:C:5:ILE:CG2	2:C:55:LEU:HD22	2.47	0.45
1:A:139:ARG:HD3	1:A:151:ILE:HG21	1.99	0.45
1:B:139:ARG:HD3	1:B:151:ILE:HG21	1.99	0.45
1:A:33:GLN:HA	1:A:33:GLN:NE2	2.31	0.45
2:D:2:VAL:HB	2:D:43:HIS:CE1	2.52	0.45
2:C:94:LYS:O	2:C:97:LEU:HB3	2.17	0.45
1:A:59:CYS:HB2	3:A:600:FAD:O2'	2.17	0.45
2:C:2:VAL:HG11	2:C:42:PHE:HE2	1.82	0.45
1:A:392:GLU:HB2	5:A:616:HOH:O	2.16	0.45
1:B:379:GLU:O	1:B:441:LEU:HD12	2.16	0.44
2:D:51:ASN:HD22	2:D:51:ASN:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.82	0.44
1:B:352:LEU:HD12	1:B:365:CYS:HB2	2.00	0.44
1:B:278:GLU:HA	5:B:561:HOH:O	2.16	0.44
1:B:172:GLY:O	1:B:176:TYR:HD2	2.01	0.44
1:A:186:LEU:HA	1:A:187:PRO:HD3	1.74	0.44
2:D:24:VAL:HG22	2:D:79:PHE:CD2	2.53	0.44
1:A:262:GLY:C	1:A:264:PRO:C	2.76	0.44
1:A:390:ALA:CB	1:A:426:ILE:HG21	2.48	0.44
2:C:2:VAL:HG13	2:C:54:PHE:C	2.38	0.44
1:B:186:LEU:HA	1:B:187:PRO:HD3	1.73	0.44
1:A:303:GLU:H	1:A:303:GLU:CD	2.20	0.44
1:B:378:LEU:HD11	1:B:442:GLY:HA2	1.99	0.44
1:A:138:HIS:HD2	1:A:154:ALA:O	2.01	0.43
1:A:406:PHE:CE1	1:A:421:CYS:HB3	2.53	0.43
1:A:368:GLU:HA	4:A:802:GOL:O2	2.18	0.43
1:A:198:ALA:HB1	1:A:224:LEU:HD23	2.00	0.43
2:C:4:GLN:HE22	2:C:56:GLU:CB	2.30	0.43
1:A:391:VAL:CG2	1:A:392:GLU:N	2.82	0.43
1:A:205:CYS:HA	1:A:208:PHE:CE2	2.54	0.43
2:D:10:ALA:O	2:D:14:ALA:HB3	2.18	0.43
1:B:319:THR:C	1:B:321:GLU:N	2.70	0.43
1:A:400:GLU:OE2	1:A:487:ARG:NE	2.43	0.43
1:B:98:TRP:NE1	1:B:102:ILE:HG13	2.33	0.43
1:B:353:LEU:O	1:B:353:LEU:HD12	2.18	0.43
1:B:35:GLY:O	1:B:36:LYS:O	2.36	0.43
1:B:110:GLY:HA2	1:B:113:ASN:HD22	1.84	0.43
1:B:117:ARG:NH1	5:B:529:HOH:O	2.35	0.43
2:C:23:VAL:HB	2:C:80:PHE:HB2	2.00	0.43
1:B:326:VAL:HA	1:B:327:PRO:HD3	1.84	0.43
2:C:3:LYS:HB3	2:C:55:LEU:CD2	2.47	0.43
2:D:14:ALA:C	2:D:16:ASP:N	2.71	0.43
1:B:411:TRP:CZ2	1:B:443:PRO:HG3	2.53	0.43
1:A:117:ARG:O	1:A:121:ARG:HG3	2.18	0.43
1:A:221:ARG:O	1:A:250:GLN:HA	2.19	0.43
1:B:326:VAL:CG1	1:B:328:TYR:CE1	3.01	0.43
1:A:471:ILE:HD11	1:B:371:PRO:HB2	2.01	0.43
1:B:391:VAL:CG2	1:B:392:GLU:N	2.82	0.43
2:D:48:LYS:HG2	2:D:48:LYS:O	2.18	0.43
1:B:309:ILE:HG13	1:B:310:ASN:N	2.33	0.43
1:A:340:VAL:CG1	1:A:345:VAL:HG21	2.49	0.42
1:B:400:GLU:OE2	1:B:487:ARG:NE	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLU:H	1:B:303:GLU:CD	2.22	0.42
1:A:378:LEU:HD11	1:A:442:GLY:HA2	2.01	0.42
1:A:379:GLU:O	1:A:441:LEU:HD12	2.18	0.42
1:A:326:VAL:CG1	1:A:328:TYR:CE1	3.02	0.42
1:B:225:LEU:O	1:B:226:ARG:C	2.57	0.42
1:A:186:LEU:CD2	1:A:190:PRO:HG3	2.48	0.42
1:B:385:LEU:HG	5:B:547:HOH:O	2.19	0.42
2:D:72:LYS:HD2	2:D:72:LYS:O	2.19	0.42
1:A:309:ILE:HG13	1:A:310:ASN:N	2.34	0.42
2:D:81:LYS:O	2:D:82:LYS:HB2	2.19	0.42
2:D:77:PHE:O	2:D:88:GLU:HA	2.19	0.42
2:C:5:ILE:CG1	2:C:57:VAL:HG22	2.49	0.42
1:A:319:THR:C	1:A:321:GLU:N	2.72	0.42
1:B:277:GLU:O	1:B:279:ILE:HG13	2.19	0.42
1:B:428:ASN:ND2	1:B:431:ASP:CB	2.81	0.42
1:B:39:MET:CE	1:B:41:LEU:HD21	2.49	0.42
1:B:35:GLY:O	1:B:36:LYS:C	2.58	0.42
2:D:80:PHE:HA	2:D:84:GLN:O	2.20	0.42
1:B:221:ARG:O	1:B:250:GLN:HA	2.20	0.42
1:B:186:LEU:CD2	1:B:190:PRO:HG3	2.50	0.42
1:A:369:ASN:N	4:A:802:GOL:O2	2.35	0.42
1:A:173:ASP:HA	1:A:177:CYS:SG	2.59	0.42
1:B:244:GLY:O	1:B:245:ILE:C	2.58	0.42
2:C:5:ILE:HD12	2:C:5:ILE:C	2.39	0.42
1:B:325:ASN:ND2	1:B:326:VAL:HG23	2.35	0.42
1:A:458:CYS:HB3	1:B:458:CYS:HB3	2.02	0.42
2:D:12:GLN:NE2	2:D:12:GLN:HA	2.35	0.42
1:A:371:PRO:HB2	1:B:471:ILE:HD11	2.03	0.41
1:B:298:ARG:HG2	1:B:298:ARG:NH1	2.35	0.41
2:C:47:GLU:O	2:C:49:TYR:N	2.54	0.41
1:A:84:ARG:HA	1:A:88:TRP:O	2.20	0.41
1:B:269:VAL:HG12	1:B:270:VAL:N	2.35	0.41
2:D:41:PHE:CD2	2:D:94:LYS:HD3	2.55	0.41
1:B:138:HIS:HD2	1:B:154:ALA:O	2.04	0.41
1:B:351:ARG:HD2	5:B:532:HOH:O	2.20	0.41
2:D:94:LYS:O	2:D:97:LEU:HB3	2.21	0.41
2:C:2:VAL:HG22	2:C:54:PHE:CB	2.50	0.41
1:B:253:PRO:HA	1:B:271:ALA:HA	2.03	0.41
1:A:37:LYS:NZ	5:A:561:HOH:O	2.53	0.41
1:B:13:TYR:HB3	1:B:37:LYS:O	2.20	0.41
1:A:333:GLY:HA3	3:A:600:FAD:O2P	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:CYS:HA	1:B:208:PHE:CE2	2.54	0.41
1:B:194:LEU:HB2	1:B:284:TYR:CE2	2.56	0.41
1:B:9:LYS:HG2	1:B:11:TYR:HB2	2.03	0.41
2:D:16:ASP:C	2:D:18:ALA:H	2.23	0.41
2:C:32:CYS:SG	2:C:35:SER:HB2	2.61	0.41
1:B:173:ASP:O	1:B:177:CYS:HB2	2.20	0.41
1:A:326:VAL:HA	1:A:327:PRO:HD3	1.85	0.41
2:D:38:ILE:O	2:D:38:ILE:HG12	2.20	0.41
2:D:16:ASP:HB2	5:D:204:HOH:O	2.20	0.41
1:A:35:GLY:O	1:A:36:LYS:O	2.38	0.41
1:A:383:CYS:SG	1:A:456:LEU:HD12	2.61	0.41
2:C:4:GLN:HA	2:C:4:GLN:NE2	2.36	0.41
1:B:9:LYS:O	1:B:11:TYR:N	2.44	0.41
1:B:356:ARG:HA	1:B:361:SER:O	2.21	0.41
1:A:344:PRO:HB2	1:B:469:ILE:CG2	2.52	0.40
2:D:60:ASP:O	2:D:63:GLN:HG3	2.21	0.40
1:B:113:ASN:O	1:B:117:ARG:HG3	2.21	0.40
1:A:467:SER:OG	1:B:457:LYS:HD2	2.21	0.40
1:A:65:ILE:HB	1:A:66:PRO:CD	2.51	0.40
1:B:47:THR:HG23	1:B:51:THR:O	2.21	0.40
1:A:13:TYR:O	1:A:154:ALA:CA	2.64	0.40
1:B:390:ALA:CB	1:B:426:ILE:HG21	2.51	0.40
1:A:356:ARG:HA	1:A:361:SER:O	2.22	0.40
1:A:35:GLY:O	1:A:36:LYS:C	2.59	0.40
1:B:168:LEU:HB3	1:B:170:ILE:HG23	2.04	0.40
1:B:67:LYS:HB3	1:B:67:LYS:HE3	1.92	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	493/519 (95%)	446 (90%)	40 (8%)	7 (1%)	14 28
1	B	489/519 (94%)	433 (88%)	48 (10%)	8 (2%)	12 24
2	C	103/116 (89%)	83 (81%)	11 (11%)	9 (9%)	1 1
2	D	103/116 (89%)	91 (88%)	9 (9%)	3 (3%)	6 9
All	All	1188/1270 (94%)	1053 (89%)	108 (9%)	27 (2%)	8 14

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	B	36	LYS
1	B	92	GLU
2	C	69	CYS
1	A	301	GLY
1	A	311	GLU
1	B	10	SER
1	B	245	ILE
1	B	301	GLY
2	C	19	GLY
1	A	6	ASP
1	A	276	SER
1	B	311	GLU
2	C	17	ALA
2	C	48	LYS
2	C	50	SER
2	C	88	GLU
2	D	22	LEU
1	A	299	LYS
1	B	133	GLN
1	B	299	LYS
2	D	17	ALA
2	D	21	LYS
2	C	68	GLU
2	C	103	GLU
2	C	59	VAL
1	A	223	ILE

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	406/426 (95%)	390 (96%)	16 (4%)	39	68
1	B	402/426 (94%)	386 (96%)	16 (4%)	38	67
2	C	92/101 (91%)	89 (97%)	3 (3%)	45	73
2	D	92/101 (91%)	88 (96%)	4 (4%)	35	64
All	All	992/1054 (94%)	953 (96%)	39 (4%)	39	68

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	93	THR
1	A	100	ARG
1	A	122	GLU
1	A	145	ASN
1	A	175	GLU
1	A	311	GLU
1	A	336	LEU
1	A	341	GLU
1	A	348	GLN
1	A	364	LYS
1	A	376	THR
1	A	397	GLU
1	A	403	HIS
1	A	474	VAL
1	A	491	SER
1	B	14	ASP
1	B	76	LEU
1	B	85	ASN
1	B	100	ARG
1	B	121	ARG
1	B	122	GLU
1	B	145	ASN
1	B	175	GLU
1	B	311	GLU
1	B	348	GLN
1	B	364	LYS
1	B	376	THR

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Mol	Chain	Res	Type
1	B	397	GLU
1	B	403	HIS
1	B	432	ASN
1	B	474	VAL
2	C	30	THR
2	C	63	GLN
2	C	94	LYS
2	D	4	GLN
2	D	5	ILE
2	D	20	ASP
2	D	64	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	81	GLN
1	A	107	ASN
1	A	113	ASN
1	A	138	HIS
1	A	258	GLN
1	A	348	GLN
1	A	355	GLN
1	A	398	ASN
1	A	428	ASN
1	A	439	HIS
1	A	450	GLN
1	B	33	GLN
1	B	81	GLN
1	B	85	ASN
1	B	96	HIS
1	B	107	ASN
1	B	113	ASN
1	B	133	GLN
1	B	138	HIS
1	B	275	ASN
1	B	348	GLN
1	B	355	GLN
1	B	398	ASN
1	B	428	ASN
1	B	432	ASN
1	B	439	HIS

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Mol	Chain	Res	Type
1	B	450	GLN
2	C	4	GLN
2	C	12	GLN
2	C	102	ASN
2	D	4	GLN
2	D	12	GLN
2	D	51	ASN
2	D	102	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	$\#\|Z\| > 2$
3	FAD	A	600	-	48,58,58	1.74	9 (18%)	54,89,89	1.92	3 (5%)
4	GOL	A	801	-	5,5,5	4.79	5 (100%)	5,5,5	5.70	3 (60%)
4	GOL	A	802	-	5,5,5	4.87	5 (100%)	5,5,5	5.71	3 (60%)
4	GOL	A	804	-	5,5,5	4.78	5 (100%)	5,5,5	5.72	3 (60%)
4	GOL	A	806	-	5,5,5	4.74	5 (100%)	5,5,5	5.72	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FAD	B	600	-	48,58,58	1.81	8 (16%)	54,89,89	1.95	3 (5%)
4	GOL	B	807	-	5,5,5	4.81	5 (100%)	5,5,5	5.68	3 (60%)
4	GOL	B	808	-	5,5,5	4.73	5 (100%)	5,5,5	5.73	3 (60%)

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
3	FAD	A	600	-	-	0/30/50/50	0/6/6/6
4	GOL	A	801	-	-	0/4/4/4	0/0/0/0
4	GOL	A	802	-	-	0/4/4/4	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	FAD	B	600	-	-	0/30/50/50	0/6/6/6
4	GOL	B	807	-	-	0/4/4/4	0/0/0/0
4	GOL	B	808	-	-	0/4/4/4	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	GOL	C3-C2	-8.14	1.21	1.52
4	B	807	GOL	C3-C2	-8.05	1.21	1.52
4	A	801	GOL	C3-C2	-8.02	1.21	1.52
4	A	804	GOL	C3-C2	-7.93	1.22	1.52
4	B	808	GOL	C3-C2	-7.82	1.22	1.52
4	A	806	GOL	C3-C2	-7.81	1.22	1.52
4	A	802	GOL	C1-C2	-3.32	1.39	1.52
4	A	802	GOL	O2-C2	-3.24	1.33	1.43
4	A	806	GOL	O2-C2	-3.22	1.33	1.43
4	A	801	GOL	O2-C2	-3.12	1.34	1.43
4	A	804	GOL	O2-C2	-3.01	1.34	1.43
4	B	807	GOL	C1-C2	-3.00	1.40	1.52
4	B	807	GOL	O2-C2	-3.00	1.34	1.43
4	A	804	GOL	C1-C2	-2.89	1.41	1.52
4	B	808	GOL	O2-C2	-2.89	1.34	1.43
4	B	808	GOL	C1-C2	-2.83	1.41	1.52
4	A	801	GOL	C1-C2	-2.80	1.41	1.52
4	A	806	GOL	C1-C2	-2.74	1.41	1.52
3	B	600	FAD	C4X-C10	2.01	1.44	1.41
3	A	600	FAD	C2A-N3A	2.27	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	FAD	C9-C8	2.57	1.44	1.37
3	A	600	FAD	O4B-C1B	2.60	1.44	1.41
3	A	600	FAD	C4X-C10	2.66	1.46	1.41
3	A	600	FAD	C9-C8	2.73	1.45	1.37
3	B	600	FAD	O4B-C1B	2.75	1.44	1.41
4	A	802	GOL	O3-C3	3.18	1.56	1.42
3	B	600	FAD	C5X-N5	3.24	1.40	1.35
3	A	600	FAD	C4A-N3A	3.27	1.40	1.35
4	A	801	GOL	O3-C3	3.33	1.56	1.42
4	A	806	GOL	O3-C3	3.46	1.57	1.42
4	B	807	GOL	O3-C3	3.46	1.57	1.42
4	B	808	GOL	O3-C3	3.48	1.57	1.42
3	A	600	FAD	C5X-N5	3.50	1.40	1.35
4	A	804	GOL	O3-C3	3.51	1.57	1.42
3	B	600	FAD	C4A-N3A	3.91	1.41	1.35
3	B	600	FAD	C4-N3	4.12	1.40	1.33
3	A	600	FAD	C4-N3	4.15	1.40	1.33
4	A	802	GOL	O1-C1	4.52	1.61	1.42
4	B	807	GOL	O1-C1	4.57	1.62	1.42
4	A	806	GOL	O1-C1	4.64	1.62	1.42
4	A	801	GOL	O1-C1	4.66	1.62	1.42
4	A	804	GOL	O1-C1	4.67	1.62	1.42
4	B	808	GOL	O1-C1	4.71	1.62	1.42
3	A	600	FAD	C4X-N5	5.05	1.41	1.33
3	B	600	FAD	C9A-N10	5.52	1.46	1.38
3	A	600	FAD	C9A-N10	5.66	1.46	1.38
3	B	600	FAD	C4X-N5	5.73	1.42	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	FAD	C4X-C4-N3	-6.06	115.31	123.59
3	B	600	FAD	C4X-C4-N3	-5.81	115.65	123.59
3	B	600	FAD	O2B-C2B-C3B	2.09	118.61	111.83
3	A	600	FAD	C2B-C1B-N9A	2.23	117.69	114.29
4	A	802	GOL	O1-C1-C2	3.12	125.31	110.18
4	A	804	GOL	O1-C1-C2	3.13	125.36	110.18
4	B	808	GOL	O1-C1-C2	3.17	125.54	110.18
4	A	806	GOL	O1-C1-C2	3.22	125.80	110.18
4	B	807	GOL	O1-C1-C2	3.27	126.03	110.18
4	A	801	GOL	O1-C1-C2	3.35	126.43	110.18
4	A	806	GOL	O2-C2-C3	6.38	137.92	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	804	GOL	O2-C2-C3	6.43	138.14	108.65
4	A	801	GOL	O2-C2-C3	6.44	138.19	108.65
4	B	808	GOL	O2-C2-C3	6.49	138.43	108.65
4	A	802	GOL	O2-C2-C3	6.55	138.67	108.65
4	B	807	GOL	O2-C2-C3	6.56	138.74	108.65
4	B	807	GOL	O3-C3-C2	10.34	160.32	110.18
4	A	801	GOL	O3-C3-C2	10.45	160.86	110.18
4	A	802	GOL	O3-C3-C2	10.49	161.07	110.18
4	B	808	GOL	O3-C3-C2	10.55	161.37	110.18
4	A	806	GOL	O3-C3-C2	10.58	161.50	110.18
4	A	804	GOL	O3-C3-C2	10.59	161.53	110.18
3	A	600	FAD	C4-N3-C2	11.15	124.89	115.25
3	B	600	FAD	C4-N3-C2	11.15	124.89	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	FAD	2	0
4	A	802	GOL	2	0
3	B	600	FAD	1	0

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, 95^{th} 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	495/519 (95%)	-0.22	2 (0%) 93 91	19, 43, 72, 100	0
1	B	491/519 (94%)	-0.01	15 (3%) 52 45	22, 48, 79, 95	0
2	C	105/116 (90%)	0.45	7 (6%) 21 15	35, 69, 104, 107	0
2	D	105/116 (90%)	0.59	12 (11%) 7 4	36, 74, 107, 112	0
All	All	1196/1270 (94%)	-0.01	36 (3%) 54 47	19, 50, 91, 112	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	3	LYS	3.9
1	B	10	SER	3.8
2	D	17	ALA	3.2
2	C	82	LYS	3.2
2	D	53	ILE	3.1
1	B	330	TYR	3.1
1	B	13	TYR	3.1
2	D	15	LEU	3.0
1	B	328	TYR	2.9
2	C	81	LYS	2.8
1	B	9	LYS	2.6
1	B	11	TYR	2.5
2	C	21	LYS	2.5
1	A	5	GLU	2.5
2	D	20	ASP	2.5
1	B	156	ARG	2.4
2	D	55	LEU	2.4
1	B	254	ILE	2.4
2	D	9	THR	2.3
1	B	316	ILE	2.3
2	D	7	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	18	ALA	2.3
2	D	25	VAL	2.3
2	C	19	GLY	2.2
2	D	82	LYS	2.1
1	B	320	ASP	2.1
1	B	268	ARG	2.1
1	B	329	ILE	2.1
1	B	142	ALA	2.1
1	B	354	ALA	2.1
2	D	2	VAL	2.1
2	C	3	LYS	2.1
2	C	53	ILE	2.1
1	B	327	PRO	2.1
2	C	20	ASP	2.0
1	A	6	ASP	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 carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	804	6/6	0.61	0.46	10.12	72,73,74,74	0
4	GOL	A	806	6/6	0.80	0.36	7.88	54,56,58,59	0
4	GOL	A	801	6/6	0.54	0.33	6.33	67,71,71,71	0
4	GOL	B	807	6/6	0.76	0.21	2.03	65,65,65,66	0
4	GOL	B	808	6/6	0.81	0.29	1.72	60,62,63,64	0
3	FAD	B	600	53/53	0.93	0.18	0.62	58,62,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FAD	A	600	53/53	0.96	0.14	-0.28	32,37,40,42	0
4	GOL	A	802	6/6	0.92	0.12	-1.27	44,46,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.