WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 AM GMT

|		
PDB ID	:	2VMK
Title	:	CRYSTAL STRUCTURE OF E. COLI RNASE E APOPROTEIN - CATALYTIC DOMAIN
Authors	:	Koslover, D.J.; Callaghan, A.J.; Marcaida, M.J.; Martick, M.; Scott, W.G.; Luisi, B.F.
Deposited on	:	2008-01-28
Resolution	:	3.30 Å(reported)

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 3.30 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.
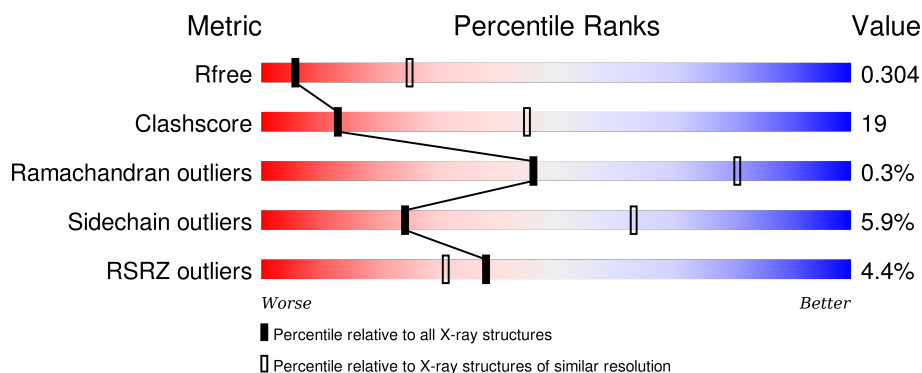
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	515	
1	B	515	
1	C	515	
1	D	515	

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	SO4	A	1509	-	-	X	-
2	SO4	C	1507	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14187 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 RIBONUCLEASE E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3507	2207	621	669	10			
1	B	495	Total	C	N	O	S	0	0	0
			3653	2303	657	681	12			
1	C	474	Total	C	N	O	S	0	0	0
			3507	2198	633	665	11			
1	D	472	Total	C	N	O	S	0	0	0
			3503	2210	626	655	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
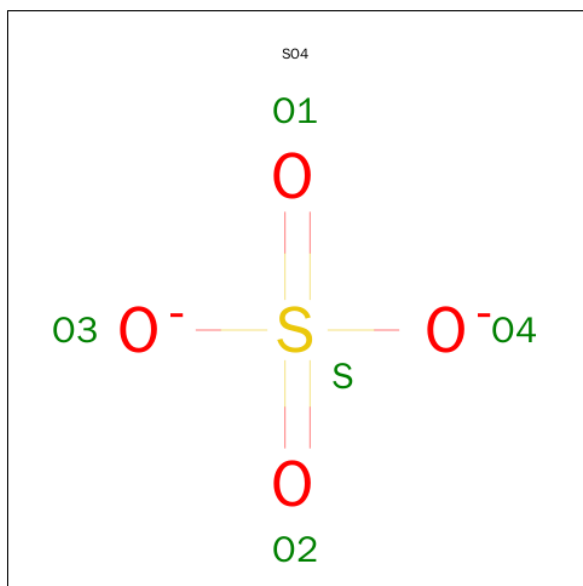
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

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: RIBONUCLEASE E
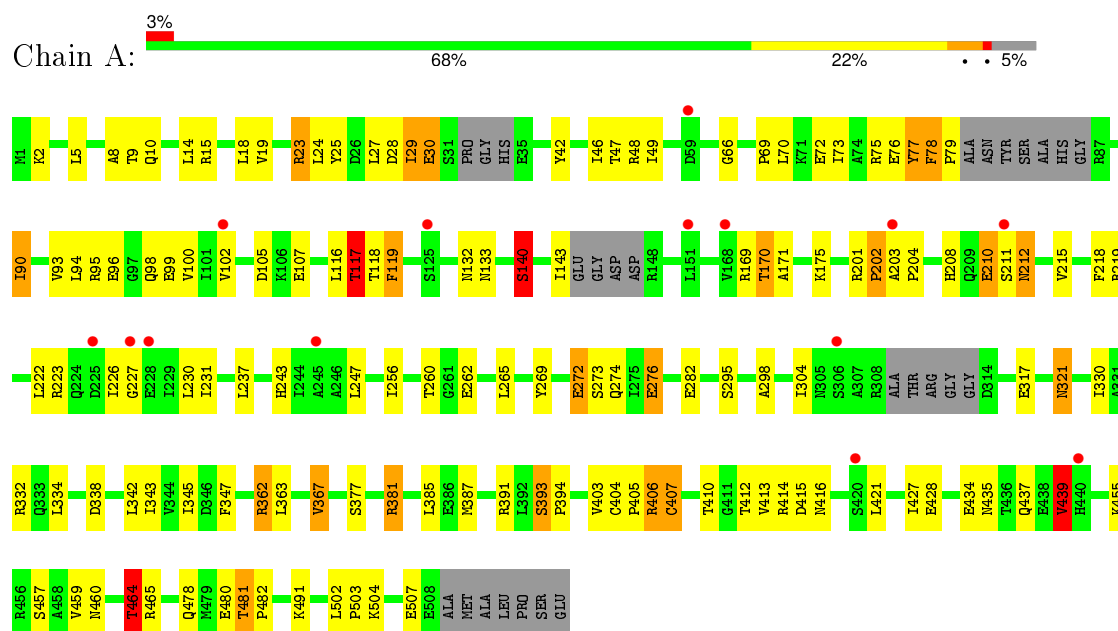
- Molecule 1: RIBONUCLEASE E

● Molecule 1: RIBONUCLEASE E

Chain C:

● Molecule 1: RIBONUCLEASE E

Chain D:
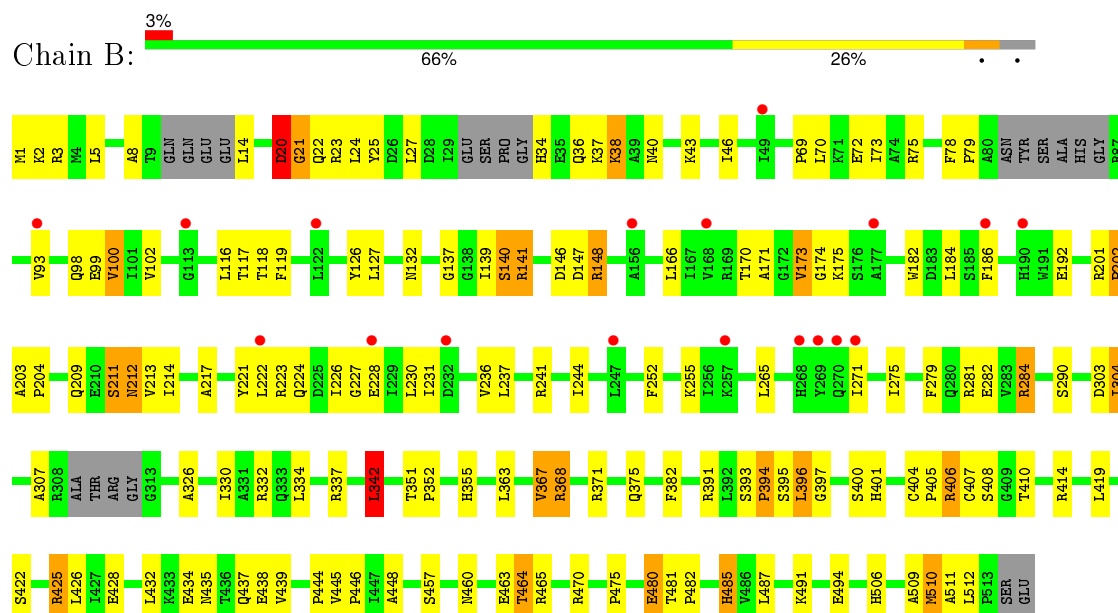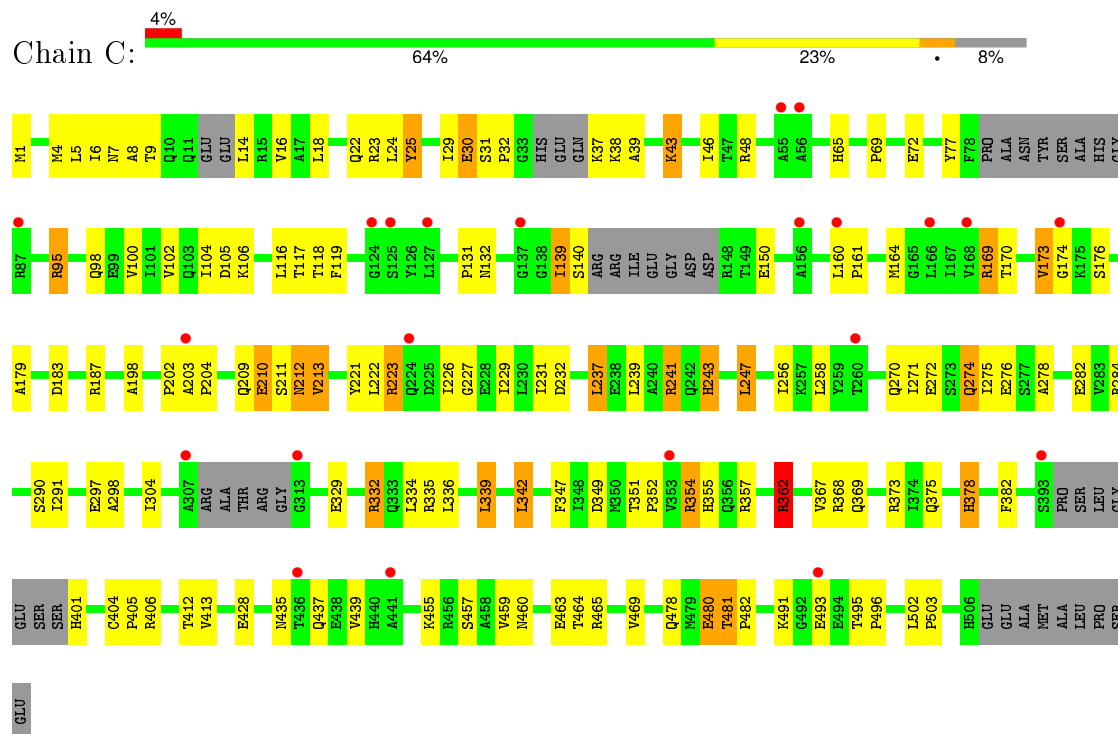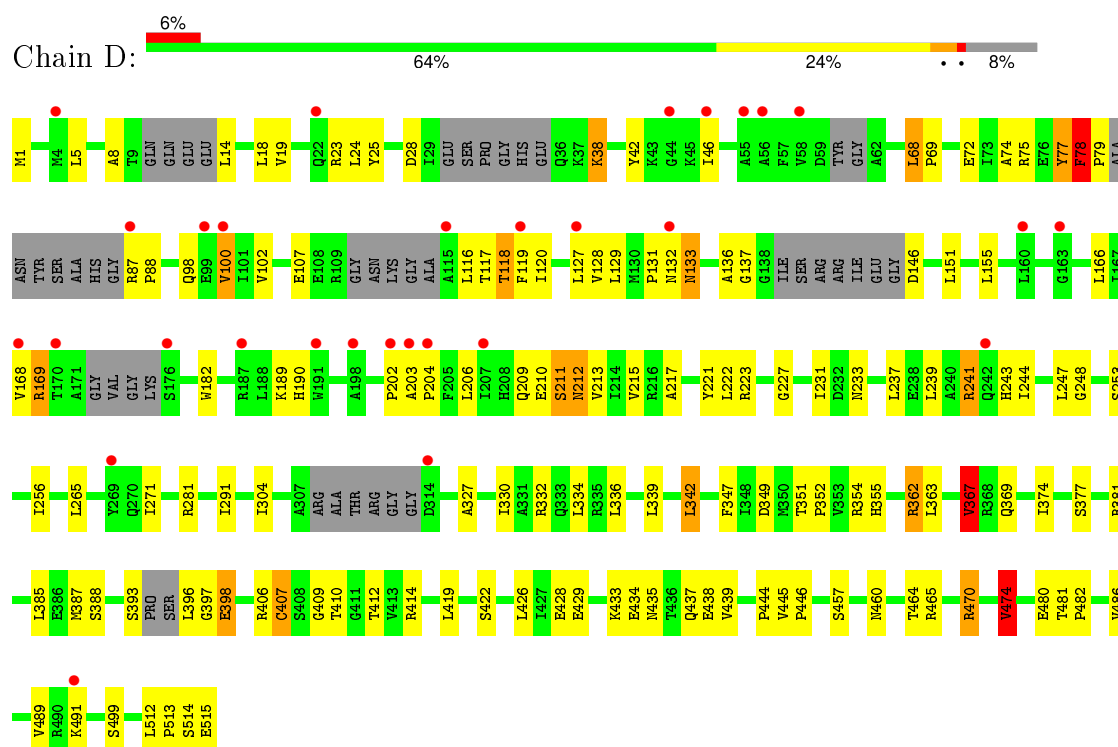
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.24Å 75.57Å 109.37Å 94.95° 102.03° 91.77°	Depositor
Resolution (Å)	47.84 – 3.30 45.54 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.84-3.30) 94.0 (45.54-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.267 , 0.293 0.274 , 0.304	Depositor DCC
R_{free} test set	1664 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	96.3	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Outliers	0 of 33275 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14187	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	1.15	20/3560 (0.6%)	0.50	0/4859
1	B	1.06	15/3711 (0.4%)	0.50	0/5048
1	C	1.25	24/3558 (0.7%)	0.56	0/4835
1	D	1.05	13/3553 (0.4%)	0.46	0/4828
All	All	1.13	72/14382 (0.5%)	0.51	0/19570

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	B	1	6
1	C	0	13
1	D	0	6
All	All	1	38

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	SER	CA-CB	-12.14	1.34	1.52
1	D	474	VAL	CB-CG2	-11.44	1.28	1.52
1	D	77	TYR	CG-CD1	-11.34	1.24	1.39
1	D	77	TYR	CE1-CZ	-11.33	1.23	1.38
1	A	439	VAL	CB-CG1	-11.10	1.29	1.52
1	A	439	VAL	CB-CG2	-10.85	1.30	1.52
1	D	77	TYR	CE2-CZ	-10.68	1.24	1.38
1	D	474	VAL	CB-CG1	-10.66	1.30	1.52
1	A	77	TYR	CE2-CZ	-10.52	1.24	1.38
1	C	77	TYR	CE2-CZ	-10.48	1.25	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	TYR	CG-CD2	-10.45	1.25	1.39
1	C	77	TYR	CE1-CZ	-10.45	1.25	1.38
1	C	77	TYR	CG-CD2	-10.18	1.25	1.39
1	C	77	TYR	CG-CD1	-10.16	1.25	1.39
1	D	367	VAL	CB-CG1	-10.10	1.31	1.52
1	A	77	TYR	CG-CD1	-9.77	1.26	1.39
1	A	140	SER	CA-CB	-9.30	1.39	1.52
1	A	95	ARG	CZ-NH1	9.17	1.45	1.33
1	A	77	TYR	CG-CD2	-9.03	1.27	1.39
1	C	342	LEU	CG-CD1	-8.72	1.19	1.51
1	D	100	VAL	CB-CG2	-8.62	1.34	1.52
1	D	100	VAL	CB-CG1	-8.62	1.34	1.52
1	B	342	LEU	CG-CD1	-8.45	1.20	1.51
1	C	25	TYR	CE2-CZ	-8.25	1.27	1.38
1	A	77	TYR	CE1-CZ	-8.14	1.27	1.38
1	A	342	LEU	CG-CD1	-8.08	1.22	1.51
1	D	367	VAL	CB-CG2	-7.96	1.36	1.52
1	D	342	LEU	CG-CD2	-7.91	1.22	1.51
1	B	140	SER	CB-OG	-7.66	1.32	1.42
1	D	342	LEU	CG-CD1	-7.26	1.25	1.51
1	A	276	GLU	CB-CG	-7.07	1.38	1.52
1	B	282	GLU	CG-CD	7.07	1.62	1.51
1	A	117	THR	CB-CG2	-6.90	1.29	1.52
1	C	95	ARG	NE-CZ	6.79	1.41	1.33
1	C	100	VAL	CB-CG2	-6.76	1.38	1.52
1	C	298	ALA	CA-CB	-6.71	1.38	1.52
1	A	407	CYS	CB-SG	-6.57	1.71	1.82
1	A	321	ASN	CG-OD1	-6.48	1.09	1.24
1	A	367	VAL	CB-CG2	-6.43	1.39	1.52
1	A	272	GLU	CG-CD	-6.40	1.42	1.51
1	C	274	GLN	CG-CD	-6.39	1.36	1.51
1	B	307	ALA	C-O	-6.31	1.11	1.23
1	C	439	VAL	CB-CG2	-6.21	1.39	1.52
1	C	493	GLU	CB-CG	-6.15	1.40	1.52
1	A	342	LEU	CG-CD2	-6.08	1.29	1.51
1	B	367	VAL	CB-CG2	-5.99	1.40	1.52
1	C	258	LEU	CG-CD2	-5.94	1.29	1.51
1	A	140	SER	CB-OG	-5.89	1.34	1.42
1	C	247	LEU	CG-CD1	-5.89	1.30	1.51
1	B	485	HIS	CA-CB	-5.85	1.41	1.53
1	B	439	VAL	CB-CG2	-5.79	1.40	1.52
1	A	464	THR	CB-CG2	-5.72	1.33	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	463	GLU	CD-OE1	5.69	1.31	1.25
1	C	439	VAL	CB-CG1	-5.68	1.41	1.52
1	A	95	ARG	CZ-NH2	5.67	1.40	1.33
1	B	192	GLU	CG-CD	-5.65	1.43	1.51
1	B	25	TYR	CE1-CZ	-5.58	1.31	1.38
1	D	439	VAL	CB-CG2	-5.52	1.41	1.52
1	C	362	ARG	CZ-NH1	5.51	1.40	1.33
1	C	342	LEU	CG-CD2	-5.46	1.31	1.51
1	A	321	ASN	CG-ND2	-5.40	1.19	1.32
1	C	276	GLU	CG-CD	5.36	1.59	1.51
1	C	339	LEU	C-O	5.33	1.33	1.23
1	B	1	MET	CG-SD	-5.32	1.67	1.81
1	C	367	VAL	CB-CG1	-5.32	1.41	1.52
1	B	100	VAL	CB-CG2	-5.31	1.41	1.52
1	C	247	LEU	CG-CD2	-5.25	1.32	1.51
1	C	278	ALA	CA-CB	5.17	1.63	1.52
1	B	141	ARG	N-CA	-5.17	1.36	1.46
1	C	100	VAL	CB-CG1	-5.13	1.42	1.52
1	B	439	VAL	CB-CG1	-5.13	1.42	1.52
1	C	493	GLU	CD-OE1	-5.09	1.20	1.25

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	412	THR	CB

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLN	Mainchain
1	A	140	SER	Mainchain
1	A	202	PRO	Peptide
1	A	210	GLU	Peptide
1	A	212	ASN	Peptide
1	A	23	ARG	Peptide
1	A	243	HIS	Sidechain
1	A	29	ILE	Peptide
1	A	30	GLU	Peptide
1	A	393	SER	Mainchain
1	A	42	TYR	Peptide
1	A	480	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	9	THR	Mainchain
1	B	140	SER	Mainchain
1	B	20	ASP	Peptide
1	B	202	PRO	Peptide
1	B	21	GLY	Peptide
1	B	211	SER	Peptide
1	B	480	GLU	Peptide
1	C	139	ILE	Peptide
1	C	202	PRO	Peptide
1	C	210	GLU	Peptide
1	C	212	ASN	Peptide
1	C	243	HIS	Sidechain
1	C	284	ARG	Sidechain
1	C	29	ILE	Mainchain
1	C	30	GLU	Mainchain
1	C	354	ARG	Mainchain
1	C	37	LYS	Peptide
1	C	378	HIS	Mainchain
1	C	405	PRO	Peptide
1	C	480	GLU	Peptide
1	D	118	THR	Peptide
1	D	136	ALA	Peptide
1	D	202	PRO	Peptide
1	D	212	ASN	Mainchain
1	D	480	GLU	Peptide
1	D	78	PHE	Sidechain

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	3507	0	3268	134	1
1	B	3653	0	3525	159	0
1	C	3507	0	3350	137	3
1	D	3503	0	3359	144	0
2	A	5	0	0	4	0
2	B	5	0	0	1	0
2	C	5	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	14187	0	13502	530	3

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 19.

All (530) 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:C:23:ARG:NH2	1:C:332:ARG:HG2	1.36	1.41
1:B:14:LEU:HD23	1:B:213:VAL:CG1	1.59	1.32
1:D:128:VAL:O	1:D:166:LEU:HD12	1.28	1.32
1:D:14:LEU:HD23	1:D:213:VAL:CG1	1.66	1.24
1:B:391:ARG:NH1	1:B:397:GLY:HA2	1.54	1.21
1:C:209:GLN:HG2	1:C:212:ASN:ND2	1.56	1.19
1:B:485:HIS:HD2	1:B:487:LEU:HD11	1.04	1.18
1:B:391:ARG:HH11	1:B:397:GLY:HA2	0.99	1.16
1:C:222:LEU:O	1:C:223:ARG:HG3	1.45	1.15
1:D:14:LEU:HD23	1:D:213:VAL:HG11	1.25	1.14
1:D:169:ARG:HH11	1:D:169:ARG:HG2	1.07	1.13
1:C:209:GLN:CG	1:C:212:ASN:HD22	1.62	1.13
1:A:231:ILE:HD12	1:A:237:LEU:HD12	1.23	1.12
1:B:391:ARG:HH11	1:B:397:GLY:CA	1.66	1.08
1:B:78:PHE:HE2	1:B:93:VAL:HG11	1.04	1.07
1:B:485:HIS:CD2	1:B:487:LEU:HD11	1.90	1.04
1:B:485:HIS:HD2	1:B:487:LEU:CD1	1.69	1.04
1:C:23:ARG:NH2	1:C:332:ARG:CG	2.21	1.04
1:B:209:GLN:HG2	1:B:212:ASN:OD1	1.59	1.03
1:B:78:PHE:CE2	1:B:93:VAL:HG11	1.95	1.01
1:C:25:TYR:HB2	1:C:335:ARG:HH21	1.21	1.00
1:D:231:ILE:HD12	1:D:237:LEU:HD12	1.39	0.99
1:B:14:LEU:HD23	1:B:213:VAL:HG11	1.00	0.99
1:B:166:LEU:HD21	1:B:184:LEU:HD13	1.41	0.99
1:B:78:PHE:HE2	1:B:93:VAL:CG1	1.75	0.98
1:A:5:LEU:HD22	1:A:265:LEU:HD11	1.44	0.98
1:D:128:VAL:O	1:D:166:LEU:CD1	2.11	0.97
1:D:128:VAL:C	1:D:166:LEU:CD1	2.33	0.96
1:B:3:ARG:NE	1:B:228:GLU:OE2	1.98	0.95
1:B:14:LEU:CD2	1:B:213:VAL:HG11	1.96	0.95
1:B:34:HIS:CE1	1:B:36:GLN:HB2	2.01	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:VAL:HG11	1:C:373:ARG:HG2	1.49	0.94
1:A:78:PHE:HE2	1:A:93:VAL:HG11	1.32	0.94
1:D:129:LEU:HA	1:D:166:LEU:HD13	1.50	0.94
1:B:14:LEU:CD2	1:B:213:VAL:CG1	2.47	0.93
1:D:169:ARG:CG	1:D:169:ARG:HH11	1.81	0.93
1:A:78:PHE:CE2	1:A:93:VAL:HG11	2.04	0.92
1:B:78:PHE:CE2	1:B:93:VAL:CG1	2.55	0.90
1:A:99:GLU:HG2	1:A:203:ALA:HB2	1.53	0.90
1:A:273:SER:HB3	1:B:426:LEU:CD1	2.02	0.89
1:C:272:GLU:HB3	1:D:429:GLU:CD	1.93	0.89
1:D:128:VAL:C	1:D:166:LEU:HD12	1.93	0.88
1:C:209:GLN:HG2	1:C:212:ASN:HD22	0.73	0.88
1:A:70:LEU:HD13	1:A:90:ILE:HG12	1.53	0.88
1:C:118:THR:O	1:C:132:ASN:ND2	2.07	0.88
1:B:406:ARG:HH21	1:B:481:THR:HG22	1.40	0.87
1:C:23:ARG:HH22	1:C:332:ARG:HG2	1.36	0.86
1:C:30:GLU:HB3	1:C:213:VAL:HG21	1.56	0.86
1:C:23:ARG:CZ	1:C:332:ARG:HG2	2.04	0.86
1:D:169:ARG:NH1	1:D:169:ARG:HG2	1.78	0.86
1:A:460:ASN:O	1:A:464:THR:HG23	1.76	0.86
1:C:382:PHE:CZ	1:D:387:MET:HA	2.10	0.85
1:C:22:GLN:O	1:C:274:GLN:NE2	2.10	0.85
1:D:363:LEU:O	1:D:367:VAL:HG23	1.76	0.85
1:D:1:MET:CE	1:D:227:GLY:HA3	2.07	0.85
1:D:237:LEU:HD11	1:D:256:ILE:HG22	1.57	0.84
1:A:78:PHE:CD2	1:A:93:VAL:HG13	2.12	0.84
1:A:18:LEU:HB3	1:A:25:TYR:CZ	2.13	0.84
1:A:407:CYS:HB2	1:A:410:THR:O	1.78	0.83
1:B:3:ARG:HG2	1:B:228:GLU:HB2	1.60	0.83
1:C:30:GLU:HB3	1:C:213:VAL:CG2	2.09	0.83
1:D:367:VAL:HG11	1:D:374:ILE:HD13	1.60	0.83
1:D:118:THR:O	1:D:132:ASN:ND2	2.11	0.83
1:C:24:LEU:HD22	1:C:275:ILE:HG13	1.58	0.82
1:B:2:LYS:HD3	1:B:20:ASP:HB2	1.61	0.82
1:A:78:PHE:CE2	1:A:93:VAL:CG1	2.64	0.81
1:A:77:TYR:O	1:A:79:PRO:HD3	1.80	0.80
1:D:514:SER:O	1:D:515:GLU:HB2	1.81	0.80
1:C:382:PHE:HB3	1:D:342:LEU:HD22	1.63	0.80
1:B:460:ASN:O	1:B:464:THR:HG22	1.82	0.80
1:B:14:LEU:HD23	1:B:213:VAL:HG13	1.61	0.80
1:D:474:VAL:HG21	1:D:499:SER:O	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:HG2	1:A:203:ALA:CB	2.12	0.78
1:D:407:CYS:HB2	1:D:409:GLY:H	1.48	0.78
1:C:102:VAL:HG11	1:C:116:LEU:HD13	1.66	0.78
1:A:99:GLU:CG	1:A:203:ALA:HB2	2.13	0.78
1:A:273:SER:HB3	1:B:426:LEU:HD11	1.65	0.77
1:D:78:PHE:O	1:D:78:PHE:CD2	2.38	0.77
1:D:78:PHE:HD2	1:D:78:PHE:O	1.67	0.77
1:C:7:ASN:ND2	1:C:232:ASP:OD1	2.15	0.77
1:D:129:LEU:CA	1:D:166:LEU:HD13	2.15	0.77
1:B:24:LEU:HB2	1:B:271:ILE:CG2	2.13	0.77
1:D:367:VAL:CG1	1:D:374:ILE:HD13	2.15	0.76
1:C:173:VAL:HG11	1:C:373:ARG:CG	2.15	0.76
1:B:22:GLN:HG2	1:B:22:GLN:O	1.85	0.76
1:D:14:LEU:CD2	1:D:213:VAL:CG1	2.57	0.76
1:B:352:PRO:HG2	1:B:355:HIS:CD2	2.20	0.76
1:D:68:LEU:HD11	1:D:118:THR:CG2	2.16	0.75
1:A:77:TYR:O	1:A:79:PRO:CD	2.35	0.75
1:C:24:LEU:HG	1:C:336:LEU:HD21	1.68	0.75
1:B:102:VAL:HG11	1:B:116:LEU:HD13	1.68	0.75
1:A:272:GLU:HG2	1:B:425:ARG:HB2	1.69	0.75
1:D:68:LEU:HD11	1:D:118:THR:HG23	1.66	0.74
1:C:382:PHE:CD2	1:D:388:SER:HB3	2.22	0.74
1:A:231:ILE:CD1	1:A:237:LEU:HD12	2.12	0.74
1:D:155:LEU:HD13	1:D:168:VAL:CG2	2.18	0.73
1:D:14:LEU:HD23	1:D:213:VAL:HG13	1.65	0.73
1:C:460:ASN:O	1:C:464:THR:HG22	1.89	0.73
1:B:284:ARG:HH12	1:B:290:SER:HB3	1.53	0.73
1:B:284:ARG:NH1	1:B:290:SER:HB3	2.04	0.73
1:B:363:LEU:O	1:B:367:VAL:HG22	1.88	0.72
1:D:151:LEU:HD11	1:D:168:VAL:HG11	1.71	0.72
1:D:209:GLN:HG2	1:D:212:ASN:HD22	1.55	0.72
1:A:231:ILE:HD12	1:A:237:LEU:CD1	2.12	0.71
1:A:237:LEU:HD11	1:A:256:ILE:CG2	2.20	0.71
1:A:49:ILE:HG23	1:A:90:ILE:HG22	1.71	0.71
1:D:75:ARG:HA	1:D:78:PHE:CD1	2.25	0.71
1:C:139:ILE:O	1:C:140:SER:HB3	1.91	0.70
1:C:382:PHE:HB3	1:D:342:LEU:CD2	2.22	0.69
1:D:75:ARG:HA	1:D:78:PHE:CE1	2.26	0.69
1:B:5:LEU:HD23	1:B:230:LEU:HB2	1.74	0.69
1:D:438:GLU:HG2	1:D:470:ARG:HB2	1.75	0.69
1:A:460:ASN:O	1:A:464:THR:CG2	2.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:CD	1:A:203:ALA:HB2	2.12	0.69
1:B:166:LEU:CD2	1:B:184:LEU:HD13	2.20	0.69
1:C:173:VAL:HB	1:C:373:ARG:HG3	1.74	0.69
1:B:43:LYS:NZ	1:B:99:GLU:OE2	2.25	0.69
1:D:102:VAL:HG11	1:D:116:LEU:HD13	1.75	0.69
1:D:237:LEU:HD11	1:D:256:ILE:CG2	2.22	0.68
1:D:182:TRP:CZ2	1:D:223:ARG:HA	2.28	0.68
1:D:239:LEU:O	1:D:243:HIS:ND1	2.25	0.68
1:A:170:THR:OG1	2:A:1509:SO4:O2	2.11	0.68
1:A:78:PHE:CD2	1:A:93:VAL:CG1	2.76	0.68
1:C:46:ILE:HD12	1:C:98:GLN:HB3	1.75	0.68
1:A:78:PHE:HD2	1:A:93:VAL:HG13	1.55	0.67
1:D:460:ASN:O	1:D:464:THR:HG22	1.93	0.67
1:B:14:LEU:CD2	1:B:213:VAL:HG13	2.22	0.67
1:A:237:LEU:HD11	1:A:256:ILE:HG22	1.77	0.67
1:C:18:LEU:HD11	1:C:221:TYR:HD2	1.59	0.67
1:A:273:SER:HB3	1:B:426:LEU:HD13	1.74	0.67
1:D:410:THR:OG1	1:D:412:THR:HG22	1.95	0.66
1:A:377:SER:HB3	1:B:382:PHE:HE1	1.60	0.66
1:C:169:ARG:NH1	2:C:1507:SO4:O2	2.28	0.66
1:C:222:LEU:C	1:C:223:ARG:HG3	2.11	0.66
1:B:485:HIS:CD2	1:B:487:LEU:CD1	2.62	0.65
1:A:5:LEU:HD21	1:A:230:LEU:HD12	1.78	0.65
1:D:1:MET:HE3	1:D:227:GLY:HA3	1.78	0.65
1:C:9:THR:HG23	1:C:232:ASP:CG	2.16	0.65
1:A:46:ILE:HD12	1:A:98:GLN:HB3	1.79	0.65
1:C:173:VAL:CG1	1:C:373:ARG:CG	2.75	0.65
1:D:211:SER:O	1:D:211:SER:OG	2.06	0.65
1:B:20:ASP:OD1	1:B:20:ASP:C	2.35	0.65
1:C:382:PHE:CE2	1:D:388:SER:HB3	2.32	0.64
1:B:509:ALA:O	1:B:511:ALA:N	2.30	0.64
1:C:179:ALA:HB2	1:C:368:ARG:HH21	1.62	0.64
1:C:237:LEU:O	1:C:241:ARG:HG3	1.97	0.64
1:A:210:GLU:CD	1:A:219:ARG:HH12	2.02	0.63
1:A:19:VAL:HA	1:A:23:ARG:O	1.98	0.63
1:B:20:ASP:O	1:B:23:ARG:N	2.31	0.63
1:C:139:ILE:O	1:C:140:SER:CB	2.47	0.63
1:A:169:ARG:CG	2:A:1509:SO4:O4	2.47	0.63
1:A:437:GLN:HB2	1:A:491:LYS:HA	1.81	0.63
1:A:100:VAL:HG12	1:A:102:VAL:HG23	1.80	0.62
1:B:175:LYS:N	1:B:175:LYS:HD2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:THR:O	1:A:412:THR:HG23	1.98	0.62
1:D:419:LEU:HD21	1:D:481:THR:O	1.98	0.62
1:A:75:ARG:HA	1:A:78:PHE:HD1	1.64	0.62
1:C:351:THR:N	1:C:352:PRO:CD	2.63	0.62
1:D:137:GLY:HA2	1:D:166:LEU:O	2.00	0.62
1:A:298:ALA:HB2	1:B:303:ASP:HB2	1.81	0.61
1:D:129:LEU:HA	1:D:166:LEU:CD1	2.28	0.61
1:D:129:LEU:N	1:D:166:LEU:CD1	2.63	0.61
1:A:15:ARG:NH1	1:A:272:GLU:OE2	2.24	0.61
1:B:166:LEU:HD21	1:B:184:LEU:CD1	2.22	0.61
1:A:421:LEU:HD13	1:B:279:PHE:CE2	2.36	0.61
1:B:244:ILE:HD13	1:B:252:PHE:HB3	1.83	0.61
1:A:5:LEU:HD23	1:A:230:LEU:HB2	1.82	0.60
1:B:46:ILE:HD12	1:B:98:GLN:HB3	1.82	0.60
1:C:170:THR:HG22	1:C:373:ARG:HD2	1.84	0.60
1:B:509:ALA:C	1:B:511:ALA:H	2.04	0.60
1:A:481:THR:N	1:A:482:PRO:HD2	2.15	0.60
1:C:173:VAL:CG1	1:C:373:ARG:HG3	2.31	0.60
1:A:119:PHE:HA	1:A:132:ASN:HD22	1.67	0.60
1:B:78:PHE:CE2	1:B:93:VAL:HG13	2.37	0.60
1:C:25:TYR:HB2	1:C:335:ARG:NH2	2.05	0.60
1:A:404:CYS:HB2	1:B:407:CYS:SG	2.43	0.59
1:B:146:ASP:OD1	1:B:147:ASP:N	2.35	0.59
1:A:404:CYS:CB	1:B:407:CYS:SG	2.90	0.59
1:A:428:GLU:OE1	1:A:465:ARG:NH1	2.34	0.59
1:C:8:ALA:N	1:C:232:ASP:OD2	2.28	0.59
1:B:24:LEU:HB2	1:B:271:ILE:HG21	1.83	0.59
1:C:69:PRO:HG2	1:C:72:GLU:HG2	1.85	0.59
1:B:99:GLU:O	1:B:100:VAL:HG23	2.02	0.59
1:D:222:LEU:O	1:D:223:ARG:HG2	2.02	0.59
1:B:5:LEU:HD22	1:B:265:LEU:HD11	1.85	0.59
1:D:128:VAL:C	1:D:166:LEU:HD11	2.23	0.59
1:A:210:GLU:CD	1:A:219:ARG:NH1	2.57	0.58
1:B:70:LEU:HA	1:B:73:ILE:HD12	1.83	0.58
1:D:190:HIS:ND1	1:D:247:LEU:HA	2.18	0.58
1:D:14:LEU:CD2	1:D:213:VAL:HG13	2.31	0.58
1:B:36:GLN:HG2	1:B:211:SER:HB3	1.84	0.58
1:C:43:LYS:HD2	1:C:203:ALA:HA	1.86	0.58
1:C:23:ARG:HH21	1:C:332:ARG:HB3	1.69	0.57
1:A:49:ILE:CG2	1:A:90:ILE:HG22	2.33	0.57
1:C:23:ARG:HG2	1:C:332:ARG:NH2	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:HA	1:B:78:PHE:HB2	1.86	0.57
1:D:1:MET:HE2	1:D:227:GLY:HA3	1.82	0.57
1:A:169:ARG:HG2	2:A:1509:SO4:O4	2.04	0.57
1:A:5:LEU:CD2	1:A:230:LEU:HD12	2.34	0.57
1:A:404:CYS:HB3	1:A:407:CYS:SG	2.44	0.57
1:D:406:ARG:HH21	1:D:481:THR:HG22	1.70	0.57
1:B:437:GLN:HB2	1:B:491:LYS:HA	1.86	0.56
1:C:243:HIS:O	1:C:247:LEU:HD12	2.05	0.56
1:D:127:LEU:HD13	1:D:166:LEU:HD21	1.85	0.56
1:B:5:LEU:CD2	1:B:230:LEU:HB2	2.35	0.56
1:A:47:THR:O	1:A:96:GLU:OE1	2.23	0.56
1:C:481:THR:N	1:C:482:PRO:HD2	2.20	0.56
1:C:437:GLN:HB2	1:C:491:LYS:HA	1.88	0.56
1:B:34:HIS:HE1	1:B:36:GLN:OE1	1.89	0.56
1:C:213:VAL:O	1:C:213:VAL:CG2	2.54	0.56
1:D:239:LEU:HB3	1:D:243:HIS:HE1	1.71	0.56
1:C:239:LEU:O	1:C:243:HIS:ND1	2.39	0.56
1:D:69:PRO:HG2	1:D:72:GLU:HG2	1.87	0.56
1:A:5:LEU:HD11	1:A:269:TYR:CG	2.40	0.56
1:B:391:ARG:NH2	1:B:395:SER:CB	2.69	0.56
1:D:119:PHE:HD1	1:D:133:ASN:HB3	1.71	0.55
1:C:95:ARG:HG2	1:C:98:GLN:HB2	1.88	0.55
1:B:407:CYS:HB3	1:B:410:THR:H	1.71	0.55
1:A:18:LEU:HB3	1:A:25:TYR:OH	2.06	0.55
1:C:173:VAL:CG1	1:C:174:GLY:N	2.69	0.55
1:D:474:VAL:HG12	1:D:474:VAL:O	2.05	0.55
1:D:474:VAL:CG2	1:D:499:SER:O	2.52	0.55
1:A:69:PRO:HG2	1:A:72:GLU:HG2	1.89	0.55
1:C:173:VAL:CB	1:C:373:ARG:HG3	2.36	0.55
1:B:391:ARG:NH2	1:B:395:SER:HB3	2.21	0.55
1:D:291:ILE:HG22	1:D:304:ILE:HG12	1.88	0.55
1:A:406:ARG:NH1	1:B:480:GLU:OE2	2.41	0.54
1:C:30:GLU:HG2	1:C:213:VAL:HB	1.88	0.54
1:D:426:LEU:HD23	1:D:486:VAL:HG21	1.90	0.54
1:C:23:ARG:CG	1:C:332:ARG:NH2	2.70	0.54
1:B:2:LYS:HB2	1:B:226:ILE:HA	1.89	0.54
1:A:66:GLY:HA3	1:A:116:LEU:HD11	1.89	0.54
1:D:334:LEU:HD23	1:D:339:LEU:HD12	1.90	0.54
1:B:141:ARG:HD2	1:B:141:ARG:N	2.22	0.54
1:A:208:HIS:CE1	1:A:215:VAL:HG11	2.44	0.54
1:D:428:GLU:OE1	1:D:465:ARG:NH1	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ALA:HB2	1:B:371:ARG:O	2.08	0.53
1:D:237:LEU:CD1	1:D:256:ILE:CG2	2.86	0.53
1:B:127:LEU:CD1	1:B:184:LEU:HB2	2.39	0.53
1:C:24:LEU:CD2	1:C:275:ILE:HA	2.38	0.53
1:B:170:THR:OG1	2:B:1515:SO4:O2	2.25	0.53
1:D:414:ARG:HH22	1:D:422:SER:HB2	1.73	0.53
1:C:231:ILE:HD12	1:C:237:LEU:HD12	1.90	0.53
1:D:209:GLN:HG2	1:D:212:ASN:ND2	2.22	0.53
1:C:18:LEU:CD1	1:C:221:TYR:HD2	2.20	0.53
1:D:239:LEU:HB3	1:D:243:HIS:CE1	2.43	0.53
1:A:282:GLU:CD	1:B:512:LEU:HB3	2.29	0.53
1:A:381:ARG:HH12	1:B:375:GLN:NE2	2.06	0.53
1:D:46:ILE:HD12	1:D:98:GLN:HB3	1.91	0.53
1:D:14:LEU:CD2	1:D:213:VAL:HG11	2.18	0.53
1:A:18:LEU:HB3	1:A:25:TYR:CE2	2.44	0.53
1:B:170:THR:O	1:B:173:VAL:HB	2.09	0.53
1:D:119:PHE:CD1	1:D:133:ASN:HB3	2.43	0.52
1:A:212:ASN:C	1:A:212:ASN:OD1	2.46	0.52
1:D:352:PRO:HG2	1:D:355:HIS:CD2	2.44	0.52
1:D:367:VAL:CG1	1:D:374:ILE:CD1	2.87	0.52
1:B:2:LYS:CD	1:B:20:ASP:HB2	2.37	0.52
1:A:102:VAL:HG11	1:A:116:LEU:HD13	1.90	0.52
1:A:407:CYS:CB	1:A:410:THR:O	2.55	0.52
1:B:24:LEU:HB2	1:B:271:ILE:HG22	1.89	0.52
1:A:49:ILE:HG23	1:A:90:ILE:CG2	2.38	0.52
1:C:304:ILE:HD12	1:C:347:PHE:HA	1.91	0.52
1:D:24:LEU:HD21	1:D:336:LEU:HD22	1.92	0.52
1:B:43:LYS:CE	1:B:99:GLU:OE2	2.58	0.52
1:A:46:ILE:HD13	1:A:94:LEU:HD13	1.90	0.52
1:C:291:ILE:HG22	1:C:304:ILE:HG12	1.90	0.52
1:A:317:GLU:O	1:A:321:ASN:HB2	2.09	0.52
1:C:382:PHE:CE2	1:D:388:SER:CB	2.93	0.52
1:C:270:GLN:HE22	1:D:433:LYS:HG2	1.74	0.52
1:C:382:PHE:HD2	1:D:388:SER:HB3	1.74	0.51
1:D:155:LEU:HD13	1:D:168:VAL:HG23	1.92	0.51
1:C:406:ARG:O	1:C:406:ARG:HG2	2.10	0.51
1:B:224:GLN:HG2	1:B:224:GLN:O	2.09	0.51
1:D:377:SER:O	1:D:385:LEU:HD11	2.09	0.51
1:A:2:LYS:O	1:A:227:GLY:N	2.40	0.51
1:A:404:CYS:SG	1:B:406:ARG:HB3	2.49	0.51
1:C:30:GLU:HB3	1:C:213:VAL:HG23	1.89	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:PHE:CE2	1:D:388:SER:N	2.78	0.51
1:C:131:PRO:HA	1:C:164:MET:HB3	1.92	0.51
1:C:463:GLU:HG2	1:C:469:VAL:O	2.10	0.51
1:B:352:PRO:HG2	1:B:355:HIS:HD2	1.69	0.51
1:C:5:LEU:HD12	1:C:271:ILE:HD13	1.93	0.51
1:C:25:TYR:O	1:C:335:ARG:NE	2.35	0.51
1:A:18:LEU:CB	1:A:25:TYR:CZ	2.89	0.51
1:A:363:LEU:O	1:A:367:VAL:HG22	2.11	0.51
1:A:70:LEU:HD12	1:A:73:ILE:HD12	1.93	0.51
1:D:239:LEU:O	1:D:243:HIS:CE1	2.64	0.51
1:D:481:THR:N	1:D:482:PRO:HD2	2.25	0.51
1:C:352:PRO:HG2	1:C:355:HIS:CD2	2.46	0.51
1:D:203:ALA:N	1:D:204:PRO:HD3	2.26	0.51
1:D:217:ALA:O	1:D:221:TYR:HB2	2.10	0.51
1:A:75:ARG:HA	1:A:78:PHE:CD1	2.45	0.51
1:B:330:ILE:O	1:B:334:LEU:HG	2.11	0.50
1:A:273:SER:CB	1:B:426:LEU:HD11	2.40	0.50
1:B:27:LEU:HD22	1:B:275:ILE:HG12	1.92	0.50
1:D:437:GLN:HB2	1:D:491:LYS:HA	1.91	0.50
1:C:412:THR:HG21	1:D:281:ARG:HE	1.76	0.50
1:A:427:ILE:HG23	1:A:439:VAL:HG11	1.94	0.50
1:B:3:ARG:HA	1:B:228:GLU:O	2.10	0.50
1:C:131:PRO:HA	1:C:164:MET:CB	2.41	0.50
1:C:30:GLU:CB	1:C:213:VAL:CG2	2.88	0.50
1:D:407:CYS:HB2	1:D:410:THR:H	1.76	0.50
1:B:337:ARG:NH1	1:B:400:SER:CB	2.74	0.50
1:B:231:ILE:HB	1:B:237:LEU:HD12	1.94	0.50
1:D:514:SER:O	1:D:515:GLU:CB	2.56	0.50
1:B:171:ALA:C	1:B:173:VAL:H	2.15	0.50
1:A:105:ASP:OD2	1:A:117:THR:HG21	2.12	0.50
1:C:23:ARG:NH2	1:C:332:ARG:CB	2.74	0.49
1:C:428:GLU:OE1	1:C:465:ARG:NH1	2.41	0.49
1:C:173:VAL:HG21	1:C:373:ARG:HE	1.77	0.49
1:A:208:HIS:HE1	1:A:215:VAL:HG11	1.75	0.49
1:C:23:ARG:HH22	1:C:332:ARG:CG	2.08	0.49
1:A:212:ASN:OD1	1:A:215:VAL:HB	2.13	0.49
1:A:15:ARG:NH2	1:A:272:GLU:OE1	2.29	0.49
1:C:4:MET:HE1	1:C:221:TYR:HB2	1.95	0.49
1:D:304:ILE:HD12	1:D:347:PHE:HA	1.93	0.49
1:C:212:ASN:OD1	1:C:212:ASN:O	2.30	0.49
1:C:119:PHE:HA	1:C:132:ASN:HD22	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:OD2	1:A:117:THR:CG2	2.61	0.49
1:A:414:ARG:HG3	1:B:401:HIS:CE1	2.47	0.49
1:D:129:LEU:CA	1:D:166:LEU:CD1	2.88	0.49
1:A:481:THR:N	1:A:482:PRO:CD	2.76	0.49
1:A:212:ASN:O	1:A:212:ASN:OD1	2.30	0.49
1:B:438:GLU:HG2	1:B:470:ARG:CB	2.43	0.49
1:D:77:TYR:O	1:D:79:PRO:HD3	2.13	0.49
1:D:127:LEU:HB3	1:D:166:LEU:HD21	1.95	0.48
1:B:391:ARG:HH21	1:B:395:SER:HB2	1.77	0.48
1:B:393:SER:O	1:B:395:SER:O	2.31	0.48
1:C:272:GLU:HB3	1:D:429:GLU:OE2	2.11	0.48
1:A:282:GLU:OE2	1:B:512:LEU:HB3	2.13	0.48
1:C:406:ARG:HD3	1:C:413:VAL:HG21	1.95	0.48
1:C:173:VAL:HG12	1:C:174:GLY:N	2.28	0.48
1:A:405:PRO:HG2	1:B:406:ARG:NH1	2.28	0.48
1:D:5:LEU:HB3	1:D:265:LEU:HD21	1.94	0.48
1:A:237:LEU:CD1	1:A:256:ILE:CG2	2.92	0.48
1:B:391:ARG:NH1	1:B:397:GLY:CA	2.39	0.48
1:D:512:LEU:O	1:D:515:GLU:N	2.45	0.48
1:B:8:ALA:HB2	1:B:14:LEU:CD1	2.43	0.48
1:B:137:GLY:CA	1:B:166:LEU:O	2.62	0.48
1:A:412:THR:HG21	1:B:281:ARG:HD2	1.96	0.48
1:A:502:LEU:N	1:A:503:PRO:CD	2.76	0.48
1:B:432:LEU:HG	1:B:432:LEU:O	2.13	0.48
1:A:77:TYR:O	1:A:79:PRO:HD2	2.11	0.48
1:C:272:GLU:HB3	1:D:429:GLU:OE1	2.14	0.48
1:C:95:ARG:CG	1:C:98:GLN:HB2	2.43	0.48
1:B:69:PRO:HG2	1:B:72:GLU:HG2	1.95	0.48
1:B:119:PHE:HA	1:B:132:ASN:HD22	1.79	0.47
1:D:38:LYS:HB2	1:D:107:GLU:OE1	2.14	0.47
1:C:18:LEU:HD21	1:C:221:TYR:HB3	1.97	0.47
1:C:203:ALA:N	1:C:204:PRO:HD3	2.29	0.47
1:D:351:THR:N	1:D:352:PRO:CD	2.78	0.47
1:B:174:GLY:O	1:B:368:ARG:HD3	2.14	0.47
1:B:139:ILE:HB	1:B:148:ARG:HH11	1.79	0.47
1:C:6:ILE:HG12	1:C:16:VAL:HG22	1.97	0.47
1:B:391:ARG:HH12	1:B:397:GLY:HA2	1.68	0.47
1:B:34:HIS:O	1:B:34:HIS:CG	2.67	0.47
1:B:406:ARG:HG3	1:B:482:PRO:HG3	1.96	0.47
1:C:8:ALA:HB2	1:C:14:LEU:CD1	2.44	0.47
1:A:8:ALA:HB2	1:A:14:LEU:CD1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HB3	1:A:30:GLU:O	2.14	0.47
1:D:42:TYR:CD2	1:D:206:LEU:HA	2.49	0.47
1:A:118:THR:O	1:A:132:ASN:ND2	2.48	0.47
1:B:391:ARG:NH2	1:B:395:SER:HB2	2.29	0.47
1:C:160:LEU:HD12	1:C:161:PRO:HD2	1.97	0.47
1:B:485:HIS:HD2	1:B:487:LEU:HD12	1.72	0.47
1:C:213:VAL:HG22	1:C:213:VAL:O	2.15	0.47
1:B:182:TRP:NE1	1:B:186:PHE:HE2	2.13	0.47
1:D:407:CYS:CB	1:D:410:THR:H	2.28	0.46
1:C:369:GLN:O	1:C:369:GLN:HG3	2.15	0.46
1:B:100:VAL:HG12	1:B:102:VAL:HG23	1.97	0.46
1:D:8:ALA:HB2	1:D:14:LEU:CD1	2.46	0.46
1:C:43:LYS:HZ3	1:C:198:ALA:C	2.18	0.46
1:C:179:ALA:HB2	1:C:368:ARG:NH2	2.30	0.46
1:B:182:TRP:O	1:B:186:PHE:HD2	1.99	0.46
1:C:282:GLU:OE1	1:D:513:PRO:HD2	2.15	0.46
1:C:375:GLN:NE2	1:D:381:ARG:HH12	2.14	0.46
1:A:27:LEU:HG	1:A:28:ASP:N	2.30	0.46
1:D:354:ARG:HG2	1:D:354:ARG:HH11	1.79	0.46
1:B:182:TRP:CZ2	1:B:223:ARG:HA	2.50	0.46
1:C:455:LYS:O	1:C:459:VAL:HG23	2.16	0.46
1:D:129:LEU:N	1:D:166:LEU:HD13	2.30	0.46
1:C:334:LEU:HD23	1:C:339:LEU:HD12	1.96	0.46
1:D:189:LYS:HB3	1:D:248:GLY:O	2.15	0.46
1:B:201:ARG:HG2	1:B:202:PRO:HD2	1.98	0.46
1:B:34:HIS:HE1	1:B:36:GLN:HB2	1.71	0.46
1:C:382:PHE:HE2	1:D:388:SER:CB	2.28	0.46
1:B:139:ILE:HB	1:B:148:ARG:NH1	2.31	0.46
1:C:24:LEU:HD22	1:C:275:ILE:CG1	2.39	0.46
1:C:43:LYS:NZ	1:C:198:ALA:O	2.46	0.46
1:D:367:VAL:HG12	1:D:374:ILE:CD1	2.45	0.46
1:B:118:THR:O	1:B:132:ASN:ND2	2.49	0.46
1:C:6:ILE:HD12	1:C:229:ILE:CG2	2.46	0.46
1:C:31:SER:HA	1:C:32:PRO:HD3	1.81	0.46
1:A:70:LEU:HB2	1:A:90:ILE:CG1	2.46	0.45
1:A:143:ILE:HG22	1:A:143:ILE:O	2.16	0.45
1:B:217:ALA:O	1:B:221:TYR:HB2	2.17	0.45
1:A:338:ASP:O	1:A:391:ARG:HD2	2.16	0.45
1:D:212:ASN:OD1	1:D:215:VAL:HG23	2.17	0.45
1:A:210:GLU:OE1	1:A:219:ARG:NH1	2.49	0.45
1:D:127:LEU:HD22	1:D:166:LEU:HD21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:SER:OG	1:C:140:SER:O	2.30	0.45
1:A:203:ALA:N	1:A:204:PRO:CD	2.80	0.45
1:C:160:LEU:HD11	1:C:164:MET:HG3	1.99	0.45
1:C:351:THR:N	1:C:352:PRO:HD3	2.30	0.45
1:A:24:LEU:HD23	1:A:274:GLN:HB3	1.98	0.45
1:A:393:SER:HA	1:A:394:PRO:HD2	1.51	0.45
1:A:223:ARG:H	1:A:226:ILE:HD12	1.82	0.45
1:D:237:LEU:O	1:D:241:ARG:HG3	2.17	0.45
1:A:478:GLN:NE2	1:C:478:GLN:OE1	2.50	0.45
1:B:404:CYS:HA	1:B:405:PRO:HD3	1.77	0.45
1:C:404:CYS:SG	1:D:406:ARG:HB3	2.57	0.45
1:A:276:GLU:OE1	1:B:422:SER:OG	2.35	0.45
1:B:222:LEU:HA	1:B:226:ILE:HD12	1.99	0.44
1:B:203:ALA:N	1:B:204:PRO:HD3	2.32	0.44
1:C:290:SER:HB3	1:D:513:PRO:HG2	1.99	0.44
1:D:18:LEU:HB3	1:D:25:TYR:CZ	2.53	0.44
1:C:209:GLN:CG	1:C:212:ASN:ND2	2.43	0.44
1:C:222:LEU:HA	1:C:226:ILE:HD12	1.99	0.44
1:A:78:PHE:HA	1:A:79:PRO:HD2	1.80	0.44
1:D:182:TRP:CH2	1:D:222:LEU:O	2.70	0.44
1:B:8:ALA:HB2	1:B:14:LEU:HD13	2.00	0.44
1:A:99:GLU:O	1:A:100:VAL:HG23	2.18	0.44
1:B:509:ALA:C	1:B:511:ALA:N	2.69	0.44
1:A:208:HIS:HE1	1:A:215:VAL:CG1	2.31	0.44
1:D:87:ARG:HA	1:D:88:PRO:HD3	1.85	0.44
1:B:37:LYS:O	1:B:38:LYS:C	2.56	0.44
1:B:428:GLU:OE1	1:B:465:ARG:NH1	2.50	0.44
1:A:273:SER:CB	1:B:426:LEU:CD1	2.87	0.44
1:C:272:GLU:CB	1:D:429:GLU:OE1	2.64	0.44
1:A:407:CYS:HB3	1:B:404:CYS:SG	2.57	0.44
1:B:126:TYR:CE1	1:B:175:LYS:HE2	2.52	0.44
1:A:406:ARG:HD3	1:A:413:VAL:HG21	1.98	0.44
1:C:38:LYS:O	1:C:104:ILE:O	2.35	0.44
1:C:223:ARG:NH1	1:C:369:GLN:HE21	2.16	0.44
1:A:345:ILE:HD12	1:A:385:LEU:HD23	2.00	0.44
1:D:146:ASP:CG	1:D:146:ASP:O	2.56	0.44
1:C:342:LEU:HA	1:C:342:LEU:HD12	1.73	0.44
1:A:218:PHE:O	1:A:222:LEU:HB2	2.17	0.44
1:A:99:GLU:OE2	1:A:203:ALA:HB2	2.18	0.44
1:C:30:GLU:HG2	1:C:213:VAL:CG2	2.48	0.44
1:C:169:ARG:HG2	2:C:1507:SO4:O4	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:HG2	1:C:332:ARG:HH21	1.82	0.43
1:C:382:PHE:CZ	1:D:387:MET:CA	2.92	0.43
1:D:330:ILE:O	1:D:334:LEU:HG	2.18	0.43
1:B:37:LYS:HA	1:B:40:ASN:ND2	2.33	0.43
1:C:481:THR:N	1:C:482:PRO:CD	2.82	0.43
1:A:304:ILE:HD12	1:A:347:PHE:HA	2.01	0.43
1:B:20:ASP:OD1	1:B:21:GLY:N	2.52	0.43
1:A:363:LEU:HD22	1:A:385:LEU:CD2	2.49	0.43
1:B:304:ILE:HD12	1:B:326:ALA:HB1	1.99	0.43
1:B:444:PRO:HG2	1:B:481:THR:HA	2.01	0.43
1:B:352:PRO:CG	1:B:355:HIS:CD2	2.98	0.43
1:B:393:SER:OG	1:B:395:SER:HB2	2.19	0.43
1:B:434:GLU:O	1:B:435:ASN:HB3	2.19	0.43
1:B:445:VAL:N	1:B:446:PRO:HD2	2.33	0.43
1:C:1:MET:CE	1:C:227:GLY:HA3	2.49	0.42
1:C:23:ARG:HG3	1:C:332:ARG:NH2	2.34	0.42
1:A:363:LEU:CD2	1:A:385:LEU:HD21	2.49	0.42
1:C:502:LEU:N	1:C:503:PRO:CD	2.82	0.42
1:B:351:THR:N	1:B:352:PRO:CD	2.82	0.42
1:D:203:ALA:N	1:D:204:PRO:CD	2.83	0.42
1:A:343:ILE:HB	1:A:387:MET:HG3	2.00	0.42
1:D:120:ILE:O	1:D:131:PRO:HD2	2.19	0.42
1:D:244:ILE:HD12	1:D:256:ILE:HD11	2.02	0.42
1:C:39:ALA:O	1:C:210:GLU:HB2	2.20	0.42
1:D:127:LEU:HD22	1:D:166:LEU:CD2	2.49	0.42
1:A:201:ARG:CG	1:A:202:PRO:HD2	2.50	0.42
1:A:46:ILE:CD1	1:A:94:LEU:HD13	2.50	0.42
1:D:377:SER:O	1:D:385:LEU:CD1	2.68	0.42
1:A:404:CYS:HA	1:A:405:PRO:HD2	1.94	0.42
1:C:169:ARG:HG3	2:C:1507:SO4:O3	2.19	0.42
1:A:412:THR:O	1:A:412:THR:CG2	2.67	0.42
1:B:24:LEU:HD22	1:B:271:ILE:HB	2.01	0.42
1:B:227:GLY:O	1:B:255:LYS:HG2	2.19	0.42
1:A:407:CYS:SG	1:A:410:THR:O	2.77	0.41
1:B:414:ARG:HD3	1:B:419:LEU:HD13	2.02	0.41
1:B:481:THR:N	1:B:482:PRO:HD2	2.35	0.41
1:D:407:CYS:HB2	1:D:409:GLY:N	2.26	0.41
1:A:169:ARG:HA	2:A:1509:SO4:O4	2.20	0.41
1:A:119:PHE:CD1	1:A:133:ASN:HB3	2.55	0.41
1:D:28:ASP:OD2	1:D:221:TYR:HE1	2.02	0.41
1:B:506:HIS:O	1:B:510:MET:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLU:CB	1:C:213:VAL:HG23	2.50	0.41
1:D:434:GLU:O	1:D:435:ASN:HB3	2.20	0.41
1:B:448:ALA:HB3	1:B:475:PRO:HB3	2.02	0.41
1:A:362:ARG:HG2	1:A:362:ARG:NH1	2.34	0.41
1:C:105:ASP:HB3	1:C:106:LYS:HG3	2.01	0.41
1:B:214:ILE:HD11	1:B:236:VAL:HG13	2.02	0.41
1:C:412:THR:HG21	1:D:281:ARG:NE	2.35	0.41
1:A:455:LYS:O	1:A:459:VAL:HG23	2.21	0.41
1:C:354:ARG:CG	1:C:354:ARG:O	2.69	0.41
1:D:74:ALA:HB2	1:D:132:ASN:ND2	2.36	0.41
1:B:43:LYS:O	1:B:203:ALA:O	2.37	0.41
1:C:183:ASP:OD1	1:C:187:ARG:NH1	2.53	0.41
1:C:23:ARG:HH22	1:C:329:GLU:HA	1.86	0.41
1:B:78:PHE:CD2	1:B:93:VAL:HG13	2.54	0.41
1:B:419:LEU:HD21	1:B:481:THR:O	2.20	0.41
1:C:237:LEU:HD11	1:C:256:ILE:HG22	2.03	0.41
1:A:201:ARG:HG2	1:A:202:PRO:HD2	2.03	0.41
1:B:406:ARG:HH21	1:B:481:THR:CG2	2.21	0.41
1:B:99:GLU:C	1:B:100:VAL:HG23	2.41	0.41
1:D:414:ARG:NH2	1:D:422:SER:HB2	2.35	0.41
1:B:224:GLN:O	1:B:224:GLN:CG	2.68	0.41
1:D:146:ASP:OD1	1:D:146:ASP:O	2.39	0.41
1:D:445:VAL:N	1:D:446:PRO:HD2	2.36	0.41
1:A:504:LYS:O	1:A:507:GLU:CB	2.68	0.41
1:C:495:THR:HB	1:C:496:PRO:HD2	2.01	0.41
1:A:330:ILE:O	1:A:334:LEU:HG	2.20	0.41
1:D:231:ILE:HG22	1:D:233:ASN:H	1.86	0.41
1:B:137:GLY:HA2	1:B:166:LEU:O	2.21	0.41
1:D:438:GLU:HB2	1:D:489:VAL:HB	2.02	0.41
1:B:396:LEU:HD13	1:B:396:LEU:HA	1.78	0.41
1:B:438:GLU:OE2	1:B:494:GLU:HB2	2.21	0.41
1:D:327:ALA:HB3	1:D:362:ARG:HG3	2.02	0.41
1:B:407:CYS:O	1:B:408:SER:CB	2.69	0.40
1:C:203:ALA:N	1:C:204:PRO:CD	2.84	0.40
1:B:393:SER:O	1:B:394:PRO:C	2.60	0.40
1:A:15:ARG:HG2	1:A:29:ILE:HG12	2.03	0.40
1:A:169:ARG:C	1:A:171:ALA:N	2.74	0.40
1:B:337:ARG:HH11	1:B:400:SER:CB	2.34	0.40
1:B:182:TRP:CH2	1:B:223:ARG:HA	2.56	0.40
1:D:393:SER:C	1:D:396:LEU:N	2.74	0.40
1:B:24:LEU:CB	1:B:271:ILE:HG22	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:O	1:A:29:ILE:HA	2.21	0.40
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.64	0.40
1:D:397:GLY:C	1:D:398:GLU:HG3	2.41	0.40
1:A:434:GLU:O	1:A:435:ASN:HB3	2.21	0.40
1:C:401:HIS:ND1	1:D:412:THR:OG1	2.49	0.40
1:D:444:PRO:HG2	1:D:481:THR:HA	2.04	0.40
1:D:19:VAL:HG21	1:D:271:ILE:HD13	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:THR:CG2	1:C:241:ARG:NH1[1_665]	1.81	0.39
1:C:65:HIS:ND1	1:C:351:THR:OG1[1_545]	1.95	0.25
1:C:362:ARG:NH2	1:C:435:ASN:OD1[1_455]	2.18	0.02

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	479/515 (93%)	452 (94%)	24 (5%)	3 (1%)	30	68
1	B	485/515 (94%)	454 (94%)	28 (6%)	3 (1%)	30	68
1	C	460/515 (89%)	428 (93%)	32 (7%)	0	100	100
1	D	452/515 (88%)	431 (95%)	21 (5%)	0	100	100
All	All	1876/2060 (91%)	1765 (94%)	105 (6%)	6 (0%)	46	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	THR
1	B	510	MET
1	A	119	PHE
1	A	78	PHE
1	B	394	PRO

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	333/438 (76%)	311 (93%)	22 (7%)	21	59
1	B	361/438 (82%)	344 (95%)	17 (5%)	32	70
1	C	347/438 (79%)	326 (94%)	21 (6%)	23	62
1	D	346/438 (79%)	324 (94%)	22 (6%)	22	60
All	All	1387/1752 (79%)	1305 (94%)	82 (6%)	24	63

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	76	GLU
1	A	90	ILE
1	A	107	GLU
1	A	117	THR
1	A	140	SER
1	A	175	LYS
1	A	211	SER
1	A	247	LEU
1	A	262	GLU
1	A	295	SER
1	A	332	ARG
1	A	362	ARG
1	A	381	ARG
1	A	403	VAL
1	A	406	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	415	ASP
1	A	416	ASN
1	A	439	VAL
1	A	457	SER
1	A	464	THR
1	A	481	THR
1	B	20	ASP
1	B	38	LYS
1	B	117	THR
1	B	148	ARG
1	B	173	VAL
1	B	212	ASN
1	B	241	ARG
1	B	284	ARG
1	B	304	ILE
1	B	332	ARG
1	B	342	LEU
1	B	368	ARG
1	B	396	LEU
1	B	406	ARG
1	B	425	ARG
1	B	457	SER
1	B	464	THR
1	C	43	LYS
1	C	48	ARG
1	C	117	THR
1	C	150	GLU
1	C	169	ARG
1	C	173	VAL
1	C	176	SER
1	C	211	SER
1	C	213	VAL
1	C	223	ARG
1	C	237	LEU
1	C	241	ARG
1	C	297	GLU
1	C	332	ARG
1	C	349	ASP
1	C	357	ARG
1	C	362	ARG
1	C	378	HIS
1	C	457	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	480	GLU
1	C	481	THR
1	D	23	ARG
1	D	38	LYS
1	D	68	LEU
1	D	78	PHE
1	D	100	VAL
1	D	117	THR
1	D	133	ASN
1	D	169	ARG
1	D	210	GLU
1	D	211	SER
1	D	241	ARG
1	D	253	SER
1	D	332	ARG
1	D	349	ASP
1	D	362	ARG
1	D	367	VAL
1	D	369	GLN
1	D	398	GLU
1	D	407	CYS
1	D	457	SER
1	D	470	ARG
1	D	474	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	208	HIS
1	A	242	GLN
1	A	243	HIS
1	A	280	GLN
1	A	355	HIS
1	A	416	ASN
1	A	483	HIS
1	B	34	HIS
1	B	65	HIS
1	B	132	ASN
1	B	242	GLN
1	B	280	GLN
1	B	355	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	375	GLN
1	B	401	HIS
1	B	416	ASN
1	B	485	HIS
1	C	65	HIS
1	C	132	ASN
1	C	212	ASN
1	C	280	GLN
1	C	355	HIS
1	C	369	GLN
1	C	375	GLN
1	C	416	ASN
1	C	483	HIS
1	D	65	HIS
1	D	280	GLN
1	D	355	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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).

Full wwPDB X-ray Structure Validation Report

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	1509	-	4,4,4	0.79	0	6,6,6	0.11	0
2	SO4	B	1515	-	4,4,4	0.31	0	6,6,6	0.18	0
2	SO4	C	1507	-	4,4,4	0.63	0	6,6,6	0.22	0

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	SO4	A	1509	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1515	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1507	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1509	SO4	4	0
2	B	1515	SO4	1	0
2	C	1507	SO4	3	0

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	489/515 (94%)	0.15	14 (2%)	55	49	44, 99, 133, 176	0
1	B	495/515 (96%)	0.26	18 (3%)	46	39	56, 98, 129, 171	0
1	C	474/515 (92%)	0.31	22 (4%)	36	30	59, 99, 130, 172	0
1	D	472/515 (91%)	0.32	30 (6%)	23	19	54, 101, 130, 172	0
All	All	1930/2060 (93%)	0.26	84 (4%)	38	31	44, 99, 130, 176	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	ILE	5.5
1	C	393	SER	4.3
1	B	269	TYR	4.0
1	D	204	PRO	3.7
1	D	56	ALA	3.7
1	D	168	VAL	3.7
1	D	46	ILE	3.5
1	C	124	GLY	3.5
1	A	225	ASP	3.5
1	C	87	ARG	3.5
1	C	260	THR	3.4
1	C	441	ALA	3.4
1	D	87	ARG	3.4
1	C	493	GLU	3.4
1	C	224	GLN	3.3
1	B	268	HIS	3.3
1	D	203	ALA	3.3
1	D	187	ARG	3.3
1	B	247	LEU	3.1
1	C	313	GLY	3.1
1	D	44	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	125	SER	3.1
1	C	307	ALA	3.0
1	D	176	SER	3.0
1	B	156	ALA	3.0
1	B	257	LYS	3.0
1	D	100	VAL	2.9
1	D	127	LEU	2.9
1	D	202	PRO	2.8
1	B	168	VAL	2.8
1	C	174	GLY	2.8
1	B	232	ASP	2.8
1	B	93	VAL	2.7
1	C	137	GLY	2.7
1	D	55	ALA	2.7
1	B	113	GLY	2.6
1	D	115	ALA	2.6
1	D	4	MET	2.6
1	D	191	TRP	2.6
1	D	207	ILE	2.6
1	A	203	ALA	2.6
1	D	491	LYS	2.6
1	C	127	LEU	2.6
1	D	99	GLU	2.6
1	A	245	ALA	2.6
1	C	203	ALA	2.6
1	C	168	VAL	2.5
1	B	190	HIS	2.5
1	A	227	GLY	2.5
1	C	56	ALA	2.5
1	B	122	LEU	2.5
1	A	228	GLU	2.4
1	C	160	LEU	2.4
1	C	353	VAL	2.4
1	A	151	LEU	2.4
1	A	59	ASP	2.4
1	C	156	ALA	2.4
1	A	168	VAL	2.4
1	C	55	ALA	2.3
1	D	163	GLY	2.2
1	C	436	THR	2.2
1	A	211	SER	2.2
1	B	271	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	242	GLN	2.2
1	D	314	ASP	2.2
1	A	102	VAL	2.2
1	D	132	ASN	2.1
1	D	160	LEU	2.1
1	B	228	GLU	2.1
1	C	166	LEU	2.1
1	B	177	ALA	2.1
1	A	306	SER	2.1
1	A	420	SER	2.1
1	D	198	ALA	2.1
1	D	22	GLN	2.1
1	A	440	HIS	2.0
1	D	58	VAL	2.1
1	D	170	THR	2.0
1	B	270	GLN	2.0
1	B	222	LEU	2.0
1	A	125	SER	2.0
1	D	269	TYR	2.0
1	B	186	PHE	2.0
1	D	119	PHE	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	B	1514	1/1	0.98	0.19	-0.10	58,58,58,58	1

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	ZN	D	1516	1/1	0.97	0.18	-0.39	64,64,64,64	1
2	SO4	B	1515	5/5	0.90	0.15	-0.59	134,136,140,145	0
2	SO4	A	1509	5/5	0.81	0.18	-1.35	148,150,154,159	0
2	SO4	C	1507	5/5	0.91	0.15	-	108,116,118,124	0

6.5 Other polymers (i)

There are no such residues in this entry.