



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:00 PM UTC

PDB ID : 1XP4 / pdb_00001xp4
Title : Crystal structure of a peptidoglycan synthesis regulatory factor (PBP3) from *Streptococcus pneumoniae*
Authors : Morlot, C.; Pernot, L.; Le Gouellec, A.; Di Guilmi, A.M.; Vernet, T.; Dideberg, O.; Dessen, A.
Deposited on : 2004-10-08
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

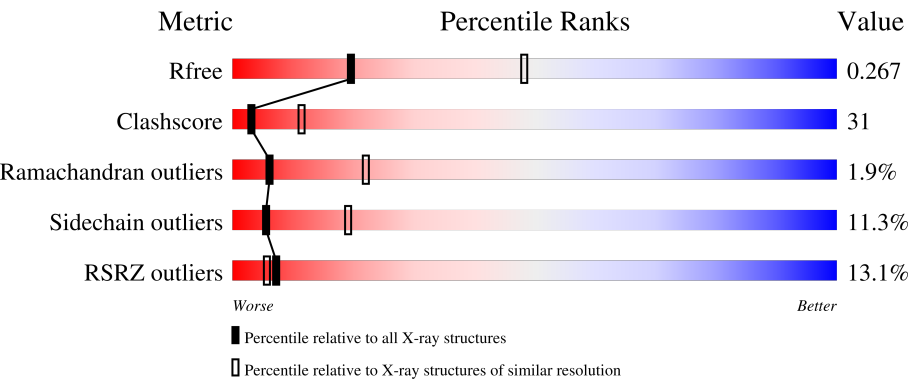
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	379	12% 56% 30% 7% . .
1	B	379	14% 46% 31% 9% . 11%
1	C	379	11% 54% 32% 6% . 5%
1	D	379	10% 44% 32% 6% . 15%

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
3	IOD	A	468	-	-	X	-
3	IOD	B	472	-	-	X	-
3	IOD	C	476	-	-	X	-
3	IOD	D	481	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11150 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 D-alanyl-D-alanine carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	Se	0	0	0
			2821	1775	457	580	9			
1	B	339	Total	C	N	O	Se	49	0	0
			2602	1642	420	531	9			
1	C	359	Total	C	N	O	Se	72	0	0
			2750	1731	445	565	9			
1	D	321	Total	C	N	O	Se	27	0	0
			2480	1571	398	502	9			

There are 36 discrepancies between the modelled and reference sequences:

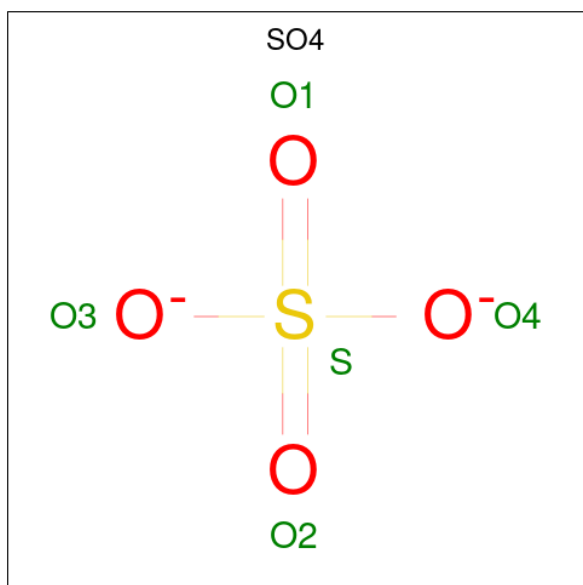
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MSE	MET	modified residue	UNP Q8DQ99
A	141	MSE	MET	modified residue	UNP Q8DQ99
A	142	MSE	MET	modified residue	UNP Q8DQ99
A	216	MSE	MET	modified residue	UNP Q8DQ99
A	224	MSE	MET	modified residue	UNP Q8DQ99
A	228	MSE	MET	modified residue	UNP Q8DQ99
A	259	MSE	MET	modified residue	UNP Q8DQ99
A	286	MSE	MET	modified residue	UNP Q8DQ99
A	386	MSE	MET	modified residue	UNP Q8DQ99
B	101	MSE	MET	modified residue	UNP Q8DQ99
B	141	MSE	MET	modified residue	UNP Q8DQ99
B	142	MSE	MET	modified residue	UNP Q8DQ99
B	216	MSE	MET	modified residue	UNP Q8DQ99
B	224	MSE	MET	modified residue	UNP Q8DQ99
B	228	MSE	MET	modified residue	UNP Q8DQ99
B	259	MSE	MET	modified residue	UNP Q8DQ99
B	286	MSE	MET	modified residue	UNP Q8DQ99
B	386	MSE	MET	modified residue	UNP Q8DQ99
C	101	MSE	MET	modified residue	UNP Q8DQ99
C	141	MSE	MET	modified residue	UNP Q8DQ99
C	142	MSE	MET	modified residue	UNP Q8DQ99

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	216	MSE	MET	modified residue	UNP Q8DQ99
C	224	MSE	MET	modified residue	UNP Q8DQ99
C	228	MSE	MET	modified residue	UNP Q8DQ99
C	259	MSE	MET	modified residue	UNP Q8DQ99
C	286	MSE	MET	modified residue	UNP Q8DQ99
C	386	MSE	MET	modified residue	UNP Q8DQ99
D	101	MSE	MET	modified residue	UNP Q8DQ99
D	141	MSE	MET	modified residue	UNP Q8DQ99
D	142	MSE	MET	modified residue	UNP Q8DQ99
D	216	MSE	MET	modified residue	UNP Q8DQ99
D	224	MSE	MET	modified residue	UNP Q8DQ99
D	228	MSE	MET	modified residue	UNP Q8DQ99
D	259	MSE	MET	modified residue	UNP Q8DQ99
D	286	MSE	MET	modified residue	UNP Q8DQ99
D	386	MSE	MET	modified residue	UNP Q8DQ99

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total I 4 4	0	0
3	B	4	Total I 4 4	0	0
3	C	4	Total I 4 4	0	0
3	D	4	Total I 4 4	0	0

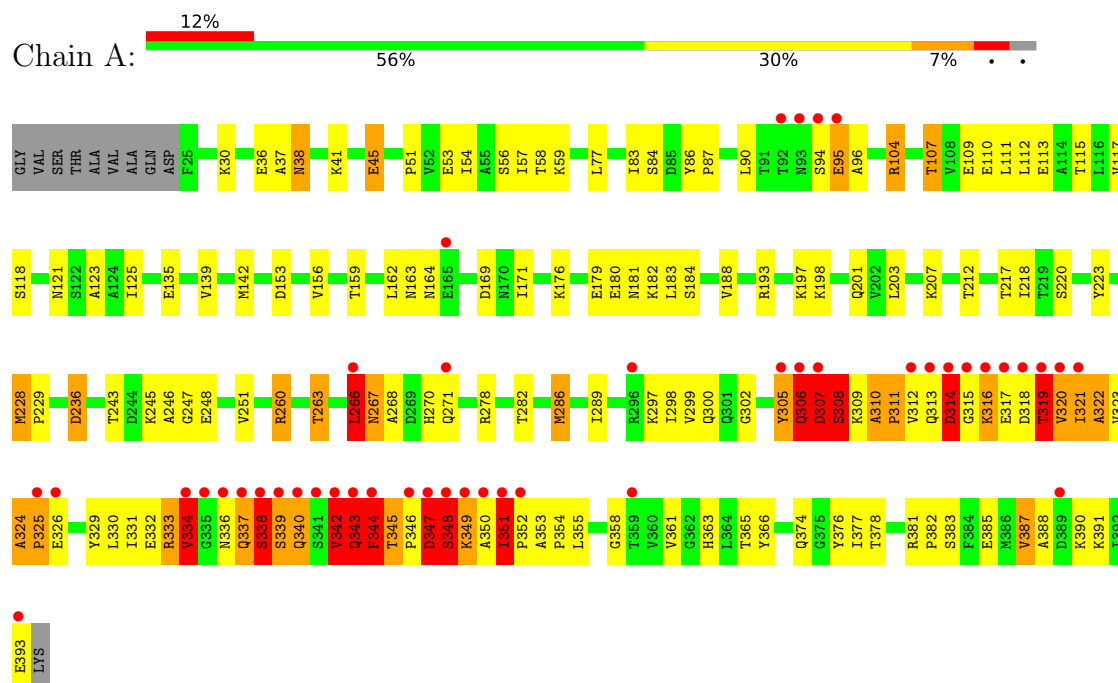
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	139	Total O 139 139	1	0
4	B	98	Total O 98 98	0	0
4	C	121	Total O 121 121	0	0
4	D	103	Total O 103 103	0	0

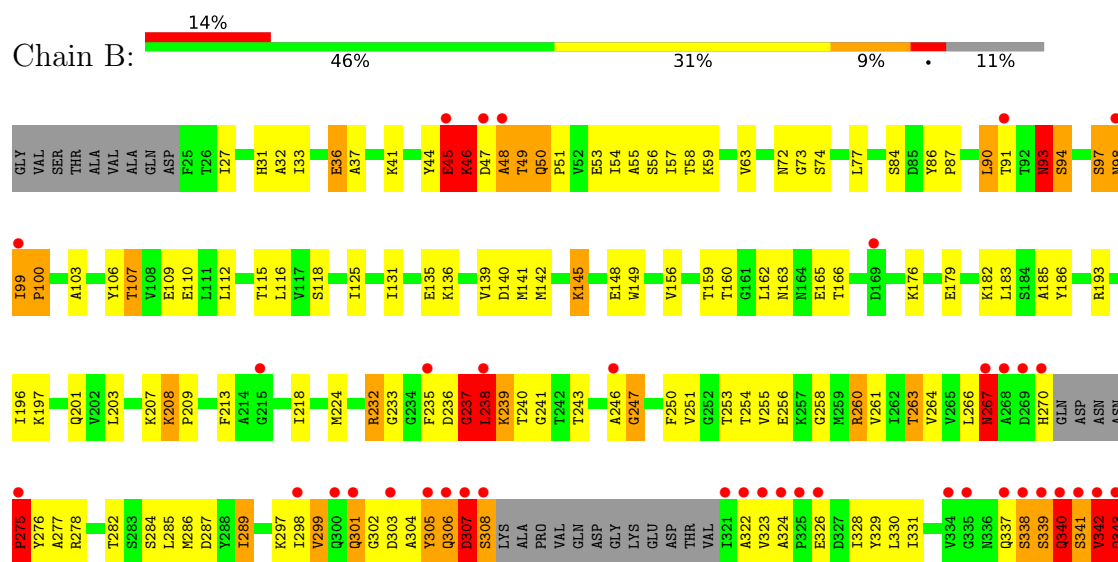
3 Residue-property plots [i](#)

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

• Molecule 1: D-alanyl-D-alanine carboxypeptidase

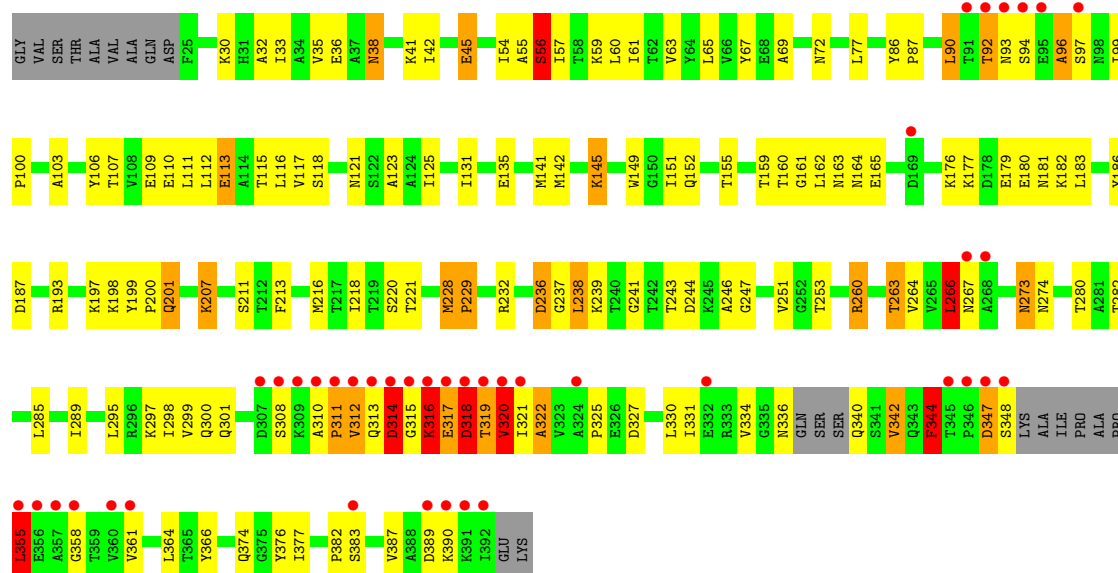


• Molecule 1: D-alanyl-D-alanine carboxypeptidase

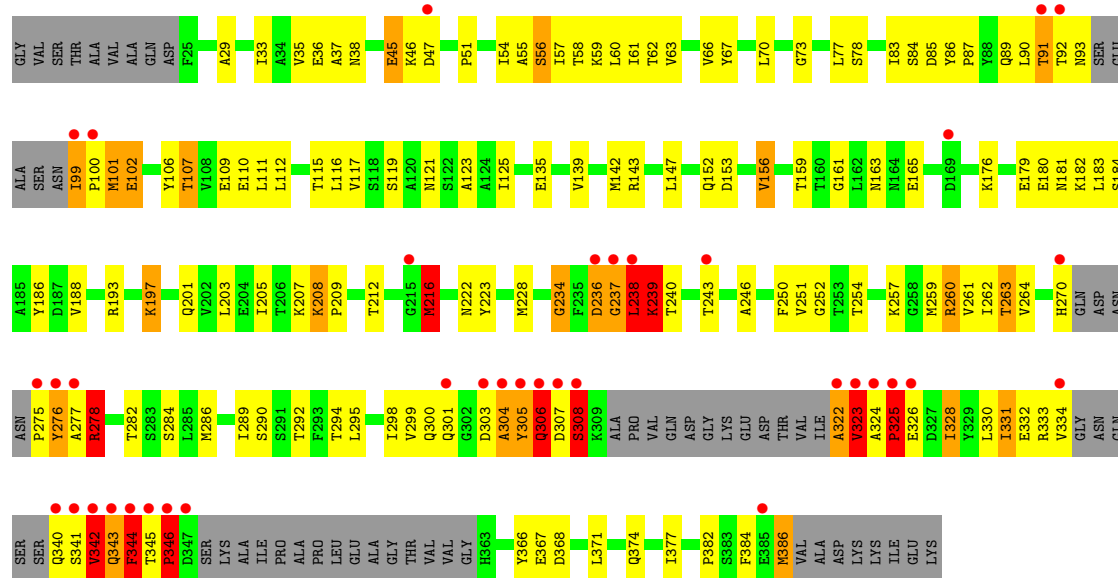
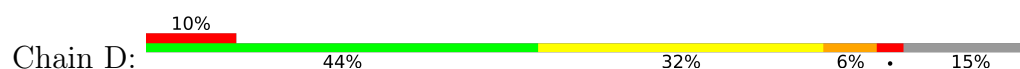




• Molecule 1: D-alanyl-D-alanine carboxypeptidase



• Molecule 1: D-alanyl-D-alanine carboxypeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.61Å 120.84Å 177.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.84 – 2.80 65.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.84-2.80) 99.9 (65.84-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.278 0.228 , 0.267	Depositor DCC
R_{free} test set	3309 reflections (7.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11150	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, 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	0.85	1/2857 (0.0%)	1.46	46/3868 (1.2%)
1	B	0.66	0/2632	1.36	36/3555 (1.0%)
1	C	0.76	3/2782 (0.1%)	1.41	33/3762 (0.9%)
1	D	0.63	5/2508 (0.2%)	1.25	33/3384 (1.0%)
All	All	0.74	9/10779 (0.1%)	1.37	148/14569 (1.0%)

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	14
1	B	0	15
1	C	2	8
1	D	0	6
All	All	2	43

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	PHE	C-N	26.92	1.77	1.33
1	C	266	LEU	C-O	22.82	1.55	1.24
1	D	304	ALA	CA-C	9.56	1.64	1.52
1	C	266	LEU	C-N	-7.97	1.23	1.34
1	C	334	VAL	C-N	6.44	1.40	1.33
1	D	304	ALA	C-N	5.73	1.41	1.33
1	D	306	GLN	N-CA	-5.24	1.39	1.46
1	D	216	MSE	CG-SE	-5.14	1.80	1.95
1	D	216	MSE	SE-CE	-5.08	1.80	1.95

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SER	O-C-N	-24.30	94.19	122.86
1	C	266	LEU	O-C-N	-23.02	94.86	122.25
1	A	351	ILE	O-C-N	-21.29	96.83	121.10
1	C	266	LEU	CA-C-N	-19.09	94.61	121.33
1	C	266	LEU	C-N-CA	-19.09	94.61	121.33
1	C	340	GLN	CA-C-N	-17.52	96.31	121.72
1	C	340	GLN	C-N-CA	-17.52	96.31	121.72
1	B	275	PRO	CA-N-CD	-17.31	87.76	112.00
1	D	275	PRO	CA-N-CD	-17.21	87.91	112.00
1	C	311	PRO	CA-N-CD	-15.13	90.82	112.00
1	C	266	LEU	CA-C-O	-14.56	102.41	119.59
1	A	344	PHE	CA-C-N	-14.18	99.71	121.83
1	A	344	PHE	C-N-CA	-14.18	99.71	121.83
1	C	320	VAL	O-C-N	-14.07	106.64	123.10
1	B	338	SER	N-CA-C	13.46	130.16	108.63
1	A	322	ALA	O-C-N	13.04	138.01	123.27
1	B	361	VAL	CA-C-N	-12.61	108.11	121.48
1	B	361	VAL	C-N-CA	-12.61	108.11	121.48
1	A	308	SER	O-C-N	-11.57	107.84	123.12
1	D	92	THR	N-CA-C	-11.12	91.69	109.59
1	A	318	ASP	CA-C-N	10.88	138.33	122.99
1	A	318	ASP	C-N-CA	10.88	138.33	122.99
1	B	366	TYR	O-C-N	-10.77	110.94	123.22
1	A	324	ALA	CA-C-N	-10.73	106.42	119.84
1	A	324	ALA	C-N-CA	-10.73	106.42	119.84
1	B	337	GLN	OE1-CD-NE2	-10.50	112.10	122.60
1	D	306	GLN	OE1-CD-NE2	-10.36	112.24	122.60
1	C	340	GLN	OE1-CD-NE2	-10.31	112.28	122.60
1	C	314	ASP	CA-CB-CG	10.31	122.91	112.60
1	B	94	SER	O-C-N	-10.21	109.01	122.59
1	C	313	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	A	306	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	B	306	GLN	OE1-CD-NE2	-9.62	112.98	122.60
1	A	342	VAL	N-CA-C	-9.20	103.43	112.17
1	B	237	GLY	CA-C-N	9.03	138.78	121.54
1	B	237	GLY	C-N-CA	9.03	138.78	121.54
1	C	318	ASP	N-CA-C	8.94	125.88	107.37
1	D	278	ARG	O-C-N	8.93	131.57	122.10
1	D	278	ARG	N-CA-C	-8.81	103.37	114.56
1	A	306	GLN	CA-CB-CG	-8.63	96.84	114.10
1	A	343	GLN	CA-C-N	-8.38	105.53	121.54
1	A	343	GLN	C-N-CA	-8.38	105.53	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	PHE	CA-CB-CG	-8.12	105.68	113.80
1	D	216	MSE	O-C-N	-7.77	113.79	123.27
1	B	45	GLU	N-CA-C	7.62	121.64	108.76
1	D	346	PRO	O-C-N	-7.44	112.60	122.64
1	C	96	ALA	N-CA-C	-7.32	97.50	108.99
1	A	344	PHE	O-C-N	7.28	132.27	122.59
1	D	343	GLN	CA-C-N	-7.26	111.91	122.44
1	D	343	GLN	C-N-CA	-7.26	111.91	122.44
1	B	337	GLN	CG-CD-NE2	7.23	127.24	116.40
1	A	306	GLN	CG-CD-NE2	7.15	127.12	116.40
1	A	334	VAL	CA-C-N	-7.06	112.68	122.63
1	A	334	VAL	C-N-CA	-7.06	112.68	122.63
1	D	239	LYS	O-C-N	-7.04	115.39	123.42
1	A	320	VAL	CA-C-N	-7.02	110.64	121.18
1	A	320	VAL	C-N-CA	-7.02	110.64	121.18
1	B	36	GLU	N-CA-C	-6.99	98.56	109.25
1	C	317	GLU	CA-C-N	-6.96	111.41	122.76
1	C	317	GLU	C-N-CA	-6.96	111.41	122.76
1	C	322	ALA	O-C-N	6.93	131.13	123.22
1	B	308	SER	CB-CA-C	6.92	123.26	110.10
1	D	278	ARG	CD-NE-CZ	-6.83	114.84	124.40
1	D	306	GLN	CG-CD-NE2	6.76	126.53	116.40
1	B	306	GLN	CG-CD-NE2	6.75	126.52	116.40
1	D	277	ALA	N-CA-C	6.75	120.79	111.55
1	D	342	VAL	CA-C-N	-6.73	112.70	122.06
1	D	342	VAL	C-N-CA	-6.73	112.70	122.06
1	A	268	ALA	CA-C-N	-6.65	111.42	120.87
1	A	268	ALA	C-N-CA	-6.65	111.42	120.87
1	C	313	GLN	CG-CD-NE2	6.65	126.37	116.40
1	C	313	GLN	CA-C-N	6.63	134.21	121.54
1	C	313	GLN	C-N-CA	6.63	134.21	121.54
1	B	342	VAL	CA-C-N	-6.42	112.80	123.33
1	B	342	VAL	C-N-CA	-6.42	112.80	123.33
1	D	161	GLY	N-CA-C	-6.42	106.07	115.63
1	D	305	TYR	O-C-N	6.38	131.15	122.48
1	D	325	PRO	N-CA-C	-6.31	105.30	113.57
1	C	340	GLN	CG-CD-NE2	6.25	125.78	116.40
1	C	355	LEU	O-C-N	-6.18	113.11	123.00
1	B	208	LYS	N-CA-C	6.13	117.37	109.65
1	C	316	LYS	CA-C-N	6.05	132.21	121.75
1	C	316	LYS	C-N-CA	6.05	132.21	121.75
1	C	318	ASP	CA-C-N	6.02	133.03	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ASP	C-N-CA	6.02	133.03	121.54
1	D	304	ALA	N-CA-C	5.99	118.69	108.02
1	D	308	SER	CA-C-O	5.98	126.89	120.32
1	B	131	ILE	N-CA-C	5.97	117.00	111.45
1	A	333	ARG	CD-NE-CZ	-5.95	116.06	124.40
1	A	305	TYR	CA-C-N	5.94	132.88	121.54
1	A	305	TYR	C-N-CA	5.94	132.88	121.54
1	D	344	PHE	CA-CB-CG	-5.92	107.88	113.80
1	C	38	ASN	N-CA-C	5.91	118.20	111.11
1	D	73	GLY	N-CA-C	-5.89	107.26	114.92
1	A	267	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	310	ALA	CA-C-N	5.83	127.13	119.84
1	A	310	ALA	C-N-CA	5.83	127.13	119.84
1	A	342	VAL	CA-C-O	5.83	125.68	119.91
1	A	347	ASP	CA-C-N	-5.76	114.78	122.72
1	A	347	ASP	C-N-CA	-5.76	114.78	122.72
1	B	305	TYR	N-CA-C	-5.75	102.95	110.53
1	A	319	THR	CA-C-N	-5.72	116.10	123.19
1	A	319	THR	C-N-CA	-5.72	116.10	123.19
1	A	306	GLN	CB-CA-C	5.71	121.78	110.42
1	B	55	ALA	CB-CA-C	-5.70	110.01	116.63
1	C	55	ALA	CB-CA-C	-5.70	109.99	116.54
1	C	161	GLY	N-CA-C	-5.68	107.14	115.72
1	D	208	LYS	N-CA-C	5.67	119.71	109.44
1	B	347	ASP	CA-CB-CG	-5.67	106.93	112.60
1	A	311	PRO	CA-C-N	5.67	130.87	122.71
1	A	311	PRO	C-N-CA	5.67	130.87	122.71
1	A	38	ASN	N-CA-C	5.66	117.90	111.11
1	B	98	ASN	N-CA-C	5.65	119.68	112.34
1	D	55	ALA	CB-CA-C	-5.63	110.06	116.54
1	D	305	TYR	CA-C-O	5.63	127.50	121.02
1	A	347	ASP	CA-CB-CG	-5.50	107.10	112.60
1	A	344	PHE	CA-CB-CG	-5.50	108.30	113.80
1	D	323	VAL	CA-C-N	-5.50	113.30	120.67
1	D	323	VAL	C-N-CA	-5.50	113.30	120.67
1	A	314	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	37	ALA	N-CA-C	5.49	117.69	111.11
1	B	337	GLN	CA-C-N	5.44	131.32	122.07
1	B	337	GLN	C-N-CA	5.44	131.32	122.07
1	C	221	THR	N-CA-C	-5.44	106.49	113.23
1	C	336	ASN	CA-CB-CG	-5.36	107.24	112.60
1	D	234	GLY	CA-C-N	-5.33	113.57	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	GLY	C-N-CA	-5.33	113.57	122.64
1	D	117	VAL	N-CA-C	5.27	115.49	110.53
1	D	342	VAL	N-CA-C	-5.25	98.43	109.34
1	A	309	LYS	O-C-N	-5.24	116.09	123.11
1	B	346	PRO	N-CA-CB	5.24	108.38	102.67
1	B	306	GLN	CA-C-N	5.22	131.52	121.54
1	B	306	GLN	C-N-CA	5.22	131.52	121.54
1	C	228	MSE	CA-C-N	5.22	126.37	119.84
1	C	228	MSE	C-N-CA	5.22	126.37	119.84
1	B	289	ILE	N-CA-C	5.21	115.42	110.42
1	A	339	SER	O-C-N	5.21	128.99	122.43
1	D	308	SER	O-C-N	5.19	129.40	123.27
1	B	324	ALA	N-CA-C	5.17	115.94	109.57
1	A	316	LYS	O-C-N	-5.17	116.96	122.85
1	A	387	VAL	N-CA-C	5.15	116.61	109.45
1	B	345	THR	CA-C-O	5.14	123.67	119.36
1	D	331	ILE	N-CA-C	-5.10	102.27	109.21
1	C	131	ILE	N-CA-C	5.10	116.56	111.00
1	B	302	GLY	N-CA-C	-5.09	109.02	115.08
1	B	340	GLN	CA-C-N	-5.09	115.24	122.41
1	B	340	GLN	C-N-CA	-5.09	115.24	122.41
1	A	266	LEU	N-CA-C	5.08	116.53	110.44

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	318	ASP	CA
1	C	343	GLN	CA

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LEU	Peptide
1	A	308	SER	Mainchain
1	A	314	ASP	Sidechain
1	A	315	GLY	Peptide
1	A	317	GLU	Mainchain
1	A	319	THR	Peptide
1	A	338	SER	Mainchain,Peptide
1	A	339	SER	Peptide
1	A	343	GLN	Peptide
1	A	344	PHE	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	348	SER	Peptide
1	A	350	ALA	Peptide
1	A	351	ILE	Mainchain
1	B	100	PRO	Mainchain
1	B	213	PHE	Sidechain
1	B	237	GLY	Peptide
1	B	258	GLY	Mainchain
1	B	342	VAL	Mainchain
1	B	343	GLN	Peptide
1	B	344	PHE	Sidechain
1	B	366	TYR	Mainchain,Sidechain
1	B	46	LYS	Peptide
1	B	48	ALA	Mainchain
1	B	49	THR	Mainchain
1	B	93	ASN	Peptide
1	B	94	SER	Peptide
1	B	97	SER	Peptide
1	C	266	LEU	Mainchain,Peptide
1	C	316	LYS	Peptide
1	C	318	ASP	Peptide
1	C	320	VAL	Mainchain
1	C	342	VAL	Peptide
1	C	344	PHE	Sidechain
1	C	355	LEU	Mainchain
1	D	216	MSE	Mainchain
1	D	239	LYS	Mainchain
1	D	322	ALA	Peptide
1	D	325	PRO	Mainchain
1	D	344	PHE	Sidechain
1	D	346	PRO	Mainchain

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	2821	0	2801	178	0
1	B	2602	0	2586	173	1
1	C	2750	0	2728	145	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2480	0	2467	173	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	4	0	0	2	0
3	B	4	0	0	2	0
3	C	4	0	0	2	0
3	D	4	0	0	3	0
4	A	139	0	0	6	0
4	B	98	0	0	2	0
4	C	121	0	0	8	0
4	D	103	0	0	5	0
All	All	11150	0	10582	657	1

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 31.

All (657) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PHE:C	1:A:345:THR:N	1.77	1.43
1:C:243:THR:HG22	1:C:246:ALA:CB	1.63	1.27
1:B:305:TYR:OH	1:B:343:GLN:HB3	1.28	1.25
1:B:237:GLY:HA3	1:B:253:THR:CG2	1.67	1.24
1:B:342:VAL:CG2	1:B:342:VAL:O	1.81	1.24
1:A:305:TYR:OH	1:A:343:GLN:HG3	1.39	1.23
1:B:307:ASP:O	1:B:307:ASP:OD1	1.57	1.23
1:B:237:GLY:CA	1:B:253:THR:HG22	1.71	1.20
1:A:333:ARG:CB	1:A:336:ASN:HD21	1.54	1.20
1:D:243:THR:HG22	1:D:246:ALA:CB	1.73	1.17
1:D:222:ASN:ND2	1:D:237:GLY:HA3	1.58	1.15
1:A:243:THR:HG22	1:A:246:ALA:CB	1.74	1.15
1:A:333:ARG:HB3	1:A:336:ASN:HD21	1.12	1.13
1:D:243:THR:CG2	1:D:246:ALA:H	1.61	1.13
1:B:342:VAL:O	1:B:342:VAL:HG23	1.37	1.12
1:B:304:ALA:HB2	1:B:323:VAL:HG12	1.12	1.11
1:C:243:THR:CG2	1:C:246:ALA:HB3	1.80	1.09
1:D:243:THR:HG23	1:D:246:ALA:H	0.96	1.08
1:C:243:THR:CG2	1:C:246:ALA:CB	2.32	1.08
1:A:243:THR:CG2	1:A:246:ALA:HB3	1.85	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:HG23	1:B:246:ALA:H	1.08	1.07
1:A:347:ASP:N	1:A:347:ASP:OD1	1.86	1.06
1:D:139:VAL:HA	1:D:142:MSE:HE3	1.38	1.04
1:C:243:THR:HG23	1:C:246:ALA:H	0.94	1.04
1:D:304:ALA:CB	1:D:322:ALA:HB1	1.88	1.04
1:A:336:ASN:O	1:A:337:GLN:O	1.77	1.03
1:B:330:LEU:HD13	1:B:342:VAL:HG11	1.43	1.01
1:D:243:THR:HG22	1:D:246:ALA:HB3	1.03	1.01
1:A:243:THR:HG23	1:A:246:ALA:H	1.19	1.01
1:A:243:THR:CG2	1:A:246:ALA:CB	2.38	1.00
1:D:341:SER:C	1:D:343:GLN:H	1.69	1.00
1:B:243:THR:HG22	1:B:246:ALA:HB3	1.43	1.00
1:D:222:ASN:HD21	1:D:237:GLY:HA3	1.26	0.99
1:C:243:THR:CG2	1:C:246:ALA:H	1.74	0.99
1:B:330:LEU:CD1	1:B:342:VAL:HG11	1.94	0.98
1:A:333:ARG:HB3	1:A:336:ASN:ND2	1.79	0.98
1:B:305:TYR:CZ	1:B:343:GLN:HB3	1.98	0.98
1:D:243:THR:CG2	1:D:246:ALA:CB	2.42	0.97
1:B:63:VAL:HG21	1:B:116:LEU:HD21	1.42	0.97
1:C:243:THR:HG23	1:C:246:ALA:N	1.78	0.97
1:A:243:THR:HG22	1:A:246:ALA:HB3	0.98	0.97
1:D:304:ALA:HB1	1:D:322:ALA:CB	1.93	0.97
1:C:63:VAL:HG21	1:C:116:LEU:HD21	1.48	0.95
1:D:243:THR:CG2	1:D:246:ALA:HB3	1.95	0.95
1:C:317:GLU:O	1:C:318:ASP:CB	2.15	0.95
1:D:243:THR:HG23	1:D:246:ALA:N	1.81	0.94
1:B:48:ALA:HB1	1:B:185:ALA:HB3	1.50	0.92
1:D:237:GLY:O	1:D:238:LEU:HB2	1.66	0.92
1:B:298:ILE:HD12	1:B:299:VAL:HG22	1.52	0.91
1:B:243:THR:CG2	1:B:246:ALA:H	1.82	0.91
1:B:107:THR:HG22	1:B:110:GLU:HG3	1.50	0.90
1:D:304:ALA:CB	1:D:322:ALA:CB	2.48	0.90
1:D:222:ASN:HD21	1:D:237:GLY:CA	1.82	0.90
1:A:330:LEU:CD1	1:A:342:VAL:HG11	2.01	0.90
1:C:317:GLU:O	1:C:318:ASP:CG	2.15	0.89
1:A:344:PHE:C	1:A:345:THR:CA	2.44	0.89
1:C:60:LEU:HD21	1:C:238:LEU:CD1	2.02	0.89
1:D:330:LEU:HD11	1:D:342:VAL:HB	1.55	0.89
1:B:342:VAL:O	1:B:342:VAL:HG22	1.70	0.88
1:B:345:THR:HA	1:B:363:HIS:O	1.75	0.87
1:B:247:GLY:HA3	1:B:267:ASN:HB2	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PRO:HD2	1:A:363:HIS:O	1.75	0.87
1:B:176:LYS:HB2	1:B:179:GLU:HG3	1.55	0.86
1:B:304:ALA:CB	1:B:323:VAL:HG12	2.01	0.86
1:A:305:TYR:OH	1:A:343:GLN:CG	2.23	0.86
1:B:196:ILE:HD11	1:B:238:LEU:HD21	1.55	0.86
1:C:60:LEU:CD2	1:C:238:LEU:CD1	2.53	0.86
1:C:243:THR:HG22	1:C:246:ALA:HB3	0.88	0.86
1:D:107:THR:HG22	1:D:110:GLU:H	1.41	0.86
1:A:333:ARG:CB	1:A:336:ASN:ND2	2.38	0.86
1:D:107:THR:HG22	1:D:110:GLU:HG3	1.58	0.85
1:A:306:GLN:O	1:A:308:SER:HB3	1.75	0.85
1:B:346:PRO:HD2	1:B:363:HIS:O	1.77	0.85
1:D:239:LYS:NZ	1:D:240:THR:O	2.10	0.85
1:B:304:ALA:HB2	1:B:323:VAL:CG1	2.03	0.84
1:A:349:LYS:O	1:A:351:ILE:HG22	1.78	0.84
1:B:305:TYR:OH	1:B:343:GLN:CB	2.21	0.84
1:A:330:LEU:HD11	1:A:342:VAL:HG11	1.59	0.84
1:A:107:THR:HG22	1:A:110:GLU:H	1.43	0.83
1:C:263:THR:HG21	1:C:282:THR:HG23	1.60	0.83
1:D:243:THR:CG2	1:D:246:ALA:N	2.40	0.83
1:D:298:ILE:CD1	1:D:342:VAL:HG21	2.08	0.83
1:A:343:GLN:O	1:A:344:PHE:HB2	1.78	0.82
1:D:176:LYS:HB2	1:D:179:GLU:HG3	1.61	0.82
1:A:305:TYR:HD1	1:A:305:TYR:O	1.61	0.82
1:D:99:ILE:HG12	1:D:99:ILE:O	1.78	0.82
1:D:142:MSE:CE	1:D:159:THR:HG22	2.10	0.82
1:D:263:THR:HG21	1:D:282:THR:HG23	1.62	0.82
1:A:271:GLN:OE1	1:B:73:GLY:HA3	1.80	0.81
1:D:90:LEU:O	1:D:90:LEU:HG	1.80	0.81
1:B:261:VAL:HG11	1:B:286:MSE:HE1	1.63	0.81
1:C:176:LYS:HB2	1:C:179:GLU:HG3	1.62	0.81
1:D:341:SER:C	1:D:343:GLN:N	2.37	0.81
1:B:107:THR:HG22	1:B:110:GLU:H	1.45	0.81
1:A:243:THR:HG23	1:A:246:ALA:N	1.97	0.80
1:A:313:GLN:HG3	1:A:313:GLN:O	1.80	0.80
1:B:243:THR:CG2	1:B:246:ALA:HB3	2.10	0.80
1:B:53:GLU:HB2	1:B:246:ALA:HB2	1.63	0.80
1:D:63:VAL:HG21	1:D:116:LEU:HD21	1.63	0.80
1:A:107:THR:HB	1:A:110:GLU:HG3	1.62	0.80
1:D:182:LYS:O	1:D:183:LEU:HD12	1.80	0.80
1:D:298:ILE:HD12	1:D:342:VAL:HG21	1.62	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:HG21	1:A:388:ALA:HB2	1.64	0.79
1:B:48:ALA:CB	1:B:185:ALA:HB3	2.11	0.79
1:C:317:GLU:O	1:C:318:ASP:HB3	1.82	0.79
1:B:298:ILE:HG12	1:B:330:LEU:CD1	2.12	0.79
1:B:263:THR:HG21	1:B:282:THR:HG23	1.63	0.78
1:A:286:MSE:HE3	1:A:286:MSE:HA	1.65	0.78
1:B:247:GLY:CA	1:B:267:ASN:HB2	2.14	0.78
1:B:243:THR:HG23	1:B:246:ALA:N	1.94	0.78
1:A:374:GLN:HG3	3:A:468:IOD:I	2.55	0.77
1:C:145:LYS:HE3	4:C:569:HOH:O	1.83	0.77
1:D:301:GLN:HG3	1:D:325:PRO:O	1.83	0.77
1:D:305:TYR:OH	1:D:343:GLN:HG2	1.84	0.77
1:A:390:LYS:HE3	1:C:325:PRO:O	1.83	0.77
1:A:336:ASN:C	1:A:337:GLN:O	2.27	0.77
1:D:305:TYR:CE2	1:D:343:GLN:HA	2.20	0.76
1:D:323:VAL:C	1:D:386:MSE:CE	2.59	0.75
1:A:349:LYS:HG2	1:D:147:LEU:HD11	1.68	0.75
1:B:53:GLU:CB	1:B:246:ALA:HB2	2.16	0.75
1:C:374:GLN:HG3	3:C:476:IOD:I	2.57	0.74
1:B:286:MSE:HE2	1:B:289:ILE:HD12	1.69	0.74
1:A:305:TYR:O	1:A:305:TYR:CD1	2.40	0.74
1:B:308:SER:CB	1:B:322:ALA:O	2.35	0.74
1:D:139:VAL:HA	1:D:142:MSE:CE	2.16	0.74
1:A:333:ARG:HB2	1:A:336:ASN:HD21	1.51	0.73
1:D:222:ASN:HD22	1:D:237:GLY:HA3	1.51	0.73
1:C:297:LYS:HE3	1:C:300:GLN:HB3	1.69	0.73
1:B:86:TYR:HB3	1:B:87:PRO:HD3	1.70	0.72
1:B:307:ASP:O	1:B:307:ASP:CG	2.32	0.72
1:D:38:ASN:HA	1:D:197:LYS:HE3	1.71	0.72
1:C:243:THR:CG2	1:C:246:ALA:N	2.45	0.72
1:C:312:VAL:HG21	1:C:320:VAL:HG22	1.70	0.72
1:D:142:MSE:HE2	1:D:159:THR:HG22	1.72	0.72
1:A:263:THR:HG21	1:A:282:THR:HG23	1.72	0.71
1:B:107:THR:CG2	1:B:110:GLU:HG3	2.20	0.71
1:B:342:VAL:HA	1:B:366:TYR:HA	1.72	0.71
1:C:59:LYS:O	1:C:63:VAL:HG23	1.89	0.71
1:C:107:THR:HB	1:C:110:GLU:HG3	1.71	0.71
1:D:342:VAL:O	1:D:342:VAL:HG22	1.89	0.71
1:A:77:LEU:O	1:A:107:THR:HG23	1.91	0.71
1:C:60:LEU:HD21	1:C:238:LEU:HD13	1.74	0.70
1:C:107:THR:HG21	4:C:599:HOH:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:VAL:CG2	1:C:320:VAL:HG22	2.21	0.70
1:D:86:TYR:HB3	1:D:87:PRO:HD3	1.72	0.70
1:C:298:ILE:HD13	1:C:330:LEU:HD11	1.73	0.70
1:D:304:ALA:HB1	1:D:322:ALA:HB1	1.55	0.70
1:A:316:LYS:HE3	1:C:301:GLN:CG	2.21	0.70
1:A:90:LEU:O	1:A:94:SER:HB2	1.91	0.70
1:A:243:THR:CG2	1:A:246:ALA:HB2	2.22	0.70
1:B:298:ILE:HD12	1:B:299:VAL:CG2	2.21	0.70
1:D:286:MSE:HE2	1:D:289:ILE:HD12	1.74	0.69
1:A:343:GLN:O	1:A:344:PHE:CB	2.40	0.69
1:A:358:GLY:HA2	1:A:387:VAL:CG1	2.23	0.69
1:D:323:VAL:C	1:D:386:MSE:HE3	2.17	0.69
1:A:325:PRO:O	1:A:326:GLU:HG3	1.93	0.68
1:D:374:GLN:HG3	3:D:481:IOD:I	2.64	0.68
1:C:273:ASN:HB2	4:C:488:HOH:O	1.94	0.67
1:A:41:LYS:HD3	1:A:331:ILE:HD12	1.76	0.67
1:C:243:THR:CG2	1:C:246:ALA:HB2	2.24	0.67
1:A:363:HIS:NE2	1:A:385:GLU:HG2	2.09	0.67
1:B:36:GLU:HG3	1:B:331:ILE:HD11	1.77	0.67
1:D:107:THR:CG2	1:D:110:GLU:HG3	2.25	0.67
1:C:312:VAL:CG2	1:C:320:VAL:CG2	2.72	0.67
1:D:222:ASN:ND2	1:D:237:GLY:CA	2.42	0.67
1:C:347:ASP:OD1	1:C:347:ASP:N	2.26	0.67
1:B:246:ALA:O	1:B:247:GLY:O	2.12	0.67
1:A:358:GLY:HA2	1:A:387:VAL:HG11	1.76	0.66
1:B:344:PHE:O	1:B:346:PRO:HD3	1.94	0.66
1:B:303:ASP:O	1:B:323:VAL:HB	1.96	0.66
1:C:60:LEU:HD22	1:C:238:LEU:CD1	2.25	0.66
1:A:349:LYS:HG2	1:D:147:LEU:CD1	2.26	0.66
1:B:297:LYS:HA	1:B:329:TYR:HA	1.78	0.66
1:D:305:TYR:HE2	1:D:343:GLN:HA	1.58	0.66
1:C:298:ILE:HG21	1:C:330:LEU:CD1	2.26	0.65
1:A:314:ASP:HB2	1:A:353:ALA:HB3	1.78	0.65
1:B:308:SER:HB3	1:B:322:ALA:O	1.96	0.65
1:D:298:ILE:HD13	1:D:330:LEU:HG	1.78	0.65
1:A:333:ARG:NH2	4:A:600:HOH:O	2.29	0.65
1:D:83:ILE:HD11	1:D:106:TYR:HD1	1.59	0.65
1:A:306:GLN:O	1:A:308:SER:CB	2.44	0.65
1:C:247:GLY:HA3	1:C:267:ASN:ND2	2.12	0.65
1:B:238:LEU:HD12	1:B:251:VAL:HG11	1.79	0.65
1:A:344:PHE:CA	1:A:345:THR:N	2.57	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TYR:HB3	1:C:87:PRO:HD3	1.79	0.64
1:A:314:ASP:O	1:A:393:GLU:HB2	1.98	0.64
1:A:336:ASN:O	1:A:337:GLN:C	2.38	0.64
1:D:304:ALA:CA	1:D:322:ALA:HB1	2.28	0.64
1:B:330:LEU:HD11	1:B:342:VAL:HG11	1.76	0.64
1:A:316:LYS:HE3	1:C:301:GLN:HG2	1.79	0.64
1:A:353:ALA:HB1	1:A:354:PRO:HA	1.80	0.63
1:B:237:GLY:HA3	1:B:253:THR:HG22	0.79	0.63
1:B:341:SER:HA	1:B:343:GLN:NE2	2.14	0.63
1:C:60:LEU:HD22	1:C:238:LEU:HD11	1.80	0.63
1:D:99:ILE:O	1:D:99:ILE:CG1	2.47	0.62
1:A:286:MSE:HA	1:A:286:MSE:CE	2.28	0.62
1:B:308:SER:HB2	1:B:322:ALA:O	1.98	0.62
1:B:341:SER:C	1:B:343:GLN:H	2.06	0.62
1:B:224:MSE:HE2	1:B:232:ARG:HB2	1.80	0.62
1:D:257:LYS:HE2	1:D:290:SER:O	2.00	0.62
1:B:298:ILE:HG12	1:B:330:LEU:HD11	1.81	0.62
1:C:60:LEU:CD2	1:C:238:LEU:HD12	2.28	0.62
1:C:77:LEU:O	1:C:107:THR:HG23	1.99	0.61
1:A:267:ASN:C	1:A:267:ASN:HD22	2.06	0.61
1:D:111:LEU:HD22	1:D:123:ALA:HA	1.83	0.61
1:D:263:THR:HG21	1:D:282:THR:CG2	2.30	0.61
1:A:286:MSE:HE3	1:A:289:ILE:HB	1.82	0.61
1:A:342:VAL:HG22	1:A:342:VAL:O	2.00	0.60
1:C:160:THR:CG2	1:C:162:LEU:HG	2.31	0.60
1:C:60:LEU:HD21	1:C:238:LEU:HD12	1.80	0.60
1:A:203:LEU:O	1:A:207:LYS:HB2	2.01	0.60
1:C:298:ILE:HG21	1:C:330:LEU:HD11	1.83	0.60
1:A:83:ILE:O	1:A:104:ARG:NH1	2.34	0.60
1:B:203:LEU:O	1:B:207:LYS:HB2	2.01	0.60
1:C:63:VAL:HG13	1:C:112:LEU:HD11	1.83	0.60
1:D:261:VAL:HG11	1:D:286:MSE:HE1	1.82	0.60
1:B:31:HIS:HB2	1:B:266:LEU:HB2	1.82	0.60
1:C:107:THR:HG22	1:C:109:GLU:N	2.15	0.60
1:D:323:VAL:H	1:D:386:MSE:HE2	1.67	0.60
1:B:139:VAL:HA	1:B:142:MSE:HG2	1.83	0.60
1:C:237:GLY:HA3	1:C:253:THR:HG22	1.84	0.60
1:A:142:MSE:HE2	1:A:156:VAL:HG11	1.83	0.60
1:A:176:LYS:HB2	1:A:179:GLU:HG3	1.84	0.60
1:B:346:PRO:CD	1:B:363:HIS:O	2.48	0.60
1:D:135:GLU:HG3	1:D:159:THR:HG23	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:MSE:HE1	1:D:159:THR:HG22	1.83	0.60
1:D:243:THR:CG2	1:D:246:ALA:HB2	2.31	0.59
1:B:275:PRO:HB2	1:B:276:TYR:CD2	2.36	0.59
1:D:163:ASN:OD1	1:D:165:GLU:HG3	2.02	0.59
1:C:160:THR:HG21	1:C:162:LEU:HG	1.83	0.59
1:B:196:ILE:HD11	1:B:238:LEU:CD2	2.31	0.59
1:B:243:THR:CG2	1:B:246:ALA:N	2.59	0.59
1:B:330:LEU:HD11	1:B:342:VAL:HG21	1.85	0.59
1:C:65:LEU:HD13	1:C:141:MSE:HE2	1.84	0.59
1:A:358:GLY:C	1:A:387:VAL:HG13	2.28	0.59
1:D:135:GLU:O	1:D:139:VAL:HG23	2.02	0.59
1:B:298:ILE:HG12	1:B:330:LEU:HD12	1.85	0.58
1:D:36:GLU:HG3	1:D:331:ILE:HD11	1.85	0.58
1:D:57:ILE:HD13	1:D:251:VAL:HG23	1.84	0.58
1:A:90:LEU:HD12	1:A:94:SER:OG	2.03	0.58
1:A:305:TYR:CD1	1:A:305:TYR:C	2.82	0.58
1:A:38:ASN:HA	1:A:197:LYS:HE2	1.85	0.58
1:A:342:VAL:O	1:A:342:VAL:CG2	2.51	0.58
1:D:163:ASN:HD22	1:D:180:GLU:HG3	1.67	0.58
1:D:308:SER:HB2	1:D:322:ALA:HB2	1.85	0.58
1:A:316:LYS:HE3	1:C:301:GLN:HG3	1.86	0.58
1:B:305:TYR:CZ	1:B:343:GLN:CB	2.83	0.58
1:C:60:LEU:CD1	1:C:238:LEU:HD12	2.34	0.58
1:A:87:PRO:HG3	1:A:125:ILE:HG21	1.86	0.57
1:A:266:LEU:O	1:A:267:ASN:HB2	2.02	0.57
1:B:86:TYR:O	1:B:90:LEU:HB2	2.03	0.57
1:C:60:LEU:HD11	1:C:238:LEU:HD12	1.86	0.57
1:C:198:LYS:HB2	4:C:590:HOH:O	2.03	0.57
1:D:163:ASN:ND2	1:D:180:GLU:HG3	2.20	0.57
1:C:56:SER:HB2	1:C:241:GLY:HA2	1.87	0.57
1:D:276:TYR:CD1	1:D:276:TYR:N	2.72	0.57
1:A:86:TYR:HB3	1:A:87:PRO:HD3	1.87	0.57
1:D:91:THR:O	1:D:91:THR:OG1	2.16	0.57
1:A:310:ALA:HB3	1:A:361:VAL:CG1	2.35	0.57
1:B:341:SER:C	1:B:343:GLN:HG2	2.30	0.57
1:C:152:GLN:HA	4:C:546:HOH:O	2.05	0.57
1:A:153:ASP:HB3	1:D:344:PHE:CE1	2.40	0.56
1:D:33:ILE:HG22	1:D:264:VAL:HB	1.87	0.56
1:A:310:ALA:HB3	1:A:361:VAL:HG12	1.87	0.56
1:B:263:THR:HG21	1:B:282:THR:CG2	2.35	0.56
1:A:322:ALA:HA	1:A:387:VAL:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLN:HG3	3:B:472:IOD:I	2.75	0.56
1:D:193:ARG:O	1:D:197:LYS:HB2	2.06	0.56
1:D:77:LEU:HB3	1:D:109:GLU:HB2	1.86	0.56
1:A:59:LYS:HD3	1:A:115:THR:HG23	1.87	0.56
1:D:304:ALA:HB2	1:D:322:ALA:CB	2.33	0.56
1:A:333:ARG:HB3	1:A:336:ASN:CG	2.31	0.56
1:B:243:THR:CG2	1:B:246:ALA:CB	2.81	0.56
1:B:363:HIS:HD2	1:B:383:SER:HB2	1.70	0.56
1:D:330:LEU:HD11	1:D:342:VAL:CB	2.34	0.56
1:B:59:LYS:HD3	1:B:115:THR:HG23	1.88	0.56
1:B:45:GLU:HG3	4:B:492:HOH:O	2.07	0.55
1:D:35:VAL:HG12	1:D:262:ILE:HB	1.88	0.55
1:A:193:ARG:HH21	1:A:197:LYS:HE3	1.70	0.55
1:A:361:VAL:CG2	1:A:388:ALA:HB2	2.36	0.55
1:B:263:THR:OG1	1:B:286:MSE:HE3	2.06	0.55
1:B:297:LYS:HB3	1:B:329:TYR:CD2	2.41	0.55
1:C:244:ASP:HB2	4:C:591:HOH:O	2.06	0.55
1:C:247:GLY:HA3	1:C:267:ASN:HD21	1.71	0.55
1:A:107:THR:HB	1:A:110:GLU:CG	2.36	0.55
1:A:193:ARG:NH2	1:A:197:LYS:HE3	2.22	0.55
1:D:107:THR:CG2	1:D:110:GLU:H	2.18	0.55
1:C:207:LYS:HB3	1:C:236:ASP:HB2	1.88	0.55
1:A:198:LYS:HB2	4:A:478:HOH:O	2.06	0.54
1:C:135:GLU:HG3	1:C:159:THR:HG23	1.89	0.54
1:C:155:THR:O	1:C:181:ASN:HA	2.07	0.54
1:A:365:THR:HG22	1:A:383:SER:HB2	1.88	0.54
1:B:390:LYS:HG2	1:B:391:LYS:N	2.23	0.54
1:D:115:THR:O	1:D:119:SER:HA	2.07	0.54
1:A:306:GLN:O	1:A:308:SER:CA	2.55	0.54
1:A:344:PHE:C	1:A:345:THR:HA	2.32	0.54
1:A:348:SER:O	1:A:349:LYS:O	2.26	0.54
1:A:307:ASP:OD1	1:A:307:ASP:N	2.39	0.54
1:D:139:VAL:CA	1:D:142:MSE:HE3	2.27	0.54
1:C:266:LEU:O	1:C:267:ASN:HB2	2.07	0.54
1:D:182:LYS:C	1:D:183:LEU:HD12	2.32	0.54
1:A:243:THR:CG2	1:A:246:ALA:H	2.06	0.54
1:B:135:GLU:HG3	1:B:159:THR:HG23	1.90	0.54
1:A:305:TYR:HH	1:A:343:GLN:HG3	1.65	0.54
1:A:330:LEU:HD11	1:A:342:VAL:HG21	1.89	0.54
1:A:365:THR:HG22	1:A:383:SER:CB	2.37	0.54
1:D:238:LEU:HD23	1:D:251:VAL:HG12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:MSE:HB3	1:C:229:PRO:HD2	1.89	0.54
1:D:276:TYR:HB3	3:D:482:IOD:I	2.77	0.53
1:B:160:THR:OG1	1:B:162:LEU:HD12	2.07	0.53
1:B:250:PHE:HB2	1:B:278:ARG:CD	2.38	0.53
1:C:243:THR:HG21	1:C:246:ALA:HB2	1.90	0.53
1:C:285:LEU:O	1:C:289:ILE:HG12	2.08	0.53
1:C:251:VAL:HA	1:C:263:THR:O	2.08	0.53
1:A:248:GLU:HG2	1:A:278:ARG:HH21	1.72	0.53
1:B:163:ASN:OD1	1:B:165:GLU:HG3	2.08	0.53
1:B:193:ARG:O	1:B:197:LYS:HG3	2.07	0.53
1:C:274:ASN:ND2	1:C:280:THR:OG1	2.38	0.53
1:D:236:ASP:OD1	1:D:260:ARG:NH2	2.41	0.53
1:B:303:ASP:C	1:B:323:VAL:HB	2.34	0.53
1:C:111:LEU:HD22	1:C:123:ALA:HA	1.90	0.53
1:D:257:LYS:CE	1:D:290:SER:O	2.57	0.53
1:D:303:ASP:O	1:D:323:VAL:HA	2.09	0.53
1:A:306:GLN:O	1:A:307:ASP:C	2.51	0.53
1:A:332:GLU:HG2	1:A:333:ARG:O	2.08	0.53
1:B:267:ASN:O	1:B:267:ASN:ND2	2.41	0.53
1:C:107:THR:HG22	1:C:109:GLU:H	1.73	0.53
1:B:297:LYS:HB3	1:B:329:TYR:CE2	2.44	0.52
1:B:342:VAL:HB	1:B:366:TYR:HB2	1.90	0.52
1:A:217:THR:HG23	4:A:510:HOH:O	2.08	0.52
1:B:145:LYS:HD2	1:B:149:TRP:CE2	2.44	0.52
1:D:107:THR:HG22	1:D:110:GLU:N	2.19	0.52
1:A:299:VAL:CG2	1:A:305:TYR:HB2	2.39	0.52
1:C:182:LYS:C	1:C:183:LEU:HD12	2.35	0.52
1:D:341:SER:O	1:D:367:GLU:HG3	2.09	0.52
1:B:243:THR:HG22	1:B:246:ALA:CB	2.26	0.52
1:D:45:GLU:HG3	3:D:481:IOD:I	2.79	0.52
1:D:107:THR:HG23	1:D:109:GLU:N	2.25	0.52
1:D:107:THR:HG23	1:D:109:GLU:H	1.74	0.52
1:D:323:VAL:O	1:D:386:MSE:HE3	2.09	0.52
1:A:180:GLU:OE2	1:A:245:LYS:HD2	2.10	0.52
1:A:286:MSE:CE	1:A:289:ILE:HB	2.39	0.52
1:B:36:GLU:CG	1:B:331:ILE:HD11	2.39	0.52
1:C:198:LYS:C	1:C:200:PRO:HD3	2.34	0.52
1:C:312:VAL:HG22	1:C:320:VAL:CG2	2.40	0.52
1:D:184:SER:O	1:D:188:VAL:HG23	2.09	0.52
1:C:315:GLY:N	1:C:318:ASP:OD2	2.41	0.52
1:D:63:VAL:HG21	1:D:116:LEU:CD2	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASN:HD22	1:A:180:GLU:HG3	1.74	0.52
1:C:165:GLU:HG3	1:C:177:LYS:O	2.10	0.52
1:D:323:VAL:N	1:D:386:MSE:HE2	2.24	0.52
1:D:56:SER:HB2	4:D:585:HOH:O	2.09	0.52
1:D:67:TYR:HA	1:D:70:LEU:HD12	1.92	0.52
1:D:83:ILE:CD1	1:D:106:TYR:HD1	2.22	0.52
1:A:310:ALA:CB	1:A:361:VAL:HG12	2.39	0.51
1:A:247:GLY:HA3	1:A:267:ASN:ND2	2.25	0.51
1:D:51:PRO:HG3	1:D:153:ASP:OD2	2.11	0.51
1:B:90:LEU:HD22	1:B:91:THR:N	2.24	0.51
1:C:41:LYS:HB2	1:C:376:TYR:CE2	2.46	0.51
1:D:100:PRO:O	1:D:102:GLU:N	2.43	0.51
1:D:203:LEU:O	1:D:207:LYS:HB2	2.11	0.51
1:B:247:GLY:N	1:B:267:ASN:HB2	2.26	0.51
1:A:297:LYS:HB2	1:A:329:TYR:CE2	2.46	0.51
1:A:313:GLN:O	1:A:314:ASP:CG	2.54	0.51
1:D:294:THR:HG22	1:D:295:LEU:N	2.26	0.51
1:D:308:SER:CB	1:D:322:ALA:HB2	2.40	0.51
1:D:366:TYR:CE2	1:D:368:ASP:HB2	2.46	0.51
1:D:101:MSE:HB2	1:D:106:TYR:CE1	2.45	0.51
1:D:263:THR:OG1	1:D:286:MSE:HE3	2.10	0.51
1:D:304:ALA:CB	1:D:322:ALA:HB3	2.40	0.51
1:A:58:THR:HG21	1:A:181:ASN:ND2	2.26	0.51
1:B:162:LEU:HD22	1:B:166:THR:HG21	1.93	0.51
1:C:243:THR:CG2	1:C:246:ALA:CA	2.88	0.51
1:A:334:VAL:O	1:A:334:VAL:CG2	2.59	0.51
1:B:45:GLU:HG3	3:B:472:IOD:I	2.82	0.50
1:C:121:ASN:O	1:C:125:ILE:HG13	2.11	0.50
1:B:63:VAL:HG21	1:B:116:LEU:CD2	2.30	0.50
1:A:84:SER:O	1:A:87:PRO:HD2	2.12	0.50
1:C:163:ASN:HD22	1:C:180:GLU:HG3	1.76	0.50
1:C:121:ASN:ND2	1:C:162:LEU:HD21	2.27	0.50
1:B:47:ASP:OD1	1:B:47:ASP:O	2.29	0.50
1:C:63:VAL:HG21	1:C:116:LEU:CD2	2.30	0.50
1:A:95:GLU:OE1	1:A:95:GLU:HA	2.11	0.50
1:A:346:PRO:HB3	1:D:152:GLN:HB3	1.94	0.50
1:A:299:VAL:HG22	1:A:305:TYR:HB2	1.94	0.50
1:B:299:VAL:CG2	1:B:328:ILE:HB	2.41	0.50
1:B:107:THR:HG23	1:B:109:GLU:N	2.27	0.50
1:C:298:ILE:HG21	1:C:330:LEU:HD12	1.92	0.50
1:A:139:VAL:HA	1:A:142:MSE:CG	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MSE:HE3	1:A:289:ILE:HD12	1.93	0.50
1:A:355:LEU:O	1:A:391:LYS:HA	2.11	0.50
1:B:27:ILE:HG22	1:B:46:LYS:HD2	1.94	0.50
1:A:306:GLN:O	1:A:308:SER:N	2.45	0.49
1:B:87:PRO:HG3	1:B:125:ILE:CG2	2.43	0.49
1:B:360:VAL:O	1:B:360:VAL:HG22	2.12	0.49
1:C:117:VAL:O	1:C:220:SER:HA	2.12	0.49
1:C:121:ASN:OD1	1:C:160:THR:HG23	2.10	0.49
1:D:223:TYR:CD1	1:D:228:MSE:HE3	2.47	0.49
1:B:33:ILE:HG22	1:B:264:VAL:HB	1.94	0.49
1:B:182:LYS:C	1:B:183:LEU:HD12	2.37	0.49
1:B:238:LEU:HD12	1:B:251:VAL:CG1	2.43	0.49
1:B:27:ILE:HD12	1:B:285:LEU:HD22	1.93	0.49
1:B:261:VAL:CG1	1:B:286:MSE:HE1	2.40	0.49
1:A:87:PRO:HG3	1:A:125:ILE:CG2	2.42	0.49
1:A:302:GLY:C	1:A:323:VAL:HG13	2.38	0.49
1:B:107:THR:CG2	1:B:110:GLU:H	2.22	0.49
1:B:142:MSE:HE2	1:B:156:VAL:HG11	1.94	0.49
1:D:83:ILE:HD13	1:D:101:MSE:SE	2.62	0.49
1:B:238:LEU:O	1:B:239:LYS:HB3	2.12	0.49
1:A:153:ASP:HB3	1:D:344:PHE:CZ	2.47	0.49
1:C:86:TYR:CB	1:C:87:PRO:HD3	2.43	0.49
1:D:323:VAL:N	1:D:386:MSE:CE	2.76	0.49
1:D:324:ALA:HA	1:D:386:MSE:HE3	1.93	0.49
1:A:270:HIS:O	1:B:74:SER:HA	2.13	0.49
1:A:358:GLY:CA	1:A:387:VAL:HG13	2.43	0.49
1:C:236:ASP:OD1	1:C:260:ARG:NH2	2.45	0.49
1:B:56:SER:O	1:B:239:LYS:HD3	2.13	0.49
1:C:121:ASN:OD1	1:C:160:THR:CG2	2.60	0.49
1:D:243:THR:HG21	1:D:246:ALA:HB2	1.95	0.49
1:A:176:LYS:H	1:A:179:GLU:HG3	1.78	0.49
1:C:54:ILE:HD13	1:C:183:LEU:HB2	1.95	0.48
1:D:304:ALA:HB2	1:D:322:ALA:HB1	1.86	0.48
1:C:32:ALA:HA	1:C:264:VAL:O	2.14	0.48
1:C:151:ILE:HG23	1:C:187:ASP:OD1	2.13	0.48
1:C:182:LYS:O	1:C:183:LEU:HD12	2.13	0.48
1:D:54:ILE:HD13	1:D:183:LEU:HD22	1.95	0.48
1:B:86:TYR:CZ	1:B:125:ILE:HD13	2.49	0.48
1:D:259:MSE:HE3	1:D:261:VAL:HG22	1.96	0.48
1:A:366:TYR:HB3	1:A:382:PRO:HG2	1.94	0.48
1:B:182:LYS:O	1:B:183:LEU:HD12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:LYS:HD3	1:D:115:THR:HG23	1.95	0.48
1:A:135:GLU:HG3	1:A:159:THR:HG23	1.95	0.48
1:B:72:ASN:OD1	1:B:72:ASN:C	2.57	0.48
1:C:312:VAL:O	1:C:318:ASP:HB2	2.13	0.48
1:D:299:VAL:HG12	1:D:324:ALA:HB2	1.95	0.48
1:D:324:ALA:HB1	1:D:328:ILE:HD12	1.95	0.48
1:A:36:GLU:HG3	1:A:331:ILE:HD11	1.96	0.48
1:A:94:SER:O	1:A:96:ALA:N	2.42	0.48
1:A:142:MSE:HE2	1:A:156:VAL:CG1	2.43	0.48
1:C:65:LEU:HD21	1:C:145:LYS:HG3	1.95	0.48
1:A:358:GLY:CA	1:A:387:VAL:CG1	2.92	0.48
1:C:145:LYS:HD2	1:C:149:TRP:CE2	2.48	0.48
1:C:298:ILE:CG2	1:C:330:LEU:HD12	2.43	0.48
1:A:351:ILE:O	1:A:352:PRO:C	2.57	0.47
1:D:243:THR:CG2	1:D:246:ALA:CA	2.92	0.47
1:A:45:GLU:CG	4:A:480:HOH:O	2.62	0.47
1:A:107:THR:HG22	1:A:110:GLU:N	2.21	0.47
1:A:117:VAL:O	1:A:220:SER:HA	2.14	0.47
1:D:332:GLU:HB2	1:D:340:GLN:NE2	2.28	0.47
1:A:45:GLU:HG2	4:A:480:HOH:O	2.14	0.47
1:B:384:PHE:N	1:B:384:PHE:CD1	2.83	0.47
1:C:90:LEU:HD23	1:C:90:LEU:HA	1.76	0.47
1:B:77:LEU:HB3	1:B:109:GLU:HB2	1.96	0.47
1:C:267:ASN:ND2	4:C:575:HOH:O	2.47	0.47
1:C:297:LYS:HD2	1:C:327:ASP:OD2	2.14	0.47
1:B:360:VAL:O	1:B:360:VAL:CG2	2.63	0.47
1:D:342:VAL:HA	1:D:366:TYR:HA	1.96	0.47
1:A:107:THR:HG22	1:A:109:GLU:N	2.30	0.47
1:B:107:THR:HG22	1:B:110:GLU:N	2.21	0.47
1:B:238:LEU:O	1:B:239:LYS:CB	2.60	0.47
1:D:234:GLY:O	1:D:254:THR:HA	2.15	0.47
1:C:30:LYS:HB2	1:C:267:ASN:HB3	1.97	0.47
1:D:62:THR:O	1:D:66:VAL:HG23	2.15	0.47
1:D:84:SER:O	1:D:87:PRO:HD2	2.15	0.47
1:A:223:TYR:CD1	1:A:228:MSE:HE2	2.50	0.47
1:C:237:GLY:CA	1:C:253:THR:HG22	2.44	0.47
1:B:107:THR:HG23	1:B:109:GLU:H	1.80	0.46
1:C:59:LYS:HD3	1:C:115:THR:HG23	1.97	0.46
1:A:297:LYS:HD3	1:A:329:TYR:CZ	2.50	0.46
1:C:86:TYR:CZ	1:C:125:ILE:HD13	2.51	0.46
1:D:139:VAL:HG22	1:D:142:MSE:CE	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:CG2	1:B:46:LYS:HD2	2.45	0.46
1:C:87:PRO:HG3	1:C:125:ILE:CG2	2.46	0.46
1:D:37:ALA:HB3	1:D:260:ARG:HG2	1.97	0.46
1:C:193:ARG:NH2	1:C:197:LYS:HE3	2.30	0.46
1:A:163:ASN:HD22	1:A:180:GLU:CG	2.29	0.46
1:D:292:THR:C	1:D:334:VAL:HG23	2.41	0.46
1:A:111:LEU:HD22	1:A:123:ALA:HA	1.97	0.46
1:B:299:VAL:HG23	1:B:328:ILE:HB	1.97	0.46
1:D:85:ASP:O	1:D:89:GLN:HG3	2.16	0.46
1:A:30:LYS:HB2	1:A:267:ASN:HB3	1.97	0.46
1:B:232:ARG:NH1	1:B:256:GLU:OE2	2.48	0.46
1:C:57:ILE:HD13	1:C:251:VAL:HG23	1.96	0.46
1:D:58:THR:HG21	1:D:181:ASN:ND2	2.30	0.46
1:D:384:PHE:CD1	1:D:384:PHE:N	2.83	0.46
1:B:84:SER:O	1:B:87:PRO:HD2	2.16	0.46
1:B:341:SER:C	1:B:343:GLN:N	2.71	0.46
1:C:310:ALA:O	1:C:320:VAL:HG23	2.16	0.46
1:D:259:MSE:SE	1:D:295:LEU:HD11	2.66	0.46
1:A:325:PRO:O	1:A:326:GLU:CG	2.63	0.46
1:D:36:GLU:CG	1:D:331:ILE:HD11	2.45	0.46
1:B:87:PRO:HG3	1:B:125:ILE:HG21	1.98	0.46
1:A:45:GLU:HG3	3:A:468:IOD:I	2.86	0.45
1:A:247:GLY:HA3	1:A:267:ASN:HD21	1.81	0.45
4:A:604:HOH:O	1:D:45:GLU:HG2	2.16	0.45
1:C:77:LEU:O	1:C:107:THR:CG2	2.64	0.45
1:D:278:ARG:HH11	1:D:278:ARG:HD3	1.56	0.45
1:D:143:ARG:HG2	1:D:156:VAL:CG1	2.46	0.45
1:D:257:LYS:HE3	4:D:487:HOH:O	2.15	0.45
1:D:292:THR:O	1:D:334:VAL:HG23	2.16	0.45
1:B:260:ARG:HD2	4:B:570:HOH:O	2.17	0.45
1:C:110:GLU:HB3	1:C:213:PHE:CE1	2.51	0.45
1:B:142:MSE:HE2	1:B:156:VAL:CG1	2.46	0.45
1:C:145:LYS:HD2	1:C:149:TRP:CZ2	2.51	0.45
1:A:361:VAL:HG12	1:A:361:VAL:O	2.16	0.45
1:B:56:SER:HB2	1:B:241:GLY:HA2	1.98	0.45
1:B:118:SER:OG	1:B:218:ILE:HB	2.16	0.45
1:C:298:ILE:HG13	1:C:299:VAL:N	2.30	0.45
1:A:378:THR:O	1:A:381:ARG:NH1	2.50	0.45
1:D:305:TYR:O	1:D:306:GLN:O	2.34	0.45
1:A:228:MSE:HE2	1:A:229:PRO:HD2	1.98	0.45
1:B:86:TYR:CB	1:B:87:PRO:HD3	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:HD12	1:D:205:ILE:HG21	1.99	0.45
1:A:223:TYR:HD1	1:A:228:MSE:HE2	1.82	0.45
1:A:298:ILE:HD13	1:A:330:LEU:HD11	1.98	0.45
1:A:193:ARG:HD2	1:A:377:ILE:HD11	1.98	0.44
1:C:107:THR:HB	1:C:110:GLU:CG	2.43	0.44
1:C:364:LEU:O	1:C:383:SER:HA	2.18	0.44
1:D:119:SER:HB3	1:D:239:LYS:CE	2.48	0.44
1:A:96:ALA:HB1	1:A:121:ASN:HD22	1.82	0.44
1:C:321:ILE:O	1:C:389:ASP:HB2	2.17	0.44
1:B:360:VAL:HA	1:B:387:VAL:HA	2.00	0.44
1:C:263:THR:HG21	1:C:282:THR:CG2	2.38	0.44
1:A:139:VAL:HA	1:A:142:MSE:HG2	2.00	0.44
1:B:361:VAL:HG21	1:B:388:ALA:HB2	1.99	0.44
1:C:193:ARG:HD3	4:C:491:HOH:O	2.18	0.44
1:A:57:ILE:HD13	1:A:251:VAL:HG23	2.00	0.44
1:A:343:GLN:O	1:A:344:PHE:CD2	2.70	0.44
1:B:32:ALA:HA	1:B:264:VAL:O	2.16	0.44
1:B:390:LYS:HG2	1:B:391:LYS:H	1.81	0.44
1:B:54:ILE:HB	1:B:57:ILE:HB	2.00	0.44
1:B:365:THR:HA	1:B:382:PRO:O	2.17	0.44
1:A:271:GLN:HA	1:B:73:GLY:O	2.18	0.44
1:B:107:THR:CG2	1:B:109:GLU:HB3	2.47	0.44
1:C:87:PRO:HG3	1:C:125:ILE:HG21	2.00	0.44
1:A:121:ASN:ND2	1:A:162:LEU:HD21	2.32	0.44
1:A:312:VAL:HG22	1:A:351:ILE:HD13	2.00	0.44
1:D:156:VAL:HA	1:D:181:ASN:OD1	2.18	0.44
1:A:236:ASP:N	1:A:236:ASP:OD1	2.51	0.44
1:D:304:ALA:HA	1:D:322:ALA:HB1	2.00	0.44
1:C:358:GLY:C	1:C:387:VAL:HB	2.43	0.43
1:D:333:ARG:NH2	4:D:547:HOH:O	2.41	0.43
1:C:61:ILE:HD11	1:C:183:LEU:HD21	2.00	0.43
1:C:92:THR:OG1	1:C:93:ASN:N	2.50	0.43
1:A:387:VAL:CG1	1:A:388:ALA:N	2.80	0.43
1:D:61:ILE:HD11	1:D:183:LEU:HD21	2.00	0.43
1:D:324:ALA:HB1	1:D:326:GLU:O	2.17	0.43
1:A:53:GLU:HG2	1:A:245:LYS:HB2	1.99	0.43
1:A:95:GLU:OE1	1:A:95:GLU:CA	2.67	0.43
1:A:163:ASN:ND2	1:A:180:GLU:HG3	2.33	0.43
1:B:341:SER:CA	1:B:343:GLN:HG2	2.48	0.43
1:D:371:LEU:HA	4:D:514:HOH:O	2.18	0.43
1:A:393:GLU:O	1:A:393:GLU:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLN:HG3	1:B:326:GLU:HA	1.99	0.43
1:C:69:ALA:HA	1:C:72:ASN:HD22	1.84	0.43
1:B:239:LYS:HG3	1:B:240:THR:O	2.19	0.43
1:B:364:LEU:O	1:B:384:PHE:HD1	2.01	0.43
1:D:60:LEU:HD21	1:D:239:LYS:HB2	2.00	0.43
1:D:250:PHE:HB2	1:D:278:ARG:CD	2.48	0.43
1:B:53:GLU:HB3	1:B:246:ALA:HB2	2.00	0.43
1:C:267:ASN:C	1:C:267:ASN:HD22	2.26	0.43
1:C:314:ASP:OD1	1:C:314:ASP:O	2.37	0.43
1:B:41:LYS:HB2	1:B:376:TYR:CE2	2.53	0.42
1:B:237:GLY:CA	1:B:253:THR:CG2	2.54	0.42
1:C:45:GLU:HG3	3:C:476:IOD:I	2.89	0.42
1:A:243:THR:HG21	1:A:246:ALA:HB2	2.00	0.42
1:B:145:LYS:HD3	1:B:148:GLU:OE1	2.20	0.42
1:B:236:ASP:OD1	1:B:260:ARG:NH2	2.52	0.42
1:B:253:THR:O	1:B:253:THR:HG23	2.18	0.42
1:D:237:GLY:O	1:D:252:GLY:HA2	2.18	0.42
1:D:238:LEU:HB3	1:D:239:LYS:H	1.65	0.42
1:C:67:TYR:HB3	1:C:199:TYR:CD1	2.54	0.42
1:C:316:LYS:O	1:C:317:GLU:HG3	2.19	0.42
1:A:51:PRO:HG3	1:A:153:ASP:OD2	2.20	0.42
1:B:136:LYS:NZ	1:B:140:ASP:OD2	2.53	0.42
1:C:100:PRO:HD2	1:C:216:MSE:SE	2.69	0.42
1:C:176:LYS:CB	1:C:179:GLU:HG3	2.40	0.42
1:C:364:LEU:HD23	1:C:364:LEU:HA	1.91	0.42
1:A:107:THR:CB	1:A:110:GLU:HG3	2.40	0.42
1:A:118:SER:OG	1:A:218:ILE:HB	2.19	0.42
1:B:246:ALA:O	1:B:247:GLY:C	2.62	0.42
1:C:163:ASN:HA	1:C:180:GLU:HG2	2.01	0.42
1:D:366:TYR:HB3	1:D:382:PRO:HB2	2.00	0.42
1:B:232:ARG:HB3	1:B:235:PHE:HD2	1.85	0.42
1:C:33:ILE:HG22	1:C:264:VAL:HB	2.02	0.42
1:B:380:GLU:O	1:B:381:ARG:HD2	2.19	0.42
1:D:286:MSE:CE	1:D:289:ILE:HD12	2.46	0.42
1:A:56:SER:C	1:A:58:THR:N	2.77	0.42
1:A:323:VAL:CG1	1:A:324:ALA:N	2.83	0.42
1:B:48:ALA:O	1:B:186:TYR:HB2	2.20	0.42
1:B:340:GLN:HB2	1:B:342:VAL:HG12	2.01	0.42
1:C:36:GLU:HG3	1:C:331:ILE:HD11	2.02	0.42
1:C:142:MSE:SE	1:C:159:THR:HG22	2.70	0.42
1:D:386:MSE:HE2	1:D:386:MSE:HB3	1.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TYR:CZ	1:A:125:ILE:HD13	2.55	0.41
1:B:33:ILE:HA	1:B:44:TYR:O	2.20	0.41
1:B:50:GLN:HA	1:B:51:PRO:HD3	1.84	0.41
1:B:99:ILE:HA	1:B:100:PRO:HD3	1.82	0.41
1:B:254:THR:OG1	1:B:255:VAL:N	2.53	0.41
1:C:35:VAL:HG12	1:C:42:ILE:HA	2.02	0.41
1:C:298:ILE:CG2	1:C:330:LEU:CD1	2.97	0.41
1:B:86:TYR:CE2	1:B:125:ILE:HD13	2.55	0.41
1:B:232:ARG:O	1:B:233:GLY:C	2.61	0.41
1:C:103:ALA:HB3	1:C:106:TYR:CZ	2.54	0.41
1:C:113:GLU:OE2	1:C:211:SER:OG	2.36	0.41
1:C:38:ASN:HA	1:C:197:LYS:HE2	2.02	0.41
1:D:341:SER:O	1:D:343:GLN:N	2.49	0.41
1:A:344:PHE:HA	1:A:345:THR:N	2.33	0.41
1:B:286:MSE:CE	1:B:289:ILE:HD12	2.43	0.41
1:C:96:ALA:HB1	1:C:121:ASN:HD22	1.85	0.41
1:D:37:ALA:CB	1:D:260:ARG:HG2	2.50	0.41
1:B:56:SER:C	1:B:58:THR:N	2.76	0.41
1:B:308:SER:HB3	1:B:322:ALA:HB3	2.02	0.41
1:C:273:ASN:HD22	1:C:273:ASN:HA	1.60	0.41
1:A:37:ALA:CB	1:A:260:ARG:HG2	2.50	0.41
1:A:164:ASN:HB3	1:A:171:ILE:HG21	2.02	0.41
1:A:54:ILE:HD13	1:A:183:LEU:HB2	2.01	0.41
1:A:86:TYR:CB	1:A:87:PRO:HD3	2.50	0.41
1:B:59:LYS:HD3	1:B:115:THR:CG2	2.50	0.41
1:C:151:ILE:HG23	1:C:187:ASP:CG	2.45	0.41
1:D:322:ALA:O	1:D:323:VAL:HB	2.21	0.41
1:D:342:VAL:O	1:D:342:VAL:CG2	2.62	0.41
1:A:41:LYS:HB2	1:A:376:TYR:CE2	2.56	0.41
1:A:54:ILE:CD1	1:A:183:LEU:HD13	2.51	0.41
1:A:184:SER:O	1:A:188:VAL:HG23	2.20	0.41
1:A:321:ILE:HG22	1:A:323:VAL:HG23	2.03	0.41
1:B:53:GLU:CD	1:B:53:GLU:H	2.29	0.41
1:B:208:LYS:HA	1:B:209:PRO:HD3	1.76	0.41
1:B:232:ARG:NH2	1:B:287:ASP:OD1	2.54	0.41
1:C:186:TYR:CE1	1:C:377:ILE:HG22	2.56	0.41
1:C:308:SER:HB2	1:C:322:ALA:O	2.20	0.41
1:D:47:ASP:HA	4:D:506:HOH:O	2.20	0.41
1:D:102:GLU:H	1:D:102:GLU:HG2	1.49	0.41
1:D:298:ILE:HD13	1:D:330:LEU:CG	2.48	0.41
1:C:243:THR:O	1:C:244:ASP:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ILE:HD11	1:D:106:TYR:CD1	2.47	0.41
1:D:121:ASN:O	1:D:125:ILE:HG13	2.21	0.41
1:D:208:LYS:HA	1:D:209:PRO:HD3	1.91	0.41
1:B:139:VAL:HA	1:B:142:MSE:CG	2.51	0.40
1:C:310:ALA:CB	1:C:361:VAL:CG2	2.99	0.40
1:C:366:TYR:HB3	1:C:382:PRO:HB2	2.02	0.40
1:D:83:ILE:CD1	1:D:106:TYR:CD1	3.03	0.40
1:D:86:TYR:CB	1:D:87:PRO:HD3	2.47	0.40
1:D:186:TYR:CE1	1:D:377:ILE:HG22	2.57	0.40
1:B:145:LYS:HD3	1:B:145:LYS:HA	1.83	0.40
1:C:118:SER:OG	1:C:218:ILE:HB	2.22	0.40
1:C:164:ASN:HD22	1:C:179:GLU:HB2	1.85	0.40
1:D:29:ALA:O	1:D:46:LYS:HE2	2.21	0.40
1:D:139:VAL:HG13	1:D:156:VAL:HG22	2.02	0.40
1:D:304:ALA:HB2	1:D:322:ALA:HB3	2.02	0.40
1:A:334:VAL:O	1:A:334:VAL:HG23	2.21	0.40
1:A:340:GLN:H	1:A:340:GLN:HG3	1.65	0.40
1:A:363:HIS:CD2	1:A:385:GLU:HG2	2.56	0.40
1:B:57:ILE:HG12	1:B:251:VAL:HG23	2.04	0.40
1:B:103:ALA:HB3	1:B:106:TYR:CZ	2.56	0.40
1:C:201:GLN:H	1:C:201:GLN:CD	2.30	0.40
1:D:340:GLN:C	1:D:342:VAL:H	2.30	0.40

All (1) 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:B:51:PRO:CD	1:C:344:PHE:CZ[3_545]	1.79	0.41

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	367/379 (97%)	329 (90%)	31 (8%)	7 (2%)	6	22
1	B	331/379 (87%)	290 (88%)	33 (10%)	8 (2%)	4	17
1	C	353/379 (93%)	320 (91%)	29 (8%)	4 (1%)	11	36
1	D	309/379 (82%)	280 (91%)	22 (7%)	7 (2%)	5	18
All	All	1360/1516 (90%)	1219 (90%)	115 (8%)	26 (2%)	6	22

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASP
1	A	337	GLN
1	B	93	ASN
1	B	247	GLY
1	B	306	GLN
1	B	307	ASP
1	C	314	ASP
1	C	319	THR
1	D	101	MSE
1	D	238	LEU
1	D	306	GLN
1	A	314	ASP
1	A	325	PRO
1	B	238	LEU
1	B	267	ASN
1	D	237	GLY
1	A	236	ASP
1	A	343	GLN
1	D	307	ASP
1	A	306	GLN
1	B	277	ALA
1	B	339	SER
1	C	56	SER
1	C	236	ASP
1	D	342	VAL
1	D	346	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	310/308 (101%)	278 (90%)	32 (10%)	7	23
1	B	286/308 (93%)	247 (86%)	39 (14%)	3	13
1	C	302/308 (98%)	273 (90%)	29 (10%)	8	26
1	D	272/308 (88%)	240 (88%)	32 (12%)	5	17
All	All	1170/1232 (95%)	1038 (89%)	132 (11%)	5	19

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	95	GLU
1	A	104	ARG
1	A	107	THR
1	A	112	LEU
1	A	113	GLU
1	A	169	ASP
1	A	182	LYS
1	A	201	GLN
1	A	212	THR
1	A	228	MSE
1	A	260	ARG
1	A	263	THR
1	A	266	LEU
1	A	286	MSE
1	A	300	GLN
1	A	307	ASP
1	A	311	PRO
1	A	319	THR
1	A	320	VAL
1	A	321	ILE
1	A	334	VAL
1	A	338	SER
1	A	340	GLN
1	A	342	VAL
1	A	343	GLN
1	A	344	PHE
1	A	345	THR
1	A	347	ASP
1	A	348	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	349	LYS
1	A	351	ILE
1	B	45	GLU
1	B	46	LYS
1	B	49	THR
1	B	50	GLN
1	B	90	LEU
1	B	93	ASN
1	B	97	SER
1	B	98	ASN
1	B	99	ILE
1	B	107	THR
1	B	112	LEU
1	B	141	MSE
1	B	145	LYS
1	B	201	GLN
1	B	232	ARG
1	B	238	LEU
1	B	239	LYS
1	B	260	ARG
1	B	263	THR
1	B	267	ASN
1	B	270	HIS
1	B	275	PRO
1	B	284	SER
1	B	299	VAL
1	B	301	GLN
1	B	307	ASP
1	B	338	SER
1	B	339	SER
1	B	340	GLN
1	B	341	SER
1	B	342	VAL
1	B	343	GLN
1	B	344	PHE
1	B	347	ASP
1	B	360	VAL
1	B	361	VAL
1	B	363	HIS
1	B	364	LEU
1	B	379	THR
1	C	45	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	56	SER
1	C	90	LEU
1	C	92	THR
1	C	94	SER
1	C	97	SER
1	C	99	ILE
1	C	113	GLU
1	C	145	LYS
1	C	201	GLN
1	C	207	LYS
1	C	229	PRO
1	C	232	ARG
1	C	238	LEU
1	C	239	LYS
1	C	260	ARG
1	C	263	THR
1	C	273	ASN
1	C	295	LEU
1	C	311	PRO
1	C	312	VAL
1	C	319	THR
1	C	320	VAL
1	C	342	VAL
1	C	344	PHE
1	C	347	ASP
1	C	348	SER
1	C	355	LEU
1	C	390	LYS
1	D	45	GLU
1	D	56	SER
1	D	78	SER
1	D	91	THR
1	D	93	ASN
1	D	99	ILE
1	D	102	GLU
1	D	107	THR
1	D	112	LEU
1	D	156	VAL
1	D	197	LYS
1	D	201	GLN
1	D	212	THR
1	D	216	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	236	ASP
1	D	238	LEU
1	D	239	LYS
1	D	260	ARG
1	D	263	THR
1	D	270	HIS
1	D	276	TYR
1	D	278	ARG
1	D	284	SER
1	D	300	GLN
1	D	306	GLN
1	D	308	SER
1	D	323	VAL
1	D	328	ILE
1	D	342	VAL
1	D	344	PHE
1	D	345	THR
1	D	386	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	152	GLN
1	A	267	ASN
1	A	274	ASN
1	A	313	GLN
1	A	336	ASN
1	A	337	GLN
1	A	343	GLN
1	B	38	ASN
1	B	170	ASN
1	B	340	GLN
1	B	343	GLN
1	B	363	HIS
1	C	38	ASN
1	C	72	ASN
1	C	164	ASN
1	C	267	ASN
1	C	273	ASN
1	C	363	HIS
1	D	50	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	170	ASN
1	D	270	HIS
1	D	300	GLN
1	D	306	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	465	-	4,4,4	0.36	0	6,6,6	0.17	0
2	SO4	D	467	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	A	464	-	4,4,4	0.38	0	6,6,6	0.16	0
2	SO4	C	466	-	4,4,4	0.38	0	6,6,6	0.13	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	344:PHE	C	345:THR	N	1.77

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	360/379 (94%)	0.41	44 (12%) 8 6	7, 20, 65, 82	0
1	B	323/379 (85%)	0.57	52 (16%) 4 4	9, 22, 72, 85	0
1	C	341/379 (89%)	0.33	41 (12%) 9 6	9, 23, 67, 88	0
1	D	309/379 (81%)	0.28	37 (11%) 9 6	7, 20, 61, 88	0
All	All	1333/1516 (87%)	0.40	174 (13%) 7 6	7, 22, 68, 88	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	ASP	9.8
1	B	308	SER	9.0
1	D	91	THR	9.0
1	A	342	VAL	8.3
1	B	307	ASP	8.2
1	D	92	THR	7.6
1	C	318	ASP	7.2
1	B	342	VAL	7.1
1	A	336	ASN	7.1
1	B	269	ASP	7.0
1	C	317	GLU	6.8
1	A	319	THR	6.7
1	C	355	LEU	6.6
1	D	307	ASP	6.5
1	A	350	ALA	6.4
1	A	338	SER	6.2
1	C	319	THR	6.2
1	D	344	PHE	6.1
1	B	346	PRO	6.1
1	A	337	GLN	6.0
1	B	321	ILE	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	308	SER	5.9
1	B	275	PRO	5.9
1	A	347	ASP	5.5
1	C	348	SER	5.4
1	D	345	THR	5.3
1	D	347	ASP	5.3
1	B	306	GLN	5.3
1	A	314	ASP	5.1
1	D	342	VAL	5.0
1	A	317	GLU	4.9
1	A	343	GLN	4.9
1	D	343	GLN	4.9
1	B	305	TYR	4.8
1	B	99	ILE	4.8
1	D	306	GLN	4.8
1	A	348	SER	4.7
1	B	337	GLN	4.7
1	D	237	GLY	4.7
1	B	343	GLN	4.6
1	C	315	GLY	4.6
1	A	351	ILE	4.6
1	B	322	ALA	4.6
1	C	361	VAL	4.6
1	A	349	LYS	4.5
1	C	316	LYS	4.4
1	B	387	VAL	4.4
1	B	389	ASP	4.4
1	B	270	HIS	4.3
1	D	341	SER	4.3
1	B	98	ASN	4.2
1	D	275	PRO	4.2
1	B	344	PHE	4.2
1	A	93	ASN	4.2
1	D	340	GLN	4.2
1	A	94	SER	4.1
1	D	99	ILE	4.0
1	B	391	LYS	4.0
1	D	323	VAL	4.0
1	C	345	THR	4.0
1	B	326	GLU	4.0
1	C	312	VAL	3.9
1	B	388	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	346	PRO	3.9
1	D	169	ASP	3.8
1	B	345	THR	3.8
1	A	326	GLU	3.8
1	A	307	ASP	3.8
1	C	346	PRO	3.8
1	C	392	ILE	3.8
1	D	325	PRO	3.7
1	D	277	ALA	3.7
1	A	315	GLY	3.6
1	B	361	VAL	3.6
1	A	95	GLU	3.6
1	D	324	ALA	3.5
1	C	356	GLU	3.5
1	C	347	ASP	3.4
1	A	325	PRO	3.3
1	B	390	LYS	3.3
1	A	346	PRO	3.2
1	D	322	ALA	3.2
1	A	339	SER	3.2
1	A	320	VAL	3.2
1	C	313	GLN	3.2
1	C	358	GLY	3.2
1	C	94	SER	3.1
1	A	165	GLU	3.1
1	A	306	GLN	3.1
1	D	238	LEU	3.1
1	A	271	GLN	3.1
1	B	300	GLN	3.0
1	A	316	LYS	3.0
1	D	100	PRO	3.0
1	A	305	TYR	3.0
1	C	97	SER	3.0
1	C	309	LYS	3.0
1	A	296	ARG	3.0
1	A	341	SER	3.0
1	D	270	HIS	2.9
1	A	335	GLY	2.9
1	B	339	SER	2.9
1	A	344	PHE	2.8
1	B	341	SER	2.8
1	B	364	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	323	VAL	2.8
1	B	360	VAL	2.8
1	B	335	GLY	2.8
1	C	332	GLU	2.7
1	D	334	VAL	2.7
1	B	169	ASP	2.7
1	B	215	GLY	2.7
1	B	338	SER	2.7
1	C	93	ASN	2.7
1	B	91	THR	2.7
1	C	308	SER	2.7
1	B	238	LEU	2.7
1	B	324	ALA	2.7
1	A	313	GLN	2.7
1	A	340	GLN	2.7
1	B	340	GLN	2.7
1	C	320	VAL	2.7
1	A	321	ILE	2.6
1	B	268	ALA	2.6
1	C	169	ASP	2.6
1	B	298	ILE	2.6
1	B	334	VAL	2.6
1	A	393	GLU	2.6
1	C	268	ALA	2.6
1	C	92	THR	2.5
1	D	326	GLU	2.5
1	D	303	ASP	2.5
1	A	352	PRO	2.5
1	B	362	GLY	2.5
1	D	305	TYR	2.5
1	D	215	GLY	2.5
1	D	276	TYR	2.5
1	B	267	ASN	2.4
1	B	301	GLN	2.4
1	A	266	LEU	2.4
1	D	47	ASP	2.4
1	A	92	THR	2.4
1	B	363	HIS	2.4
1	C	311	PRO	2.4
1	C	321	ILE	2.3
1	C	389	ASP	2.3
1	A	312	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	389	ASP	2.2
1	A	334	VAL	2.2
1	C	267	ASN	2.2
1	B	47	ASP	2.2
1	D	236	ASP	2.2
1	D	385	GLU	2.2
1	D	301	GLN	2.2
1	C	314	ASP	2.2
1	C	91	THR	2.1
1	D	243	THR	2.1
1	C	324	ALA	2.1
1	C	357	ALA	2.1
1	D	304	ALA	2.1
1	C	95	GLU	2.1
1	C	383	SER	2.1
1	B	303	ASP	2.1
1	C	390	LYS	2.1
1	B	45	GLU	2.1
1	B	48	ALA	2.0
1	C	307	ASP	2.0
1	C	310	ALA	2.0
1	C	360	VAL	2.0
1	B	325	PRO	2.0
1	B	235	PHE	2.0
1	A	359	THR	2.0
1	B	246	ALA	2.0
1	C	391	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	465	5/5	0.84	0.16	48,49,51,52	0
2	SO4	A	464	5/5	0.92	0.14	48,52,54,54	0
2	SO4	C	466	5/5	0.92	0.14	60,61,63,63	0
3	IOD	C	478	1/1	0.93	0.11	76,76,76,76	1
3	IOD	B	475	1/1	0.94	0.07	56,56,56,56	1
3	IOD	C	479	1/1	0.94	0.07	44,44,44,44	1
3	IOD	A	470	1/1	0.95	0.12	66,66,66,66	1
2	SO4	D	467	5/5	0.95	0.10	38,39,41,41	0
3	IOD	D	482	1/1	0.96	0.07	56,56,56,56	1
3	IOD	D	483	1/1	0.96	0.08	44,44,44,44	1
3	IOD	B	474	1/1	0.97	0.28	9,9,9,9	1
3	IOD	A	471	1/1	0.97	0.05	38,38,38,38	1
3	IOD	C	476	1/1	0.99	0.02	22,22,22,22	0
3	IOD	D	480	1/1	0.99	0.03	43,43,43,43	0
3	IOD	C	477	1/1	0.99	0.02	38,38,38,38	0
3	IOD	A	469	1/1	0.99	0.02	39,39,39,39	0
3	IOD	A	468	1/1	1.00	0.03	19,19,19,19	0
3	IOD	D	481	1/1	1.00	0.01	17,17,17,17	0
3	IOD	B	472	1/1	1.00	0.01	19,19,19,19	0
3	IOD	B	473	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.