Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 09:24 PM EDT

PDB ID	:	2HFB
Title	:	Crystal structure of selenomethionine-labelled RafE from Streptococcus pneumoniae
Authors	:	Paterson, N.G.; Riboldi-Tunnicliffe, A.; Mitchell, T.J.; Isaacs, N.W.
Deposited on	:	2006-06-23
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

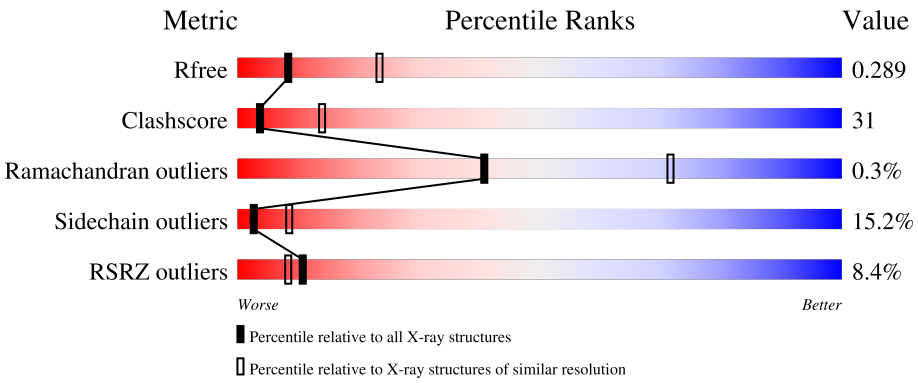
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	409	48% 38% 7% 6%
1	B	409	14% 46% 37% 10% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6045 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 Sugar ABC transporter, sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	383	3029	1937	497	584	11	69	0	0
1	B	381	3013	1927	494	581	11	376	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	CLONING ARTIFACT	UNP Q97NW2
A	-16	ARG	-	CLONING ARTIFACT	UNP Q97NW2
A	-15	GLY	-	CLONING ARTIFACT	UNP Q97NW2
A	-14	SER	-	CLONING ARTIFACT	UNP Q97NW2
A	-13	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-12	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-11	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-10	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-9	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-8	HIS	-	CLONING ARTIFACT	UNP Q97NW2
A	-7	THR	-	CLONING ARTIFACT	UNP Q97NW2
A	-6	ASP	-	CLONING ARTIFACT	UNP Q97NW2
A	-5	PRO	-	CLONING ARTIFACT	UNP Q97NW2
A	17	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	201	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	208	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	240	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	264	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	302	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	308	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	336	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	364	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	375	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
A	386	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	-17	MET	-	CLONING ARTIFACT	UNP Q97NW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	ARG	-	CLONING ARTIFACT	UNP Q97NW2
B	-15	GLY	-	CLONING ARTIFACT	UNP Q97NW2
B	-14	SER	-	CLONING ARTIFACT	UNP Q97NW2
B	-13	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-12	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-11	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-10	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-9	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-8	HIS	-	CLONING ARTIFACT	UNP Q97NW2
B	-7	THR	-	CLONING ARTIFACT	UNP Q97NW2
B	-6	ASP	-	CLONING ARTIFACT	UNP Q97NW2
B	-5	PRO	-	CLONING ARTIFACT	UNP Q97NW2
B	17	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	201	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	208	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	240	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	264	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	302	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	308	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	336	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	364	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	375	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2
B	386	MSE	MET	MODIFIED RESIDUE	UNP Q97NW2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0

- Molecule 3 is water.

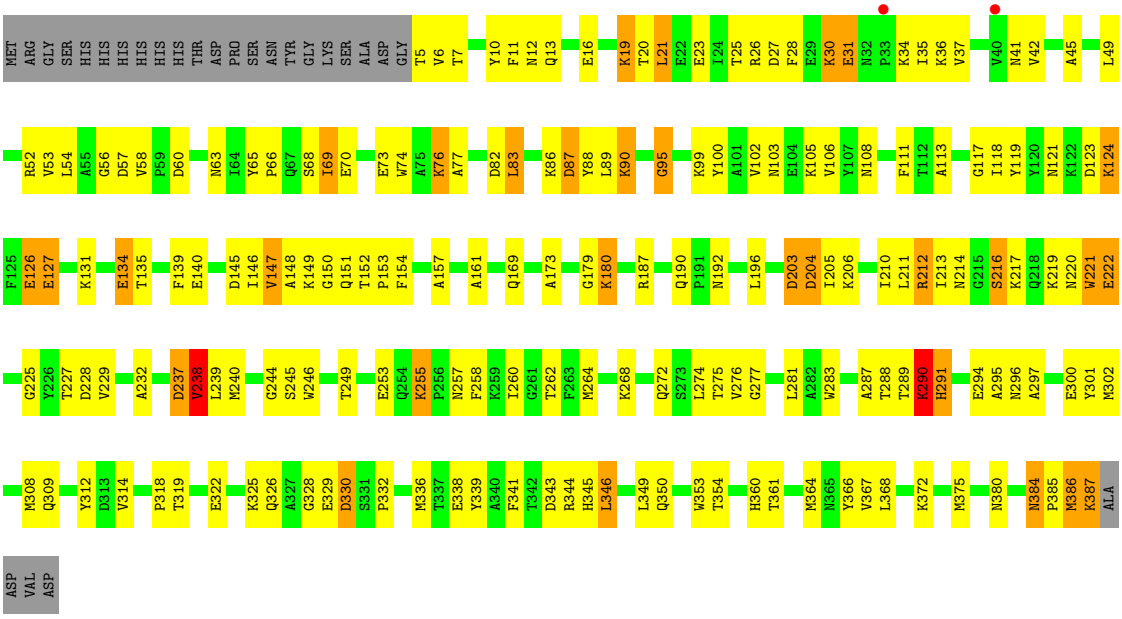
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0

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.

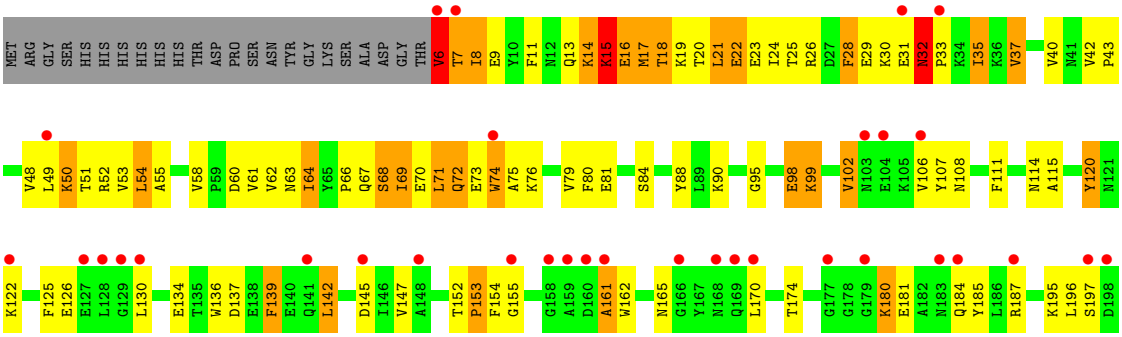
• Molecule 1: Sugar ABC transporter, sugar-binding protein

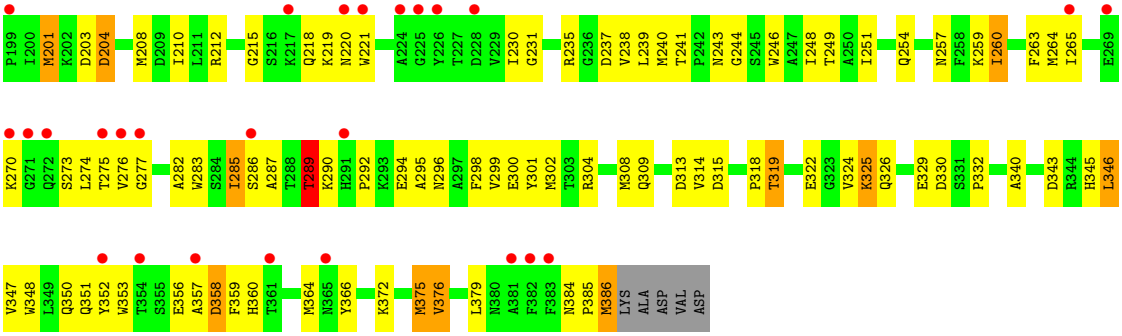
Chain A:



• Molecule 1: Sugar ABC transporter, sugar-binding protein

Chain B:




P199 I200 M201 K202 D203 D204 M208 D209 I210 L211 R212 G215 S216 K217 Q218 K219 N220 W221 A224 G225 Y226 T227 D228 V229 I230 G231 R235 G236 D237 V238 L239 M240 T241 P242 N243 G244 S245 W246 A247 I248 T249 A250 I251 Q254 N257 F258 K259 I260 F263 M264 I265 E269
K270 G271 Q272 S273 L274 T275 V276 G277 A282 W283 S284 I285 S286 A287 T288 T289 K290 H291 P292 K293 E294 A295 N296 A297 F298 V299 E300 Y301 M302 T303 R304 M308 Q309 D313 V314 D315 P318 T319 E322 G323 V324 K325 Q326 E329 D330 S331 P332 A340 D343 R344 H345 L346
V347 W348 L349 Q350 Q351 Y352 W353 T354 S355 E356 A357 D358 F359 H360 T361 M364 M365 Y366 K372 M375 V376 L379 M380 A381 F382 F383 M384 P385 M386 LYS ALA ASP VAL ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	144.54Å 144.54Å 224.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.51 – 2.90 29.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.51-2.90) 99.2 (29.51-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.50 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.248 , 0.290 0.244 , 0.289	Depositor DCC
R_{free} test set	1568 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 77.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6045	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 5.10% 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, 0.333 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: CL

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	1.20	7/3088 (0.2%)	1.15	18/4168 (0.4%)
1	B	0.95	11/3072 (0.4%)	1.24	25/4147 (0.6%)
All	All	1.08	18/6160 (0.3%)	1.20	43/8315 (0.5%)

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	1	1
1	B	0	4
All	All	1	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	GLU	CD-OE2	8.71	1.35	1.25
1	B	185	TYR	CB-CG	-7.77	1.40	1.51
1	B	16	GLU	CG-CD	7.26	1.62	1.51
1	A	322	GLU	CB-CG	7.05	1.65	1.52
1	A	36	LYS	CA-CB	-6.96	1.38	1.53
1	A	73	GLU	CG-CD	6.80	1.62	1.51
1	A	140	GLU	CB-CG	-6.67	1.39	1.52
1	B	74	TRP	CB-CG	6.32	1.61	1.50
1	B	16	GLU	CB-CG	6.27	1.64	1.52
1	B	197	SER	CA-CB	-6.24	1.43	1.52
1	B	358	ASP	CA-CB	-5.91	1.41	1.53
1	A	339	TYR	CE2-CZ	5.80	1.46	1.38
1	B	15	LYS	CE-NZ	5.71	1.63	1.49
1	B	80	PHE	CD1-CE1	5.67	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	PHE	CE1-CZ	5.54	1.47	1.37
1	B	210	ILE	CA-CB	-5.26	1.42	1.54
1	B	90	LYS	CE-NZ	5.24	1.62	1.49
1	A	322	GLU	CG-CD	5.01	1.59	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	185	TYR	CB-CG-CD1	-27.10	104.74	121.00
1	B	185	TYR	CB-CG-CD2	26.29	136.78	121.00
1	B	28	PHE	CB-CA-C	-9.38	91.63	110.40
1	A	344	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	75	ALA	CB-CA-C	-8.30	97.64	110.10
1	B	359	PHE	CB-CG-CD2	-7.76	115.37	120.80
1	A	31	GLU	N-CA-CB	-7.76	96.63	110.60
1	A	19	LYS	CB-CA-C	7.48	125.37	110.40
1	A	290	LYS	CB-CA-C	7.47	125.34	110.40
1	B	161	ALA	N-CA-C	7.16	130.32	111.00
1	B	215	GLY	N-CA-C	7.11	130.87	113.10
1	B	68	SER	CB-CA-C	-7.04	96.73	110.10
1	B	43	PRO	CB-CA-C	-6.89	94.78	112.00
1	B	204	ASP	N-CA-CB	6.79	122.82	110.60
1	B	161	ALA	CB-CA-C	-6.60	100.19	110.10
1	B	142	LEU	CB-CA-C	6.58	122.71	110.20
1	B	359	PHE	CB-CG-CD1	6.38	125.26	120.80
1	B	170	LEU	CB-CA-C	-6.25	98.33	110.20
1	B	210	ILE	N-CA-CB	6.14	124.93	110.80
1	B	313	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	185	TYR	CA-CB-CG	5.97	124.75	113.40
1	A	220	ASN	N-CA-CB	5.95	121.31	110.60
1	A	368	LEU	CB-CG-CD2	5.88	120.99	111.00
1	A	204	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	95	GLY	N-CA-C	-5.84	98.49	113.10
1	A	203	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	274	LEU	CB-CA-C	-5.76	99.25	110.20
1	A	31	GLU	N-CA-C	5.74	126.50	111.00
1	B	203	ASP	N-CA-CB	-5.73	100.28	110.60
1	B	358	ASP	CB-CA-C	5.60	121.60	110.40
1	A	272	GLN	CB-CA-C	5.58	121.57	110.40
1	B	287	ALA	N-CA-CB	5.55	117.87	110.10
1	B	139	PHE	CB-CA-C	-5.54	99.32	110.40
1	B	19	LYS	CA-CB-CG	5.53	125.57	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	LYS	CB-CA-C	-5.48	99.44	110.40
1	B	153	PRO	N-CA-C	5.46	126.31	112.10
1	A	221	TRP	CB-CA-C	-5.44	99.52	110.40
1	A	255	LYS	CA-CB-CG	5.31	125.07	113.40
1	B	18	THR	N-CA-CB	-5.26	100.30	110.30
1	A	346	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	B	14	LYS	CD-CE-NZ	-5.18	99.79	111.70
1	A	238	VAL	CB-CA-C	-5.08	101.74	111.40
1	A	214	ASN	CB-CA-C	5.05	120.50	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	386	MSE	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	GLY	Peptide
1	B	154	PHE	Peptide
1	B	289	THR	Peptide
1	B	32	ASN	Peptide
1	B	6	VAL	Peptide

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	3029	0	2968	165	0
1	B	3013	0	2948	182	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
All	All	6045	0	5916	338	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (338) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ARG:HD2	1:B:187:ARG:O	1.43	1.15
1:A:387:LYS:HE2	1:A:387:LYS:O	1.44	1.14
1:A:6:VAL:HG11	1:A:291:HIS:CD2	1.81	1.14
1:B:62:VAL:HG23	1:B:64:ILE:HG22	1.28	1.14
1:B:32:ASN:O	1:B:35:ILE:HG13	1.48	1.11
1:A:6:VAL:CG1	1:A:291:HIS:CD2	2.36	1.09
1:B:289:THR:HG21	1:B:292:PRO:HB3	1.29	1.08
1:B:31:GLU:HG3	1:B:32:ASN:ND2	1.68	1.07
1:A:10:TYR:CE2	1:A:12:ASN:HB2	1.93	1.04
1:A:309:GLN:HE22	1:A:325:LYS:H	1.09	0.97
1:B:62:VAL:HG23	1:B:64:ILE:CG2	1.96	0.95
1:B:31:GLU:HG3	1:B:32:ASN:HD21	1.21	0.95
1:B:153:PRO:O	1:B:240:MSE:HE3	1.65	0.94
1:B:289:THR:CG2	1:B:292:PRO:HB3	1.98	0.93
1:B:13:GLN:H	1:B:63:ASN:ND2	1.66	0.93
1:A:124:LYS:HG3	1:A:239:LEU:CD2	1.99	0.92
1:B:264:MSE:HE3	1:B:275:THR:HG22	1.52	0.92
1:A:86:LYS:HE3	1:A:296:ASN:OD1	1.69	0.91
1:B:42:VAL:HG21	1:B:48:VAL:HG21	1.53	0.91
1:B:32:ASN:H	1:B:32:ASN:HD22	1.19	0.90
1:B:289:THR:HG21	1:B:292:PRO:CB	2.01	0.90
1:A:290:LYS:C	1:A:291:HIS:ND1	2.25	0.89
1:B:13:GLN:N	1:B:63:ASN:HD22	1.71	0.87
1:B:375:MSE:O	1:B:379:LEU:HG	1.75	0.86
1:B:208:MSE:HB3	1:B:366:TYR:HE2	1.39	0.85
1:B:79:VAL:HG12	1:B:79:VAL:O	1.75	0.85
1:A:70:GLU:OE2	1:A:70:GLU:N	2.09	0.84
1:B:28:PHE:C	1:B:28:PHE:CD2	2.51	0.83
1:B:72:GLN:H	1:B:72:GLN:HE21	1.25	0.83
1:B:79:VAL:O	1:B:79:VAL:CG1	2.27	0.82
1:B:53:VAL:HG22	1:B:58:VAL:HG22	1.60	0.82
1:B:13:GLN:H	1:B:63:ASN:HD22	0.86	0.82
1:A:291:HIS:HB3	1:A:294:GLU:OE2	1.80	0.82
1:A:291:HIS:ND1	1:A:291:HIS:N	2.28	0.81
1:B:32:ASN:HD22	1:B:32:ASN:N	1.77	0.80
1:A:123:ASP:O	1:A:127:GLU:HG2	1.81	0.80
1:B:72:GLN:HE21	1:B:72:GLN:N	1.80	0.80
1:B:31:GLU:CG	1:B:32:ASN:HD21	1.94	0.79
1:B:32:ASN:ND2	1:B:32:ASN:N	2.30	0.79
1:B:289:THR:HG23	1:B:290:LYS:O	1.81	0.79
1:A:288:THR:HG22	1:B:22:GLU:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:HG3	1:A:239:LEU:HD21	1.64	0.79
1:B:31:GLU:CG	1:B:32:ASN:ND2	2.46	0.78
1:A:291:HIS:HB3	1:A:294:GLU:CD	2.04	0.78
1:B:208:MSE:HB3	1:B:366:TYR:CE2	2.19	0.78
1:A:192:ASN:H	1:A:384:ASN:HD21	1.30	0.78
1:A:124:LYS:HG3	1:A:239:LEU:HD22	1.64	0.78
1:B:376:VAL:HA	1:B:379:LEU:HD12	1.66	0.78
1:B:28:PHE:CD2	1:B:28:PHE:O	2.37	0.77
1:B:62:VAL:CG2	1:B:64:ILE:CG2	2.62	0.77
1:A:6:VAL:CG2	1:A:291:HIS:HD2	1.98	0.77
1:B:208:MSE:CB	1:B:366:TYR:HE2	1.97	0.77
1:B:187:ARG:O	1:B:187:ARG:CD	2.30	0.77
1:B:50:LYS:HA	1:B:74:TRP:CH2	2.19	0.77
1:B:24:ILE:HD13	1:B:302:MSE:HE1	1.67	0.76
1:B:50:LYS:HA	1:B:74:TRP:HH2	1.50	0.76
1:B:67:GLN:N	1:B:67:GLN:OE1	2.18	0.76
1:A:6:VAL:HG13	1:A:291:HIS:CD2	2.21	0.76
1:A:221:TRP:HZ3	1:A:364:MSE:HE1	1.48	0.76
1:B:17:MSE:HA	1:B:17:MSE:CE	2.16	0.75
1:A:387:LYS:O	1:A:387:LYS:CE	2.30	0.75
1:A:6:VAL:HG12	1:A:7:THR:N	2.01	0.74
1:B:17:MSE:SE	1:B:315:ASP:HB2	2.37	0.74
1:B:84:SER:OG	1:B:106:VAL:N	2.21	0.74
1:B:8:ILE:HG13	1:B:8:ILE:O	1.86	0.73
1:A:10:TYR:CZ	1:A:12:ASN:HB2	2.24	0.73
1:B:32:ASN:HB2	1:B:35:ILE:HD12	1.70	0.73
1:B:72:GLN:HB3	1:B:73:GLU:OE1	1.88	0.73
1:A:6:VAL:HG21	1:A:291:HIS:HD2	1.53	0.73
1:A:6:VAL:CG1	1:A:291:HIS:HD2	2.01	0.72
1:B:208:MSE:CB	1:B:366:TYR:CE2	2.72	0.72
1:B:32:ASN:HB2	1:B:35:ILE:CD1	2.19	0.72
1:B:11:PHE:CD1	1:B:40:VAL:HG12	2.26	0.71
1:B:32:ASN:HB3	1:B:35:ILE:HD11	1.73	0.70
1:B:134:GLU:HB3	1:B:270:LYS:HD2	1.74	0.70
1:B:32:ASN:CB	1:B:35:ILE:CD1	2.69	0.70
1:B:42:VAL:CG2	1:B:48:VAL:HG21	2.22	0.70
1:B:95:GLY:O	1:B:98:GLU:HB2	1.91	0.70
1:A:6:VAL:CG1	1:A:7:THR:N	2.54	0.70
1:A:154:PHE:O	1:A:238:VAL:HG11	1.92	0.69
1:B:17:MSE:HA	1:B:17:MSE:HE3	1.73	0.69
1:A:76:LYS:CG	1:A:76:LYS:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:CB	1:A:375:MSE:HE3	2.23	0.69
1:B:376:VAL:HA	1:B:379:LEU:CD1	2.21	0.69
1:A:34:LYS:O	1:A:35:ILE:HG13	1.93	0.69
1:B:24:ILE:HG21	1:B:302:MSE:HE1	1.75	0.69
1:B:69:ILE:O	1:B:73:GLU:HG2	1.93	0.69
1:B:51:THR:O	1:B:51:THR:OG1	2.11	0.68
1:B:289:THR:CG2	1:B:292:PRO:CB	2.67	0.68
1:A:225:GLY:O	1:A:228:ASP:HB2	1.94	0.67
1:B:309:GLN:HE22	1:B:325:LYS:H	1.42	0.67
1:A:152:THR:HB	1:A:238:VAL:HG12	1.76	0.67
1:B:318:PRO:HA	1:B:326:GLN:HE22	1.61	0.66
1:A:145:ASP:O	1:A:149:LYS:HG3	1.95	0.66
1:A:124:LYS:CG	1:A:239:LEU:HD22	2.26	0.66
1:B:111:PHE:CE1	1:B:302:MSE:HG3	2.30	0.66
1:A:108:ASN:HA	1:A:283:TRP:O	1.97	0.65
1:A:338:GLU:O	1:A:338:GLU:CG	2.45	0.65
1:A:161:ALA:HB1	1:A:360:HIS:O	1.97	0.65
1:A:12:ASN:ND2	1:A:41:ASN:OD1	2.30	0.65
1:A:152:THR:HB	1:A:238:VAL:CG1	2.26	0.65
1:B:69:ILE:HD12	1:B:69:ILE:H	1.60	0.64
1:A:77:ALA:O	1:B:15:LYS:HB3	1.98	0.64
1:A:350:GLN:HA	1:A:353:TRP:CG	2.32	0.64
1:B:294:GLU:N	1:B:294:GLU:OE1	2.31	0.64
1:B:62:VAL:CG2	1:B:64:ILE:HG22	2.14	0.64
1:A:276:VAL:HG22	1:A:277:GLY:N	2.13	0.63
1:A:56:GLY:HA3	1:B:40:VAL:HG22	1.80	0.63
1:A:283:TRP:HH2	1:A:302:MSE:HE2	1.64	0.63
1:B:153:PRO:O	1:B:240:MSE:HB2	1.98	0.63
1:B:219:LYS:O	1:B:220:ASN:HB2	1.98	0.62
1:A:366:TYR:HB3	1:A:375:MSE:HE3	1.81	0.62
1:A:6:VAL:HG11	1:A:291:HIS:CG	2.33	0.61
1:B:28:PHE:O	1:B:28:PHE:CG	2.50	0.61
1:B:155:GLY:HA3	1:B:238:VAL:HG21	1.82	0.61
1:A:179:GLY:H	1:A:346:LEU:HD22	1.65	0.61
1:A:384:ASN:N	1:A:385:PRO:HD2	2.16	0.61
1:B:50:LYS:HD3	1:B:70:GLU:HG2	1.83	0.60
1:A:366:TYR:HB3	1:A:375:MSE:CE	2.31	0.60
1:B:351:GLN:O	1:B:351:GLN:HG2	2.02	0.60
1:A:366:TYR:HB2	1:A:375:MSE:HE3	1.84	0.60
1:A:53:VAL:HA	1:A:58:VAL:HG22	1.85	0.59
1:B:289:THR:HG22	1:B:292:PRO:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:HG21	1:B:48:VAL:CG2	2.31	0.58
1:B:357:ALA:O	1:B:360:HIS:HB2	2.03	0.58
1:B:274:LEU:HB3	1:B:346:LEU:HD21	1.86	0.58
1:A:288:THR:CG2	1:B:22:GLU:HG3	2.31	0.58
1:B:102:VAL:CG2	1:B:107:TYR:HD2	2.17	0.58
1:A:190:GLN:OE1	1:A:190:GLN:HA	2.03	0.58
1:A:89:LEU:HD11	1:A:106:VAL:HG11	1.85	0.57
1:B:108:ASN:HD21	1:B:282:ALA:HB1	1.69	0.57
1:B:120:TYR:CD2	1:B:263:PHE:CD2	2.93	0.56
1:A:27:ASP:HA	1:A:30:LYS:HB2	1.88	0.56
1:A:221:TRP:CZ3	1:A:364:MSE:HE1	2.37	0.56
1:A:288:THR:CB	1:B:22:GLU:HG3	2.35	0.56
1:B:15:LYS:N	1:B:16:GLU:OE1	2.39	0.56
1:B:53:VAL:HG22	1:B:58:VAL:HG13	1.87	0.56
1:A:13:GLN:H	1:A:63:ASN:HD22	1.52	0.56
1:B:68:SER:O	1:B:68:SER:OG	2.23	0.56
1:A:6:VAL:HG11	1:A:291:HIS:HD2	1.58	0.56
1:A:76:LYS:O	1:A:76:LYS:HG3	2.05	0.56
1:B:24:ILE:HG21	1:B:302:MSE:CE	2.36	0.55
1:A:34:LYS:C	1:A:35:ILE:HG13	2.25	0.55
1:B:11:PHE:HD1	1:B:40:VAL:HG12	1.70	0.55
1:B:32:ASN:HB3	1:B:35:ILE:CD1	2.34	0.55
1:B:187:ARG:HD3	1:B:386:MSE:HE3	1.89	0.55
1:A:87:ASP:O	1:A:90:LYS:HB2	2.07	0.54
1:A:187:ARG:HD2	1:A:187:ARG:O	2.07	0.54
1:A:154:PHE:C	1:A:238:VAL:HG11	2.27	0.54
1:B:8:ILE:O	1:B:37:VAL:HA	2.07	0.54
1:B:71:LEU:O	1:B:72:GLN:C	2.46	0.54
1:B:28:PHE:O	1:B:32:ASN:ND2	2.40	0.54
1:A:294:GLU:O	1:A:297:ALA:HB3	2.07	0.54
1:A:380:ASN:O	1:A:384:ASN:HB2	2.08	0.54
1:A:291:HIS:CB	1:A:294:GLU:CD	2.75	0.53
1:B:230:ILE:HG23	1:B:251:ILE:HG13	1.90	0.53
1:B:289:THR:HG21	1:B:292:PRO:CA	2.39	0.53
1:B:201:MSE:O	1:B:201:MSE:SE	2.77	0.53
1:B:120:TYR:CD2	1:B:263:PHE:HD2	2.27	0.53
1:A:205:ILE:HD13	1:A:372:LYS:HG2	1.91	0.52
1:B:50:LYS:CA	1:B:74:TRP:HH2	2.21	0.52
1:B:285:ILE:HG23	1:B:295:ALA:HB1	1.92	0.52
1:A:192:ASN:N	1:A:384:ASN:HD21	2.03	0.52
1:A:275:THR:HG23	1:A:345:HIS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG22	1:B:58:VAL:CG2	2.36	0.52
1:B:136:TRP:HE1	1:B:174:THR:HB	1.75	0.52
1:B:384:ASN:N	1:B:384:ASN:HD22	2.08	0.52
1:A:121:ASN:ND2	1:A:124:LYS:HG2	2.25	0.51
1:A:6:VAL:CG1	1:A:7:THR:H	2.22	0.51
1:B:276:VAL:HG23	1:B:346:LEU:O	2.09	0.51
1:B:356:GLU:HG3	1:B:360:HIS:CE1	2.46	0.51
1:A:366:TYR:CB	1:A:375:MSE:CE	2.87	0.51
1:A:69:ILE:HD12	1:A:69:ILE:H	1.75	0.51
1:B:147:VAL:HG23	1:B:153:PRO:HG2	1.93	0.51
1:A:318:PRO:HA	1:A:326:GLN:HE22	1.76	0.51
1:B:69:ILE:O	1:B:72:GLN:HB2	2.11	0.51
1:B:239:LEU:O	1:B:240:MSE:HG3	2.11	0.51
1:A:121:ASN:HB3	1:A:124:LYS:HB2	1.93	0.50
1:A:161:ALA:HA	1:A:364:MSE:HG2	1.92	0.50
1:B:340:ALA:HA	1:B:345:HIS:ND1	2.27	0.50
1:A:169:GLN:HG2	1:A:349:LEU:HD12	1.94	0.50
1:A:53:VAL:HG11	1:A:74:TRP:CD2	2.46	0.50
1:B:136:TRP:HB2	1:B:137:ASP:OD1	2.12	0.50
1:B:289:THR:HG22	1:B:289:THR:O	2.11	0.50
1:B:345:HIS:O	1:B:345:HIS:CD2	2.65	0.50
1:A:387:LYS:HE2	1:A:387:LYS:C	2.24	0.49
1:A:6:VAL:CG2	1:A:291:HIS:CD2	2.88	0.49
1:B:221:TRP:HZ3	1:B:364:MSE:HE1	1.77	0.49
1:A:338:GLU:O	1:A:338:GLU:HG2	2.11	0.49
1:A:384:ASN:N	1:A:385:PRO:CD	2.76	0.49
1:B:162:TRP:O	1:B:165:ASN:HB2	2.12	0.49
1:B:308:MSE:HB3	1:B:324:VAL:HG21	1.95	0.49
1:A:25:THR:HG23	1:A:37:VAL:HB	1.95	0.48
1:A:276:VAL:HG22	1:A:277:GLY:H	1.76	0.48
1:A:283:TRP:HH2	1:A:302:MSE:CE	2.25	0.48
1:B:32:ASN:CB	1:B:35:ILE:HD12	2.35	0.48
1:A:111:PHE:HB2	1:A:281:LEU:O	2.13	0.48
1:B:181:GLU:OE1	1:B:181:GLU:N	2.38	0.48
1:A:283:TRP:CH2	1:A:302:MSE:CE	2.97	0.48
1:A:179:GLY:H	1:A:346:LEU:CD2	2.24	0.48
1:A:82:ASP:OD2	1:A:105:LYS:HG2	2.13	0.48
1:A:232:ALA:HB1	1:A:237:ASP:HB2	1.96	0.48
1:A:244:GLY:HA3	1:A:246:TRP:CZ2	2.48	0.48
1:B:221:TRP:CZ3	1:B:364:MSE:HE1	2.48	0.48
1:A:210:ILE:HA	1:A:213:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:MSE:HB2	1:B:366:TYR:CE2	2.49	0.48
1:A:113:ALA:O	1:A:318:PRO:HG2	2.15	0.47
1:B:72:GLN:HE21	1:B:72:GLN:CA	2.22	0.47
1:B:120:TYR:CD1	1:B:120:TYR:C	2.88	0.47
1:B:69:ILE:H	1:B:69:ILE:CD1	2.16	0.47
1:B:17:MSE:O	1:B:21:LEU:HD22	2.14	0.47
1:B:48:VAL:O	1:B:52:ARG:HG2	2.15	0.47
1:B:292:PRO:C	1:B:294:GLU:N	2.66	0.47
1:A:124:LYS:CG	1:A:239:LEU:CD2	2.81	0.47
1:A:264:MSE:HE3	1:A:275:THR:HG22	1.97	0.47
1:B:8:ILE:HG13	1:B:37:VAL:HG13	1.97	0.47
1:A:152:THR:CB	1:A:238:VAL:HG12	2.44	0.47
1:A:309:GLN:NE2	1:A:325:LYS:H	1.93	0.47
1:B:20:THR:O	1:B:21:LEU:C	2.53	0.47
1:B:120:TYR:HD2	1:B:263:PHE:CD2	2.32	0.47
1:B:260:ILE:HD13	1:B:332:PRO:HG3	1.97	0.47
1:B:248:ILE:HG23	1:B:249:THR:N	2.30	0.47
1:B:61:VAL:HG21	1:B:298:PHE:HD2	1.80	0.46
1:A:52:ARG:HB3	1:A:57:ASP:O	2.15	0.46
1:A:350:GLN:HA	1:A:353:TRP:CD2	2.51	0.46
1:B:11:PHE:HD1	1:B:40:VAL:CG1	2.28	0.46
1:B:31:GLU:O	1:B:33:PRO:HD3	2.15	0.46
1:B:204:ASP:O	1:B:208:MSE:HG2	2.16	0.46
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.81	0.46
1:B:6:VAL:CG2	1:B:7:THR:H	2.29	0.46
1:B:115:ALA:HA	1:B:276:VAL:O	2.16	0.46
1:B:277:GLY:O	1:B:347:VAL:HA	2.16	0.46
1:A:52:ARG:O	1:A:56:GLY:N	2.49	0.46
1:A:384:ASN:C	1:A:386:MSE:N	2.69	0.46
1:B:155:GLY:N	1:B:240:MSE:O	2.45	0.46
1:A:290:LYS:HB3	1:A:291:HIS:CE1	2.51	0.45
1:B:125:PHE:CD2	1:B:130:LEU:HB2	2.51	0.45
1:B:161:ALA:HB1	1:B:360:HIS:HB3	1.97	0.45
1:A:76:LYS:O	1:A:76:LYS:HG2	2.15	0.45
1:A:221:TRP:CG	1:A:222:GLU:N	2.85	0.45
1:A:338:GLU:O	1:A:338:GLU:HG3	2.17	0.45
1:B:187:ARG:NE	1:B:352:TYR:O	2.50	0.45
1:B:218:GLN:O	1:B:221:TRP:HD1	2.00	0.45
1:B:299:VAL:O	1:B:300:GLU:C	2.54	0.45
1:B:88:TYR:OH	1:B:296:ASN:OD1	2.28	0.45
1:A:127:GLU:HG2	1:A:127:GLU:H	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:OE1	1:A:294:GLU:N	2.48	0.44
1:A:134:GLU:O	1:A:135:THR:HG23	2.16	0.44
1:A:196:LEU:HG	1:A:196:LEU:O	2.16	0.44
1:A:244:GLY:HA3	1:A:246:TRP:CE2	2.53	0.44
1:B:114:ASN:O	1:B:277:GLY:HA3	2.18	0.44
1:A:34:LYS:O	1:A:35:ILE:CG1	2.63	0.44
1:A:88:TYR:CD2	1:A:300:GLU:HB2	2.53	0.44
1:B:352:TYR:O	1:B:353:TRP:HD1	2.01	0.44
1:A:126:GLU:OE2	1:A:126:GLU:HA	2.17	0.44
1:B:73:GLU:O	1:B:76:LYS:N	2.51	0.44
1:B:384:ASN:N	1:B:385:PRO:HD2	2.32	0.44
1:A:287:ALA:HB3	1:B:18:THR:HG21	2.00	0.44
1:A:157:ALA:N	1:A:229:VAL:HG21	2.33	0.43
1:A:290:LYS:O	1:A:291:HIS:C	2.57	0.43
1:A:354:THR:H	1:A:386:MSE:HE3	1.82	0.43
1:A:66:PRO:HB2	1:A:100:TYR:CD1	2.53	0.43
1:A:179:GLY:O	1:A:180:LYS:C	2.57	0.43
1:B:244:GLY:HA3	1:B:246:TRP:CH2	2.53	0.43
1:A:60:ASP:OD1	1:A:289:THR:OG1	2.28	0.43
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.81	0.43
1:A:364:MSE:HE3	1:A:367:VAL:HB	2.00	0.43
1:B:345:HIS:CD2	1:B:345:HIS:C	2.92	0.43
1:B:348:TRP:HB3	1:B:350:GLN:OE1	2.19	0.43
1:A:42:VAL:O	1:A:45:ALA:HB2	2.19	0.43
1:A:123:ASP:CG	1:A:258:PHE:HB2	2.39	0.43
1:A:203:ASP:O	1:A:206:LYS:HB3	2.17	0.43
1:A:384:ASN:C	1:A:386:MSE:H	2.21	0.43
1:A:11:PHE:CD2	1:A:49:LEU:HD13	2.54	0.43
1:A:65:TYR:O	1:A:68:SER:HB3	2.18	0.43
1:B:9:GLU:N	1:B:60:ASP:OD2	2.46	0.43
1:B:28:PHE:CE1	1:B:298:PHE:HA	2.54	0.43
1:A:99:LYS:HE2	1:A:343:ASP:OD1	2.18	0.43
1:A:308:MSE:O	1:A:309:GLN:C	2.57	0.42
1:A:25:THR:CG2	1:A:37:VAL:HB	2.50	0.42
1:A:119:TYR:OH	1:A:245:SER:HA	2.20	0.42
1:A:328:GLY:O	1:A:330:ASP:N	2.52	0.42
1:B:301:TYR:O	1:B:304:ARG:HG3	2.19	0.42
1:A:57:ASP:O	1:A:57:ASP:OD1	2.37	0.42
1:A:312:TYR:C	1:A:314:VAL:H	2.23	0.42
1:A:56:GLY:HA3	1:B:40:VAL:CG2	2.47	0.42
1:B:66:PRO:HB3	1:B:108:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PHE:HB2	1:A:301:TYR:CE2	2.54	0.42
1:A:276:VAL:CG2	1:A:277:GLY:N	2.81	0.42
1:B:180:LYS:HE2	1:B:184:GLN:OE1	2.20	0.42
1:B:111:PHE:HE2	1:B:283:TRP:HB2	1.85	0.42
1:B:244:GLY:HA3	1:B:246:TRP:CZ2	2.54	0.42
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.58	0.42
1:A:87:ASP:OD2	1:A:87:ASP:N	2.52	0.42
1:A:260:ILE:HB	1:A:332:PRO:HB3	2.01	0.42
1:A:283:TRP:CZ3	1:A:302:MSE:HG2	2.55	0.42
1:A:319:THR:HG23	1:A:319:THR:O	2.19	0.42
1:A:148:ALA:C	1:A:150:GLY:H	2.24	0.42
1:A:262:THR:HB	1:A:336:MSE:HB2	2.02	0.42
1:A:117:GLY:CA	1:A:336:MSE:HE2	2.49	0.42
1:A:249:THR:O	1:A:253:GLU:HG3	2.20	0.42
1:B:17:MSE:HE1	1:B:314:VAL:HG11	2.01	0.42
1:B:26:ARG:O	1:B:29:GLU:HB2	2.20	0.42
1:B:20:THR:O	1:B:22:GLU:N	2.54	0.41
1:A:295:ALA:O	1:A:296:ASN:C	2.56	0.41
1:B:308:MSE:HE2	1:B:319:THR:CB	2.50	0.41
1:A:288:THR:HA	1:B:22:GLU:HG3	2.03	0.41
1:B:49:LEU:HG	1:B:74:TRP:CZ3	2.55	0.41
1:B:76:LYS:HE2	1:B:76:LYS:HB2	1.89	0.41
1:B:102:VAL:HG23	1:B:107:TYR:HD2	1.86	0.41
1:B:231:GLY:HA2	1:B:254:GLN:OE1	2.20	0.41
1:A:65:TYR:HA	1:A:66:PRO:HD2	1.84	0.41
1:B:29:GLU:C	1:B:31:GLU:N	2.74	0.41
1:A:117:GLY:C	1:A:118:ILE:HG12	2.41	0.41
1:B:99:LYS:H	1:B:99:LYS:HG2	1.55	0.41
1:A:173:ALA:CB	1:A:346:LEU:HD11	2.51	0.41
1:A:65:TYR:O	1:A:68:SER:CB	2.68	0.41
1:A:102:VAL:HG12	1:A:103:ASN:N	2.36	0.41
1:A:153:PRO:O	1:A:240:MSE:HB2	2.21	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.62	0.41
1:A:213:ILE:O	1:A:216:SER:OG	2.39	0.41
1:B:17:MSE:HE1	1:B:314:VAL:CG1	2.51	0.41
1:B:347:VAL:HG12	1:B:348:TRP:O	2.20	0.41
1:A:83:LEU:O	1:A:89:LEU:HD13	2.20	0.41
1:B:50:LYS:HA	1:B:74:TRP:CZ2	2.56	0.41
1:B:53:VAL:CG2	1:B:58:VAL:HG13	2.51	0.41
1:A:288:THR:CA	1:B:22:GLU:HG3	2.51	0.40
1:B:187:ARG:CD	1:B:187:ARG:C	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LYS:HB2	1:B:259:LYS:O	2.21	0.40
1:B:147:VAL:CG2	1:B:153:PRO:HG2	2.52	0.40
1:B:347:VAL:HG12	1:B:348:TRP:N	2.35	0.40
1:A:152:THR:O	1:A:238:VAL:HG12	2.22	0.40
1:A:146:ILE:O	1:A:147:VAL:C	2.57	0.40
1:B:11:PHE:CD1	1:B:40:VAL:CG1	3.00	0.40
1:A:152:THR:HB	1:A:238:VAL:HG13	2.00	0.40
1:A:203:ASP:O	1:A:204:ASP:C	2.56	0.40
1:A:253:GLU:C	1:A:255:LYS:N	2.75	0.40
1:B:218:GLN:O	1:B:221:TRP:CD1	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/409 (93%)	339 (89%)	41 (11%)	1 (0%)	41	71
1	B	379/409 (93%)	325 (86%)	53 (14%)	1 (0%)	41	71
All	All	760/818 (93%)	664 (87%)	94 (12%)	2 (0%)	41	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LYS
1	B	55	ALA

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	320/330 (97%)	280 (88%)	40 (12%)	4 14
1	B	318/330 (96%)	261 (82%)	57 (18%)	2 5
All	All	638/660 (97%)	541 (85%)	97 (15%)	3 8

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	16	GLU
1	A	19	LYS
1	A	20	THR
1	A	21	LEU
1	A	23	GLU
1	A	26	ARG
1	A	30	LYS
1	A	31	GLU
1	A	54	LEU
1	A	69	ILE
1	A	76	LYS
1	A	83	LEU
1	A	87	ASP
1	A	124	LYS
1	A	126	GLU
1	A	127	GLU
1	A	131	LYS
1	A	134	GLU
1	A	139	PHE
1	A	147	VAL
1	A	151	GLN
1	A	180	LYS
1	A	212	ARG
1	A	216	SER
1	A	217	LYS
1	A	222	GLU
1	A	227	THR
1	A	237	ASP
1	A	238	VAL
1	A	257	ASN
1	A	268	LYS
1	A	290	LYS

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Mol	Chain	Res	Type
1	A	291	HIS
1	A	329	GLU
1	A	330	ASP
1	A	361	THR
1	A	384	ASN
1	A	386	MSE
1	A	387	LYS
1	B	6	VAL
1	B	7	THR
1	B	8	ILE
1	B	14	LYS
1	B	15	LYS
1	B	17	MSE
1	B	21	LEU
1	B	22	GLU
1	B	23	GLU
1	B	25	THR
1	B	30	LYS
1	B	32	ASN
1	B	35	ILE
1	B	37	VAL
1	B	50	LYS
1	B	54	LEU
1	B	64	ILE
1	B	69	ILE
1	B	71	LEU
1	B	72	GLN
1	B	98	GLU
1	B	99	LYS
1	B	102	VAL
1	B	120	TYR
1	B	126	GLU
1	B	139	PHE
1	B	142	LEU
1	B	145	ASP
1	B	152	THR
1	B	180	LYS
1	B	195	LYS
1	B	196	LEU
1	B	201	MSE
1	B	212	ARG
1	B	235	ARG

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Mol	Chain	Res	Type
1	B	237	ASP
1	B	241	THR
1	B	243	ASN
1	B	257	ASN
1	B	260	ILE
1	B	265	ILE
1	B	273	SER
1	B	285	ILE
1	B	286	SER
1	B	289	THR
1	B	319	THR
1	B	322	GLU
1	B	325	LYS
1	B	329	GLU
1	B	330	ASP
1	B	343	ASP
1	B	346	LEU
1	B	358	ASP
1	B	372	LYS
1	B	375	MSE
1	B	376	VAL
1	B	386	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	63	ASN
1	A	72	GLN
1	A	141	GLN
1	A	151	GLN
1	A	257	ASN
1	A	291	HIS
1	A	309	GLN
1	A	326	GLN
1	A	380	ASN
1	A	384	ASN
1	B	32	ASN
1	B	63	ASN
1	B	72	GLN
1	B	220	ASN
1	B	309	GLN

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Mol	Chain	Res	Type
1	B	326	GLN
1	B	380	ASN
1	B	384	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	372/409 (90%)	-0.22	2 (0%)	91	91	20, 67, 112, 160	19 (5%)
1	B	350/409 (85%)	0.73	59 (16%)	1	1	68, 121, 206, 241	51 (14%)
All	All	722/818 (88%)	0.24	61 (8%)	11	8	20, 88, 194, 241	70 (9%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	ALA	5.7
1	B	383	PHE	5.4
1	B	381	ALA	5.2
1	B	265	ILE	4.8
1	B	382	PHE	4.8
1	B	197	SER	4.7
1	B	365	ASN	4.7
1	B	159	ALA	4.6
1	B	221	TRP	4.4
1	B	169	GLN	4.1
1	B	74	TRP	3.8
1	B	129	GLY	3.8
1	A	33	PRO	3.7
1	B	33	PRO	3.6
1	B	145	ASP	3.5
1	B	199	PRO	3.4
1	B	291	HIS	3.4
1	B	183	ASN	3.3
1	B	226	TYR	3.3
1	B	271	GLY	3.2
1	B	166	GLY	3.0
1	B	269	GLU	2.9
1	B	170	LEU	2.9
1	B	220	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	127	GLU	2.8
1	B	160	ASP	2.7
1	B	224	ALA	2.7
1	B	198	ASP	2.7
1	B	184	GLN	2.7
1	B	158	GLY	2.6
1	B	187	ARG	2.6
1	B	179	GLY	2.6
1	B	177	GLY	2.6
1	A	40	VAL	2.6
1	B	6	VAL	2.6
1	B	354	THR	2.5
1	B	352	TYR	2.5
1	B	128	LEU	2.5
1	B	275	THR	2.5
1	B	286	SER	2.5
1	B	161	ALA	2.4
1	B	7	THR	2.3
1	B	270	LYS	2.3
1	B	168	ASN	2.3
1	B	228	ASP	2.3
1	B	272	GLN	2.2
1	B	130	LEU	2.2
1	B	225	GLY	2.2
1	B	104	GLU	2.2
1	B	155	GLY	2.2
1	B	361	THR	2.2
1	B	276	VAL	2.1
1	B	31	GLU	2.1
1	B	122	LYS	2.1
1	B	141	GLN	2.1
1	B	217	LYS	2.1
1	B	357	ALA	2.1
1	B	277	GLY	2.1
1	B	103	ASN	2.1
1	B	106	VAL	2.0
1	B	49	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	401	1/1	0.97	0.24	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.