



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:39 am GMT

PDB ID : 3WCB  
Title : The complex structure of TcSQS with ligand, BPH1237  
Authors : Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Ren, F.; Zheng, Y.;  
Zhu, Z.; Chen, C.C.; Guo, R.T.  
Deposited on : 2013-05-27  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

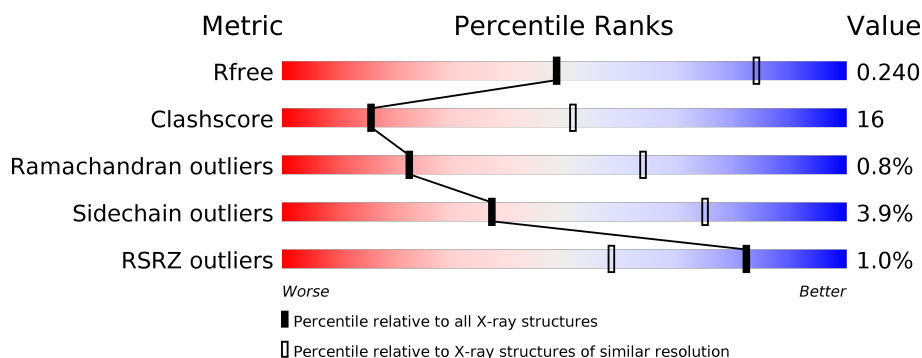
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	365	
1	B	365	
1	C	365	
1	D	365	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11273 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 Farnesyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2753	1746	473	512	22			
1	B	341	Total	C	N	O	S	0	0	0
			2753	1746	473	512	22			
1	C	341	Total	C	N	O	S	0	0	0
			2753	1746	473	512	22			
1	D	341	Total	C	N	O	S	0	0	0
			2754	1746	473	513	22			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q4CWB4
A	5	GLY	-	EXPRESSION TAG	UNP Q4CWB4
A	6	SER	-	EXPRESSION TAG	UNP Q4CWB4
A	7	SER	-	EXPRESSION TAG	UNP Q4CWB4
A	8	HIS	-	EXPRESSION TAG	UNP Q4CWB4
A	9	HIS	-	EXPRESSION TAG	UNP Q4CWB4
A	10	HIS	-	EXPRESSION TAG	UNP Q4CWB4
A	11	HIS	-	EXPRESSION TAG	UNP Q4CWB4
A	12	HIS	-	EXPRESSION TAG	UNP Q4CWB4
A	13	HIS	-	EXPRESSION TAG	UNP Q4CWB4
A	14	SER	-	EXPRESSION TAG	UNP Q4CWB4
A	15	SER	-	EXPRESSION TAG	UNP Q4CWB4
A	16	GLY	-	EXPRESSION TAG	UNP Q4CWB4
A	17	LEU	-	EXPRESSION TAG	UNP Q4CWB4
A	18	VAL	-	EXPRESSION TAG	UNP Q4CWB4
A	19	PRO	-	EXPRESSION TAG	UNP Q4CWB4
A	20	ARG	-	EXPRESSION TAG	UNP Q4CWB4
A	21	GLY	-	EXPRESSION TAG	UNP Q4CWB4
A	22	SER	-	EXPRESSION TAG	UNP Q4CWB4
A	23	HIS	-	EXPRESSION TAG	UNP Q4CWB4
A	24	MET	-	EXPRESSION TAG	UNP Q4CWB4

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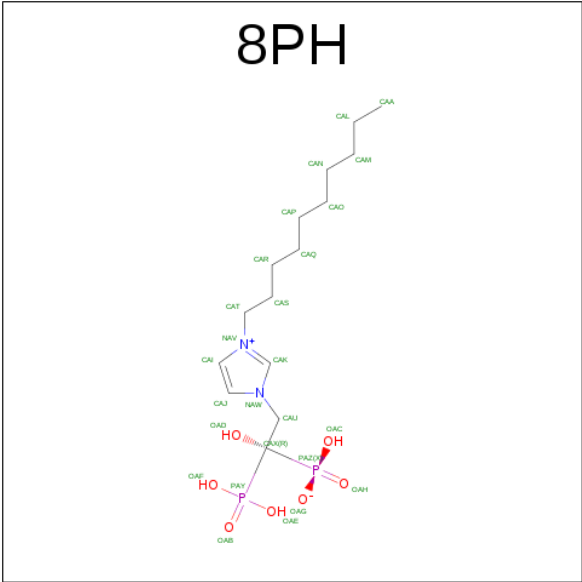
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
A	281	THR	ALA	CONFLICT	UNP Q4CWB4
B	4	MET	-	EXPRESSION TAG	UNP Q4CWB4
B	5	GLY	-	EXPRESSION TAG	UNP Q4CWB4
B	6	SER	-	EXPRESSION TAG	UNP Q4CWB4
B	7	SER	-	EXPRESSION TAG	UNP Q4CWB4
B	8	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	9	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	10	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	11	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	12	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	13	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	14	SER	-	EXPRESSION TAG	UNP Q4CWB4
B	15	SER	-	EXPRESSION TAG	UNP Q4CWB4
B	16	GLY	-	EXPRESSION TAG	UNP Q4CWB4
B	17	LEU	-	EXPRESSION TAG	UNP Q4CWB4
B	18	VAL	-	EXPRESSION TAG	UNP Q4CWB4
B	19	PRO	-	EXPRESSION TAG	UNP Q4CWB4
B	20	ARG	-	EXPRESSION TAG	UNP Q4CWB4
B	21	GLY	-	EXPRESSION TAG	UNP Q4CWB4
B	22	SER	-	EXPRESSION TAG	UNP Q4CWB4
B	23	HIS	-	EXPRESSION TAG	UNP Q4CWB4
B	24	MET	-	EXPRESSION TAG	UNP Q4CWB4
B	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
B	281	THR	ALA	CONFLICT	UNP Q4CWB4
C	4	MET	-	EXPRESSION TAG	UNP Q4CWB4
C	5	GLY	-	EXPRESSION TAG	UNP Q4CWB4
C	6	SER	-	EXPRESSION TAG	UNP Q4CWB4
C	7	SER	-	EXPRESSION TAG	UNP Q4CWB4
C	8	HIS	-	EXPRESSION TAG	UNP Q4CWB4
C	9	HIS	-	EXPRESSION TAG	UNP Q4CWB4
C	10	HIS	-	EXPRESSION TAG	UNP Q4CWB4
C	11	HIS	-	EXPRESSION TAG	UNP Q4CWB4
C	12	HIS	-	EXPRESSION TAG	UNP Q4CWB4
C	13	HIS	-	EXPRESSION TAG	UNP Q4CWB4
C	14	SER	-	EXPRESSION TAG	UNP Q4CWB4
C	15	SER	-	EXPRESSION TAG	UNP Q4CWB4
C	16	GLY	-	EXPRESSION TAG	UNP Q4CWB4
C	17	LEU	-	EXPRESSION TAG	UNP Q4CWB4
C	18	VAL	-	EXPRESSION TAG	UNP Q4CWB4
C	19	PRO	-	EXPRESSION TAG	UNP Q4CWB4
C	20	ARG	-	EXPRESSION TAG	UNP Q4CWB4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	GLY	-	EXPRESSION TAG	UNP Q4CWB4
C	22	SER	-	EXPRESSION TAG	UNP Q4CWB4
C	23	HIS	-	EXPRESSION TAG	UNP Q4CWB4
C	24	MET	-	EXPRESSION TAG	UNP Q4CWB4
C	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
C	281	THR	ALA	CONFLICT	UNP Q4CWB4
D	4	MET	-	EXPRESSION TAG	UNP Q4CWB4
D	5	GLY	-	EXPRESSION TAG	UNP Q4CWB4
D	6	SER	-	EXPRESSION TAG	UNP Q4CWB4
D	7	SER	-	EXPRESSION TAG	UNP Q4CWB4
D	8	HIS	-	EXPRESSION TAG	UNP Q4CWB4
D	9	HIS	-	EXPRESSION TAG	UNP Q4CWB4
D	10	HIS	-	EXPRESSION TAG	UNP Q4CWB4
D	11	HIS	-	EXPRESSION TAG	UNP Q4CWB4
D	12	HIS	-	EXPRESSION TAG	UNP Q4CWB4
D	13	HIS	-	EXPRESSION TAG	UNP Q4CWB4
D	14	SER	-	EXPRESSION TAG	UNP Q4CWB4
D	15	SER	-	EXPRESSION TAG	UNP Q4CWB4
D	16	GLY	-	EXPRESSION TAG	UNP Q4CWB4
D	17	LEU	-	EXPRESSION TAG	UNP Q4CWB4
D	18	VAL	-	EXPRESSION TAG	UNP Q4CWB4
D	19	PRO	-	EXPRESSION TAG	UNP Q4CWB4
D	20	ARG	-	EXPRESSION TAG	UNP Q4CWB4
D	21	GLY	-	EXPRESSION TAG	UNP Q4CWB4
D	22	SER	-	EXPRESSION TAG	UNP Q4CWB4
D	23	HIS	-	EXPRESSION TAG	UNP Q4CWB4
D	24	MET	-	EXPRESSION TAG	UNP Q4CWB4
D	82	GLU	ASP	ENGINEERED MUTATION	UNP Q4CWB4
D	281	THR	ALA	CONFLICT	UNP Q4CWB4

- Molecule 2 is HYDROGEN [(1R)-2-(3-DECYL-1H-IMIDAZOL-3-IUM-1-YL)-1-HYDROXY-1-PHOSPHONOETHYL]PHOSPHONATE (three-letter code: 8PH) (formula: C<sub>15</sub>H<sub>30</sub>N<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	15	2	7	2		
2	B	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	C	1	Total	C	O	P		0	0
			11	2	7	2			
2	D	1	Total	C	O	P		0	0
			11	2	7	2			

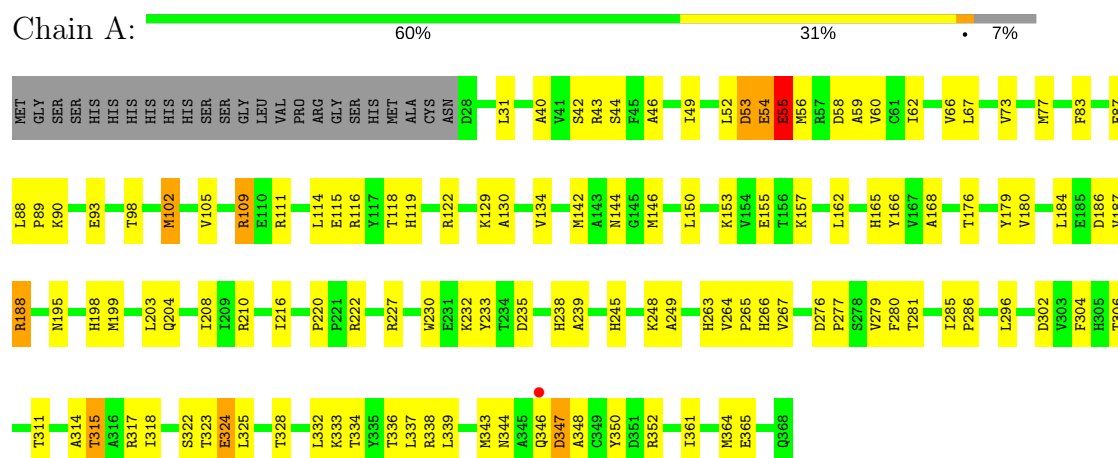
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	43	Total	O	0	0
			43	43		
3	C	47	Total	O	0	0
			47	47		
3	D	44	Total	O	0	0
			44	44		

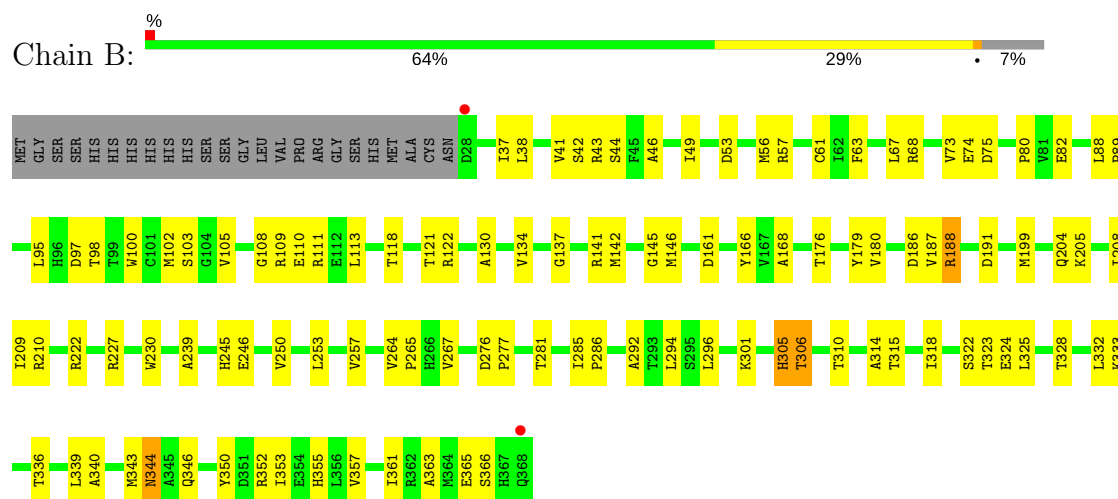
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

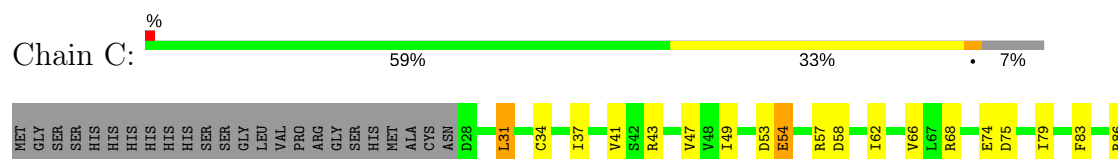
- Molecule 1: Farnesyltransferase, putative

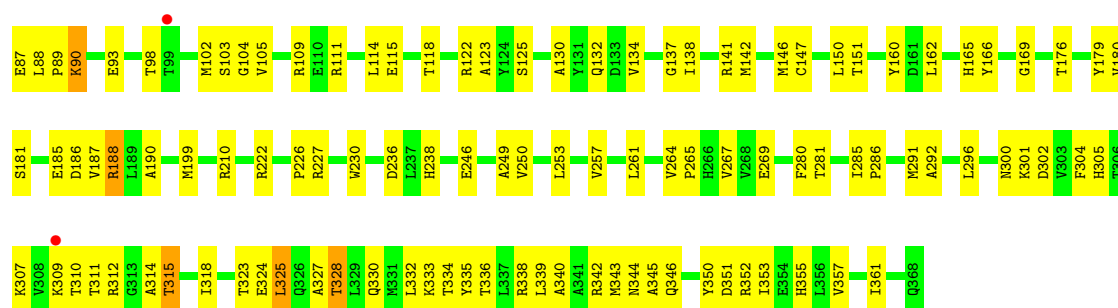


- Molecule 1: Farnesyltransferase, putative

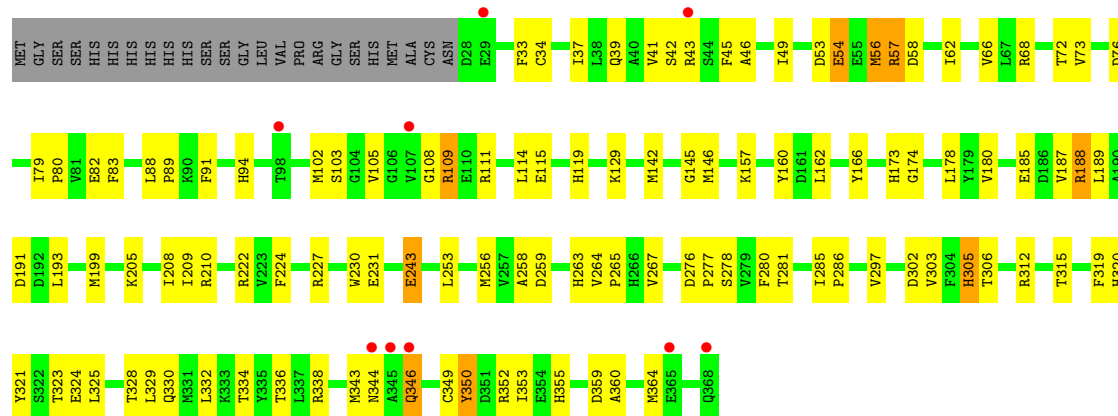


- Molecule 1: Farnesyltransferase, putative





• Molecule 1: Farnesyltransferase, putative





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.39Å 127.69Å 142.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 24.88 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-3.00) 93.0 (24.88-2.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.99Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.198 , 0.252 0.222 , 0.240	Depositor DCC
$R_{free}$ test set	1349 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.5	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 8PH

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	0.28	0/2811	0.55	2/3809 (0.1%)
1	B	0.25	0/2811	0.46	0/3809
1	C	0.25	0/2811	0.47	0/3809
1	D	0.24	0/2812	0.47	0/3809
All	All	0.25	0/11245	0.49	2/15236 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ASP	N-CA-C	8.28	133.34	111.00
1	A	347	ASP	N-CA-C	6.49	128.52	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2753	0	2700	116	0
1	B	2753	0	2700	70	0
1	C	2753	0	2700	95	0
1	D	2754	0	2700	86	0
2	A	26	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	9	3	0
2	C	11	0	4	0	0
2	D	11	0	4	2	0
3	A	62	0	0	0	0
3	B	43	0	0	0	0
3	C	47	0	0	1	0
3	D	44	0	0	1	0
All	All	11273	0	10847	359	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 16.

All (359) 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:281:THR:HG22	1:A:323:THR:HA	1.41	1.02
1:C:344:ASN:HB2	1:C:346:GLN:HE21	1.24	0.99
1:A:322:SER:HA	1:A:328:THR:HG22	1.47	0.96
1:B:322:SER:HA	1:B:328:THR:HG22	1.48	0.95
1:B:344:ASN:HB2	1:B:346:GLN:HG2	1.52	0.90
1:A:346:GLN:HG3	1:A:347:ASP:H	1.38	0.89
1:A:43:ARG:HB2	1:A:43:ARG:HH21	1.39	0.88
1:A:346:GLN:HG3	1:A:347:ASP:N	1.87	0.88
1:D:281:THR:HG22	1:D:323:THR:HA	1.57	0.86
1:C:104:GLY:HA2	1:C:111:ARG:HE	1.38	0.86
1:B:80:PRO:HB2	1:B:82:GLU:OE2	1.76	0.86
1:C:281:THR:HG22	1:C:323:THR:HA	1.59	0.85
1:C:43:ARG:HB2	1:C:43:ARG:NH2	1.91	0.85
1:A:314:ALA:HA	1:A:317:ARG:HH12	1.42	0.84
1:B:281:THR:HG22	1:B:323:THR:HA	1.61	0.80
1:D:42:SER:HB2	2:D:401:8PH:OAC	1.81	0.80
1:A:352:ARG:HD2	1:C:345:ALA:HB1	1.64	0.80
1:D:43:ARG:HB2	1:D:43:ARG:NH2	1.97	0.79
1:A:54:GLU:O	1:A:55:GLU:HB2	1.83	0.79
1:C:343:MET:HE1	1:C:350:TYR:HA	1.62	0.78
1:C:333:LYS:HE2	1:C:361:ILE:HG23	1.66	0.77
1:C:49:ILE:HG12	1:C:57:ARG:HG3	1.66	0.77
1:A:43:ARG:HB2	1:A:43:ARG:NH2	1.99	0.77
1:B:333:LYS:HE2	1:B:361:ILE:HG23	1.68	0.76
1:B:343:MET:HE1	1:B:350:TYR:HA	1.68	0.76
1:B:285:ILE:HB	1:B:286:PRO:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:OD2	1:A:188:ARG:HB2	1.86	0.75
1:C:104:GLY:HA2	1:C:111:ARG:NE	2.01	0.75
1:A:53:ASP:O	1:A:54:GLU:HB3	1.85	0.74
1:A:56:MET:O	1:A:60:VAL:HG23	1.88	0.73
1:C:43:ARG:HB2	1:C:43:ARG:HH21	1.53	0.72
1:A:102:MET:HE3	1:A:105:VAL:HG21	1.71	0.72
1:D:180:VAL:HG13	1:D:187:VAL:HA	1.72	0.71
1:D:264:VAL:HB	1:D:265:PRO:HD3	1.72	0.71
1:A:203:LEU:HD12	2:A:401:8PH:H22	1.72	0.71
1:D:285:ILE:HB	1:D:286:PRO:HD3	1.74	0.70
1:A:285:ILE:HB	1:A:286:PRO:HD3	1.73	0.69
1:A:116:ARG:HH21	1:A:119:HIS:HE1	1.40	0.69
1:C:343:MET:CE	1:C:350:TYR:HA	2.21	0.69
1:D:280:PHE:HZ	1:D:328:THR:HG21	1.57	0.69
1:D:227:ARG:HA	1:D:230:TRP:NE1	2.07	0.69
1:B:118:THR:HG22	1:B:122:ARG:HE	1.58	0.69
1:B:37:ILE:O	1:B:41:VAL:HG23	1.93	0.69
1:C:118:THR:O	1:C:122:ARG:HG2	1.94	0.68
1:B:361:ILE:O	1:B:365:GLU:HG3	1.93	0.68
1:C:227:ARG:HA	1:C:230:TRP:NE1	2.09	0.68
1:C:285:ILE:HB	1:C:286:PRO:HD3	1.76	0.67
1:B:88:LEU:HB2	1:B:89:PRO:HD3	1.75	0.67
1:D:199:MET:SD	1:D:267:VAL:HG13	2.35	0.67
1:B:102:MET:HE3	1:B:105:VAL:HG21	1.76	0.67
1:D:43:ARG:HH21	1:D:43:ARG:HB2	1.58	0.66
1:D:88:LEU:HB2	1:D:89:PRO:HD3	1.76	0.66
1:C:280:PHE:CZ	1:C:328:THR:HG21	2.31	0.66
1:A:53:ASP:O	1:A:54:GLU:CB	2.44	0.65
1:A:264:VAL:HB	1:A:265:PRO:HD3	1.78	0.65
1:C:103:SER:O	1:C:105:VAL:HG23	1.97	0.65
1:A:142:MET:O	1:A:146:MET:HG3	1.97	0.65
1:A:352:ARG:HD2	1:C:345:ALA:CB	2.26	0.65
1:D:34:CYS:O	1:D:37:ILE:HG22	1.96	0.65
1:B:186:ASP:OD2	1:B:188:ARG:HB2	1.97	0.65
1:A:344:ASN:HB2	1:A:346:GLN:HG2	1.79	0.64
1:A:232:LYS:HG2	1:C:355:HIS:HB2	1.79	0.64
1:C:344:ASN:CB	1:C:346:GLN:HE21	2.05	0.64
1:A:142:MET:HG3	1:A:166:TYR:O	1.98	0.64
1:B:42:SER:HB2	2:B:401:8PH:OAE	1.98	0.63
1:C:62:ILE:O	1:C:66:VAL:HG23	1.99	0.63
1:D:102:MET:CE	1:D:105:VAL:HG21	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ALA:O	1:C:296:LEU:HD13	1.98	0.63
1:A:98:THR:O	1:A:118:THR:HG23	1.99	0.63
1:A:58:ASP:O	1:A:62:ILE:HG12	1.98	0.63
1:B:264:VAL:HB	1:B:265:PRO:HD3	1.79	0.63
1:C:142:MET:O	1:C:146:MET:HG3	1.99	0.62
1:D:343:MET:HE1	1:D:350:TYR:HA	1.81	0.62
1:C:325:LEU:O	1:C:328:THR:HG23	2.00	0.62
1:B:102:MET:CE	1:B:105:VAL:HG21	2.29	0.62
1:A:93:GLU:OE1	1:B:141:ARG:HD2	1.99	0.61
1:A:73:VAL:HG22	1:A:102:MET:HE1	1.81	0.61
1:B:41:VAL:HG12	1:B:68:ARG:NH1	2.16	0.61
1:D:142:MET:HG3	1:D:166:TYR:O	2.00	0.61
1:D:142:MET:O	1:D:146:MET:HG3	2.00	0.61
1:A:56:MET:CE	1:A:179:TYR:CD1	2.84	0.61
1:A:227:ARG:HA	1:A:230:TRP:NE1	2.15	0.61
1:A:52:LEU:CD1	1:A:60:VAL:HG21	2.31	0.60
1:A:54:GLU:O	1:A:55:GLU:CB	2.49	0.60
1:B:137:GLY:O	1:B:141:ARG:HG3	2.01	0.60
1:C:58:ASP:O	1:C:62:ILE:HG12	2.00	0.60
1:D:344:ASN:HB2	1:D:346:GLN:HG3	1.83	0.60
1:D:360:ALA:O	1:D:364:MET:HG3	2.02	0.60
1:B:246:GLU:OE2	1:B:301:LYS:HD2	2.03	0.59
1:B:305:HIS:O	1:B:306:THR:HG22	2.02	0.59
1:B:142:MET:O	1:B:146:MET:HG3	2.01	0.59
1:C:353:ILE:O	1:C:357:VAL:HG23	2.02	0.59
1:A:324:GLU:O	1:A:328:THR:HG23	2.03	0.59
1:C:142:MET:HG3	1:C:166:TYR:O	2.03	0.59
1:A:56:MET:HE2	1:A:179:TYR:CD1	2.37	0.58
1:D:280:PHE:CZ	1:D:328:THR:HG21	2.37	0.58
1:C:179:TYR:HB3	1:C:185:GLU:CG	2.34	0.58
1:B:305:HIS:C	1:B:306:THR:HG22	2.24	0.58
1:C:300:ASN:HB2	1:C:342:ARG:NH2	2.19	0.58
1:C:88:LEU:HB2	1:C:89:PRO:HD3	1.85	0.58
1:D:102:MET:HE2	1:D:114:LEU:HD13	1.86	0.58
1:C:280:PHE:HZ	1:C:328:THR:HG21	1.69	0.58
1:A:77:MET:HG2	1:A:222:ARG:NH2	2.19	0.57
1:A:332:LEU:O	1:A:336:THR:HG23	2.04	0.57
1:C:180:VAL:HG13	1:C:187:VAL:HA	1.85	0.57
1:C:264:VAL:HB	1:C:265:PRO:HD3	1.84	0.57
1:A:42:SER:HB2	2:A:401:8PH:OAE	2.04	0.57
1:D:103:SER:HA	1:D:115:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ILE:O	1:D:66:VAL:HG23	2.03	0.57
1:A:334:THR:O	1:A:338:ARG:HG2	2.03	0.57
1:A:56:MET:CE	1:A:179:TYR:HD1	2.17	0.57
1:C:332:LEU:O	1:C:336:THR:HG23	2.04	0.57
1:B:142:MET:HG3	1:B:166:TYR:O	2.04	0.57
1:B:324:GLU:O	1:B:328:THR:HG23	2.05	0.57
1:C:179:TYR:HB3	1:C:185:GLU:HG3	1.86	0.57
1:C:300:ASN:HD21	1:C:302:ASP:HB2	1.69	0.57
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.87	0.56
1:C:246:GLU:CD	1:C:301:LYS:HD2	2.26	0.56
1:C:344:ASN:HB2	1:C:346:GLN:NE2	2.07	0.56
1:A:89:PRO:HB3	1:A:144:ASN:HD21	1.70	0.56
1:C:188:ARG:HA	1:C:188:ARG:HE	1.70	0.56
1:C:307:LYS:HD3	1:C:309:LYS:HE3	1.88	0.56
1:B:44:SER:HB2	2:B:401:8PH:OAF	2.06	0.56
1:A:179:TYR:CE1	1:A:279:VAL:HG13	2.40	0.56
1:C:246:GLU:OE2	1:C:301:LYS:HD2	2.06	0.56
1:C:79:ILE:HD11	1:C:105:VAL:HG13	1.87	0.56
1:B:332:LEU:O	1:B:336:THR:HG23	2.06	0.56
1:D:56:MET:HE1	1:D:178:LEU:O	2.06	0.56
1:A:87:GLU:OE1	1:A:90:LYS:HD2	2.06	0.55
1:A:49:ILE:O	1:A:52:LEU:HB2	2.07	0.55
1:B:353:ILE:O	1:B:357:VAL:HG23	2.06	0.55
1:A:311:THR:O	1:A:315:THR:HG22	2.07	0.55
1:A:62:ILE:O	1:A:66:VAL:HG23	2.07	0.55
1:B:343:MET:CE	1:B:350:TYR:HA	2.36	0.55
1:C:98:THR:O	1:C:118:THR:HG23	2.08	0.54
1:D:42:SER:O	1:D:46:ALA:HB2	2.07	0.54
1:A:343:MET:CE	1:A:350:TYR:HA	2.37	0.54
1:A:44:SER:HB2	2:A:401:8PH:OAF	2.07	0.54
1:B:352:ARG:HH11	1:B:352:ARG:HG2	1.71	0.54
1:D:324:GLU:O	1:D:328:THR:HG22	2.07	0.54
1:B:239:ALA:HB1	1:B:245:HIS:CD2	2.41	0.54
1:A:54:GLU:O	1:A:54:GLU:CG	2.54	0.54
1:C:300:ASN:ND2	1:C:302:ASP:HB2	2.22	0.54
1:D:43:ARG:HG2	3:D:541:HOH:O	2.07	0.54
1:A:361:ILE:O	1:A:365:GLU:HG3	2.08	0.54
1:B:180:VAL:HG13	1:B:187:VAL:HA	1.90	0.54
1:B:204:GLN:O	1:B:208:ILE:HG13	2.08	0.53
1:A:204:GLN:O	1:A:208:ILE:HG13	2.08	0.53
1:A:83:PHE:CZ	1:A:87:GLU:HG3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:O	1:C:41:VAL:HG23	2.08	0.53
1:D:227:ARG:HA	1:D:230:TRP:CE2	2.43	0.53
1:D:76:ASP:OD1	1:D:79:ILE:HG13	2.08	0.53
1:A:40:ALA:HB1	1:A:109:ARG:HG2	1.90	0.53
1:A:46:ALA:O	1:A:49:ILE:HG22	2.09	0.53
1:B:292:ALA:O	1:B:296:LEU:HD13	2.08	0.53
1:D:343:MET:CE	1:D:350:TYR:HA	2.37	0.53
1:A:322:SER:CA	1:A:328:THR:HG22	2.32	0.53
1:A:102:MET:CE	1:A:105:VAL:HG21	2.39	0.53
1:D:243:GLU:O	1:D:243:GLU:HG3	2.08	0.53
1:A:56:MET:HE2	1:A:179:TYR:CE1	2.44	0.52
1:C:227:ARG:HA	1:C:230:TRP:CD1	2.44	0.52
1:B:43:ARG:HB2	1:B:43:ARG:CZ	2.40	0.52
1:C:90:LYS:HE3	1:C:93:GLU:OE2	2.10	0.52
1:D:37:ILE:O	1:D:41:VAL:HG23	2.10	0.52
1:A:54:GLU:O	1:A:54:GLU:HG3	2.10	0.52
1:C:125:SER:HA	1:C:132:GLN:NE2	2.24	0.52
1:D:188:ARG:HG3	1:D:191:ASP:OD2	2.09	0.52
1:C:162:LEU:HG	1:C:166:TYR:CE2	2.45	0.52
1:A:222:ARG:HG3	1:A:222:ARG:HH11	1.75	0.51
1:C:334:THR:O	1:C:338:ARG:HG2	2.10	0.51
1:C:186:ASP:OD2	1:C:188:ARG:HB2	2.10	0.51
1:D:174:GLY:O	1:D:178:LEU:HG	2.11	0.51
1:B:210:ARG:HD2	1:B:210:ARG:C	2.31	0.51
1:C:176:THR:HA	1:C:179:TYR:CD2	2.45	0.51
1:D:222:ARG:HG3	1:D:222:ARG:HH11	1.75	0.51
1:D:334:THR:O	1:D:338:ARG:HG2	2.11	0.51
1:D:210:ARG:C	1:D:210:ARG:HD2	2.31	0.51
1:C:34:CYS:O	1:C:37:ILE:HG22	2.11	0.51
1:A:43:ARG:CB	1:A:43:ARG:HH21	2.17	0.51
1:B:227:ARG:HA	1:B:230:TRP:NE1	2.26	0.51
1:D:312:ARG:HA	1:D:315:THR:HG22	1.93	0.51
1:C:31:LEU:HD12	1:C:123:ALA:HB1	1.93	0.50
1:D:80:PRO:HG2	1:D:83:PHE:HB2	1.93	0.50
1:A:180:VAL:HG13	1:A:187:VAL:HA	1.92	0.50
1:D:73:VAL:HG22	1:D:102:MET:HE3	1.94	0.50
1:A:111:ARG:HG2	1:A:115:GLU:OE2	2.11	0.50
1:A:56:MET:HE1	1:A:179:TYR:CD1	2.45	0.50
1:B:205:LYS:O	1:B:209:ILE:HG13	2.11	0.50
1:D:49:ILE:O	1:D:57:ARG:HD2	2.11	0.50
1:B:246:GLU:O	1:B:250:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:HE1	1:A:179:TYR:HD1	1.76	0.50
1:D:102:MET:HG2	1:D:105:VAL:HG21	1.94	0.50
1:D:332:LEU:O	1:D:336:THR:HG23	2.12	0.50
1:A:102:MET:HB3	1:A:114:LEU:HB3	1.94	0.49
1:C:122:ARG:HG3	1:C:122:ARG:HH11	1.77	0.49
1:A:232:LYS:HE3	1:C:351:ASP:O	2.13	0.49
1:C:83:PHE:HD1	1:C:86:ARG:HH12	1.59	0.49
1:D:68:ARG:NH1	2:D:401:8PH:OAH	2.46	0.49
1:C:253:LEU:O	1:C:257:VAL:HG23	2.13	0.49
1:A:146:MET:O	1:A:150:LEU:HG	2.13	0.49
1:B:253:LEU:O	1:B:257:VAL:HG23	2.12	0.49
1:A:130:ALA:O	1:A:134:VAL:HG23	2.13	0.49
1:B:108:GLY:O	1:B:111:ARG:HB3	2.13	0.49
1:D:208:ILE:HG23	1:D:224:PHE:HB2	1.95	0.49
1:D:312:ARG:HA	1:D:315:THR:CG2	2.42	0.49
1:D:145:GLY:HA3	1:D:166:TYR:CD1	2.48	0.49
1:A:77:MET:HG3	1:A:220:PRO:HD2	1.94	0.49
1:D:54:GLU:O	1:D:57:ARG:HB3	2.13	0.49
1:C:41:VAL:HG11	1:C:68:ARG:HG2	1.95	0.49
1:D:46:ALA:O	1:D:49:ILE:HG22	2.13	0.48
1:C:236:ASP:OD2	1:C:238:HIS:HB2	2.11	0.48
1:C:312:ARG:HA	1:C:315:THR:CG2	2.42	0.48
1:D:102:MET:HG2	1:D:105:VAL:CG2	2.43	0.48
1:B:296:LEU:HD22	1:B:310:THR:HG22	1.95	0.48
1:B:49:ILE:HG12	1:B:57:ARG:HG3	1.95	0.48
1:A:52:LEU:HD13	1:A:60:VAL:HG21	1.94	0.48
1:C:280:PHE:CZ	1:C:325:LEU:HA	2.48	0.48
1:A:157:LYS:HE3	1:C:351:ASP:OD2	2.13	0.48
1:D:325:LEU:O	1:D:329:LEU:HG	2.14	0.48
1:C:352:ARG:HG2	1:C:352:ARG:HH11	1.77	0.48
1:D:256:MET:O	1:D:259:ASP:HB3	2.13	0.48
1:B:63:PHE:O	1:B:67:LEU:HG	2.14	0.48
1:B:366:SER:HA	1:D:108:GLY:HA2	1.96	0.47
1:C:122:ARG:NH1	1:C:122:ARG:HG3	2.29	0.47
1:A:227:ARG:HA	1:A:230:TRP:CE2	2.49	0.47
1:B:98:THR:O	1:B:118:THR:HG23	2.14	0.47
1:B:41:VAL:HG12	1:B:68:ARG:CZ	2.45	0.47
1:C:180:VAL:HG21	1:C:190:ALA:HB2	1.96	0.47
1:A:199:MET:CB	2:A:401:8PH:H31	2.45	0.47
1:A:314:ALA:HA	1:A:317:ARG:NH1	2.21	0.47
1:B:97:ASP:OD2	1:B:100:TRP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ARG:HG2	1:D:115:GLU:OE2	2.15	0.47
1:D:258:ALA:HB2	1:D:353:ILE:CD1	2.45	0.47
1:A:302:ASP:O	1:A:306:THR:HG22	2.15	0.47
1:A:73:VAL:HG22	1:A:102:MET:CE	2.44	0.47
1:A:333:LYS:O	1:A:337:LEU:HG	2.15	0.47
1:B:130:ALA:O	1:B:134:VAL:HG23	2.15	0.47
1:C:280:PHE:CE1	1:C:328:THR:HG21	2.50	0.46
1:C:339:LEU:HD23	1:C:339:LEU:C	2.36	0.46
1:C:102:MET:HB3	1:C:114:LEU:HB3	1.96	0.46
1:C:210:ARG:HD2	1:C:210:ARG:C	2.36	0.46
1:A:44:SER:HB2	2:A:401:8PH:H2	1.81	0.46
1:B:305:HIS:C	1:B:306:THR:CG2	2.84	0.46
1:C:314:ALA:O	1:C:318:ILE:HG13	2.15	0.46
1:D:320:HIS:HD2	1:D:321:TYR:CE2	2.34	0.46
1:A:216:ILE:HD11	1:A:238:HIS:HA	1.98	0.46
1:D:303:VAL:O	1:D:303:VAL:HG12	2.16	0.46
1:A:263:HIS:O	1:A:267:VAL:HG23	2.16	0.46
1:A:239:ALA:HB1	1:A:245:HIS:CD2	2.51	0.46
1:C:147:CYS:HA	1:C:150:LEU:HD12	1.98	0.46
1:D:160:TYR:HE2	1:D:259:ASP:OD2	1.99	0.45
1:B:43:ARG:HB2	1:B:43:ARG:NH2	2.31	0.45
1:D:227:ARG:O	1:D:231:GLU:HG2	2.16	0.45
1:D:253:LEU:HD21	1:D:297:VAL:O	2.16	0.45
1:D:91:PHE:HA	1:D:94:HIS:CD2	2.51	0.45
1:D:210:ARG:O	1:D:210:ARG:HD2	2.17	0.45
1:B:366:SER:HA	1:D:108:GLY:CA	2.47	0.45
1:C:300:ASN:HB2	1:C:342:ARG:HH21	1.81	0.45
1:B:73:VAL:HG22	1:B:102:MET:HE1	1.97	0.45
1:B:145:GLY:HA3	1:B:166:TYR:CD1	2.51	0.45
1:D:349:CYS:O	1:D:350:TYR:C	2.55	0.45
1:D:302:ASP:O	1:D:306:THR:HG22	2.16	0.45
1:A:162:LEU:O	1:A:165:HIS:HB3	2.17	0.45
1:C:31:LEU:HD12	1:C:123:ALA:CB	2.47	0.45
1:C:130:ALA:HB1	1:C:181:SER:OG	2.17	0.45
1:C:311:THR:O	1:C:315:THR:HG22	2.17	0.45
1:C:340:ALA:O	1:C:343:MET:HG2	2.17	0.45
1:D:102:MET:HE2	1:D:105:VAL:HG21	1.97	0.45
1:D:205:LYS:O	1:D:209:ILE:HG13	2.16	0.45
1:A:118:THR:O	1:A:122:ARG:HG2	2.18	0.44
1:C:291:MET:HG3	1:C:335:TYR:HB3	1.99	0.44
1:A:162:LEU:HG	1:A:166:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ARG:O	1:C:47:VAL:HG23	2.17	0.44
1:D:33:PHE:CD2	1:D:119:HIS:HB2	2.52	0.44
1:A:153:LYS:HB2	1:A:155:GLU:OE2	2.16	0.44
1:D:157:LYS:O	1:D:160:TYR:HB3	2.17	0.44
1:D:53:ASP:O	1:D:54:GLU:C	2.56	0.44
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.66	0.44
1:D:302:ASP:HA	1:D:305:HIS:NE2	2.32	0.44
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.83	0.44
1:D:58:ASP:O	1:D:62:ILE:HG12	2.16	0.44
1:D:79:ILE:HG23	1:D:80:PRO:HD2	1.99	0.44
1:A:233:TYR:HB3	1:A:248:LYS:HB3	1.99	0.44
1:C:103:SER:O	1:C:104:GLY:C	2.56	0.44
1:D:263:HIS:O	1:D:267:VAL:HG23	2.18	0.44
1:B:95:LEU:HA	1:B:121:THR:HG22	2.00	0.43
1:A:336:THR:HG21	1:A:364:MET:HE1	2.00	0.43
1:C:165:HIS:HA	1:C:169:GLY:HA3	2.01	0.43
1:C:250:VAL:O	1:C:253:LEU:HB3	2.18	0.43
1:B:339:LEU:C	1:B:339:LEU:HD23	2.39	0.43
1:C:324:GLU:O	1:C:328:THR:HG22	2.18	0.43
1:A:210:ARG:HD2	1:A:210:ARG:O	2.18	0.43
1:B:42:SER:HA	2:B:401:8PH:OAE	2.19	0.43
1:C:222:ARG:HH11	1:C:222:ARG:HG3	1.83	0.43
1:B:257:VAL:HG13	1:B:294:LEU:HD11	2.01	0.43
1:D:173:HIS:CD2	1:D:193:LEU:HB3	2.54	0.43
1:A:281:THR:HG22	1:A:323:THR:CA	2.30	0.43
1:B:42:SER:O	1:B:46:ALA:CB	2.67	0.43
1:C:137:GLY:O	1:C:141:ARG:HG3	2.18	0.43
1:D:109:ARG:HD2	1:D:109:ARG:N	2.34	0.43
1:B:314:ALA:O	1:B:318:ILE:HG13	2.19	0.43
1:C:199:MET:SD	1:C:267:VAL:HG13	2.59	0.43
1:D:162:LEU:HG	1:D:166:TYR:CE2	2.54	0.43
1:A:122:ARG:NH1	1:A:122:ARG:HG3	2.34	0.42
1:A:317:ARG:NH1	1:A:317:ARG:HB3	2.34	0.42
1:B:67:LEU:HD22	1:B:142:MET:SD	2.59	0.42
1:B:176:THR:HA	1:B:179:TYR:CD2	2.55	0.42
1:D:102:MET:O	1:D:115:GLU:HA	2.19	0.42
1:A:280:PHE:CZ	1:A:325:LEU:HA	2.55	0.42
1:A:195:ASN:OD1	1:A:266:HIS:HB3	2.19	0.42
1:A:73:VAL:CG2	1:A:102:MET:HE1	2.48	0.42
1:B:168:ALA:HB2	1:B:204:GLN:HB2	2.02	0.42
1:D:276:ASP:HA	1:D:277:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:HH11	1:A:317:ARG:HB3	1.84	0.42
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.84	0.42
1:A:339:LEU:C	1:A:339:LEU:HD23	2.40	0.42
1:A:184:LEU:HD22	1:A:276:ASP:OD2	2.20	0.42
1:A:249:ALA:HB1	1:A:304:PHE:CZ	2.55	0.42
1:C:296:LEU:HD22	1:C:310:THR:HG22	2.02	0.42
1:D:188:ARG:HA	1:D:188:ARG:HE	1.85	0.42
1:A:227:ARG:HA	1:A:230:TRP:CD1	2.55	0.41
1:D:72:THR:HG22	1:D:105:VAL:HG12	2.01	0.41
1:A:276:ASP:HA	1:A:277:PRO:HD3	1.90	0.41
1:B:276:ASP:HA	1:B:277:PRO:HD3	1.89	0.41
1:B:340:ALA:O	1:B:343:MET:HG2	2.19	0.41
1:B:363:ALA:O	1:B:366:SER:HB3	2.20	0.41
1:C:269:GLU:HG3	3:C:519:HOH:O	2.19	0.41
1:C:327:ALA:O	1:C:330:GLN:HG2	2.20	0.41
1:A:176:THR:HA	1:A:179:TYR:CD2	2.55	0.41
1:C:83:PHE:CZ	1:C:87:GLU:HG3	2.56	0.41
1:A:179:TYR:CZ	1:A:279:VAL:HG13	2.56	0.41
1:C:292:ALA:HA	1:C:335:TYR:CD1	2.56	0.41
1:D:42:SER:OG	1:D:45:PHE:HB3	2.20	0.41
1:A:168:ALA:CB	1:A:204:GLN:HB2	2.51	0.41
1:A:102:MET:O	1:A:115:GLU:HA	2.21	0.41
1:A:280:PHE:HE1	1:A:328:THR:HG21	1.86	0.41
1:B:199:MET:SD	1:B:267:VAL:HG13	2.61	0.41
1:C:249:ALA:HB1	1:C:304:PHE:CE2	2.56	0.41
1:D:336:THR:HG21	1:D:364:MET:CE	2.51	0.41
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.86	0.41
1:A:144:ASN:HD22	1:A:144:ASN:HA	1.67	0.41
1:C:160:TYR:CD1	1:C:226:PRO:HD3	2.55	0.41
1:D:185:GLU:HB3	1:D:189:LEU:HD22	2.03	0.41
1:D:258:ALA:HB2	1:D:353:ILE:HD13	2.03	0.41
1:A:67:LEU:HD22	1:A:142:MET:SD	2.61	0.40
1:B:38:LEU:HD22	1:B:61:CYS:SG	2.61	0.40
1:A:314:ALA:O	1:A:318:ILE:HG13	2.21	0.40
1:A:343:MET:HE1	1:A:350:TYR:HA	2.02	0.40
1:B:110:GLU:O	1:B:113:LEU:HB3	2.20	0.40
1:A:31:LEU:HD11	1:A:58:ASP:OD1	2.21	0.40
1:A:55:GLU:O	1:A:59:ALA:CB	2.70	0.40
1:A:343:MET:HE2	1:A:350:TYR:HA	2.04	0.40
1:C:102:MET:O	1:C:115:GLU:HA	2.20	0.40
1:C:261:LEU:HA	1:C:264:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ARG:NH1	1:D:222:ARG:HG3	2.37	0.40
1:A:195:ASN:HA	1:A:198:HIS:HD2	1.87	0.40
1:A:83:PHE:CE1	1:A:87:GLU:HG3	2.57	0.40
1:C:134:VAL:O	1:C:138:ILE:HG12	2.21	0.40
1:D:352:ARG:HD2	1:D:352:ARG:HA	1.89	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	339/365 (93%)	319 (94%)	17 (5%)	3 (1%)	20	62
1	B	339/365 (93%)	311 (92%)	26 (8%)	2 (1%)	28	70
1	C	339/365 (93%)	312 (92%)	24 (7%)	3 (1%)	20	62
1	D	339/365 (93%)	320 (94%)	16 (5%)	3 (1%)	20	62
All	All	1356/1460 (93%)	1262 (93%)	83 (6%)	11 (1%)	22	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	348	ALA
1	D	54	GLU
1	A	55	GLU
1	D	350	TYR
1	D	305	HIS
1	C	305	HIS
1	B	305	HIS
1	B	325	LEU
1	C	54	GLU

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Mol	Chain	Res	Type
1	C	325	LEU

### 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	299/319 (94%)	290 (97%)	9 (3%)	46	81
1	B	299/319 (94%)	286 (96%)	13 (4%)	33	72
1	C	299/319 (94%)	288 (96%)	11 (4%)	39	76
1	D	299/319 (94%)	285 (95%)	14 (5%)	30	69
All	All	1196/1276 (94%)	1149 (96%)	47 (4%)	37	75

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	102	MET
1	A	109	ARG
1	A	129	LYS
1	A	188	ARG
1	A	235	ASP
1	A	296	LEU
1	A	315	THR
1	A	324	GLU
1	B	53	ASP
1	B	56	MET
1	B	74	GLU
1	B	75	ASP
1	B	103	SER
1	B	109	ARG
1	B	161	ASP
1	B	188	ARG
1	B	191	ASP
1	B	306	THR
1	B	315	THR

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Mol	Chain	Res	Type
1	B	344	ASN
1	B	355	HIS
1	C	31	LEU
1	C	53	ASP
1	C	54	GLU
1	C	74	GLU
1	C	75	ASP
1	C	90	LYS
1	C	109	ARG
1	C	151	THR
1	C	188	ARG
1	C	315	THR
1	C	328	THR
1	D	39	GLN
1	D	56	MET
1	D	57	ARG
1	D	82	GLU
1	D	109	ARG
1	D	129	LYS
1	D	188	ARG
1	D	243	GLU
1	D	278	SER
1	D	319	PHE
1	D	330	GLN
1	D	346	GLN
1	D	355	HIS
1	D	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	245	HIS
1	A	358	ASN
1	B	144	ASN
1	B	204	GLN
1	B	245	HIS
1	B	344	ASN
1	B	346	GLN
1	B	358	ASN
1	C	144	ASN
1	C	238	HIS

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Mol	Chain	Res	Type
1	C	287	GLN
1	C	300	ASN
1	C	346	GLN
1	D	94	HIS
1	D	144	ASN
1	D	173	HIS
1	D	245	HIS
1	D	287	GLN
1	D	320	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	8PH	A	401	-	25,26,26	2.24	9 (36%)	31,37,37	1.32	5 (16%)
2	8PH	B	401	-	14,16,26	2.93	8 (57%)	19,26,37	1.52	5 (26%)
2	8PH	C	401	-	8,10,26	3.52	5 (62%)	11,18,37	1.60	2 (18%)
2	8PH	D	401	-	8,10,26	3.51	5 (62%)	11,18,37	1.56	2 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8PH	A	401	-	-	0/33/33/33	0/1/1/1
2	8PH	B	401	-	-	0/23/23/33	0/1/1/1
2	8PH	C	401	-	-	0/18/18/33	0/0/0/1
2	8PH	D	401	-	-	0/18/18/33	0/0/0/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	8PH	PAZ-OAC	-3.42	1.48	1.54
2	C	401	8PH	PAZ-OAC	-3.39	1.48	1.54
2	B	401	8PH	PAZ-OAC	-3.37	1.48	1.54
2	A	401	8PH	PAZ-OAC	-3.34	1.48	1.54
2	B	401	8PH	CAJ-NAW	-2.34	1.33	1.37
2	A	401	8PH	CAJ-NAW	-2.31	1.33	1.37
2	A	401	8PH	CAI-NAV	-2.30	1.33	1.37
2	A	401	8PH	PAY-CAX	2.58	1.86	1.85
2	B	401	8PH	PAY-CAX	2.59	1.87	1.85
2	A	401	8PH	PAZ-CAX	2.80	1.87	1.85
2	B	401	8PH	PAZ-CAX	2.87	1.87	1.85
2	D	401	8PH	PAY-OAF	3.57	1.61	1.54
2	C	401	8PH	PAY-OAF	3.58	1.61	1.54
2	B	401	8PH	PAY-OAE	3.58	1.61	1.54
2	C	401	8PH	PAZ-OAG	3.58	1.61	1.54
2	A	401	8PH	PAY-OAF	3.58	1.61	1.54
2	B	401	8PH	PAZ-OAG	3.59	1.61	1.54
2	D	401	8PH	PAZ-OAG	3.59	1.61	1.54
2	A	401	8PH	PAZ-OAG	3.59	1.61	1.54
2	A	401	8PH	PAY-OAE	3.60	1.61	1.54
2	D	401	8PH	PAY-OAE	3.60	1.61	1.54
2	B	401	8PH	PAY-OAF	3.61	1.61	1.54
2	C	401	8PH	PAY-OAE	3.62	1.61	1.54
2	B	401	8PH	PAZ-OAH	6.79	1.61	1.50
2	A	401	8PH	PAZ-OAH	6.79	1.61	1.50
2	D	401	8PH	PAZ-OAH	6.80	1.61	1.50
2	C	401	8PH	PAZ-OAH	6.84	1.61	1.50

All (14) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	8PH	OAG-PAZ-OAH	-3.12	106.06	113.05
2	B	401	8PH	OAG-PAZ-OAH	-3.06	106.19	113.05
2	A	401	8PH	OAG-PAZ-OAH	-3.04	106.25	113.05
2	D	401	8PH	OAG-PAZ-OAH	-3.03	106.26	113.05
2	A	401	8PH	PAZ-CAX-PAY	-2.13	108.76	112.70
2	B	401	8PH	PAZ-CAX-PAY	-2.10	108.82	112.70
2	A	401	8PH	PAZ-CAX-OAD	2.57	113.31	107.24
2	B	401	8PH	PAY-CAX-OAD	2.60	113.38	107.24
2	B	401	8PH	PAZ-CAX-OAD	2.61	113.39	107.24
2	A	401	8PH	PAY-CAX-OAD	2.62	113.42	107.24
2	B	401	8PH	OAC-PAZ-CAX	2.97	112.59	106.04
2	A	401	8PH	OAC-PAZ-CAX	2.99	112.65	106.04
2	D	401	8PH	OAC-PAZ-CAX	3.75	112.46	106.25
2	C	401	8PH	OAC-PAZ-CAX	3.83	112.60	106.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	8PH	5	0
2	B	401	8PH	3	0
2	D	401	8PH	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/365 (93%)	-0.34	1 (0%) 93 82	32, 55, 81, 99	0
1	B	341/365 (93%)	-0.23	2 (0%) 89 71	40, 71, 102, 129	0
1	C	341/365 (93%)	-0.24	2 (0%) 89 71	40, 78, 100, 120	0
1	D	341/365 (93%)	-0.00	9 (2%) 56 27	53, 89, 116, 134	0
All	All	1364/1460 (93%)	-0.20	14 (1%) 82 58	32, 73, 107, 134	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	ASP	3.9
1	D	345	ALA	3.7
1	D	344	ASN	3.6
1	D	346	GLN	2.7
1	D	43	ARG	2.5
1	D	107	VAL	2.3
1	D	368	GLN	2.3
1	D	365	GLU	2.2
1	C	99	THR	2.2
1	D	29	GLU	2.1
1	B	368	GLN	2.1
1	C	309	LYS	2.1
1	D	98	THR	2.0
1	A	346	GLN	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	8PH	A	401	26/26	0.88	0.22	0.29	47,102,112,112	0
2	8PH	B	401	16/26	0.90	0.14	-0.63	115,117,118,119	0
2	8PH	D	401	11/26	0.79	0.18	-0.94	154,155,155,155	0
2	8PH	C	401	11/26	0.57	0.30	-	165,166,167,167	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.