



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:06 pm BST

PDB ID : 5WTB
Title : Complex Structure of Staphylococcus aureus SdrE with human complement factor H
Authors : Wu, M.; Zhang, Y.; Hang, T.; Wang, C.; Yang, Y.; Zang, J.; Zhang, M.; Zhang, X.
Deposited on : 2016-12-10
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

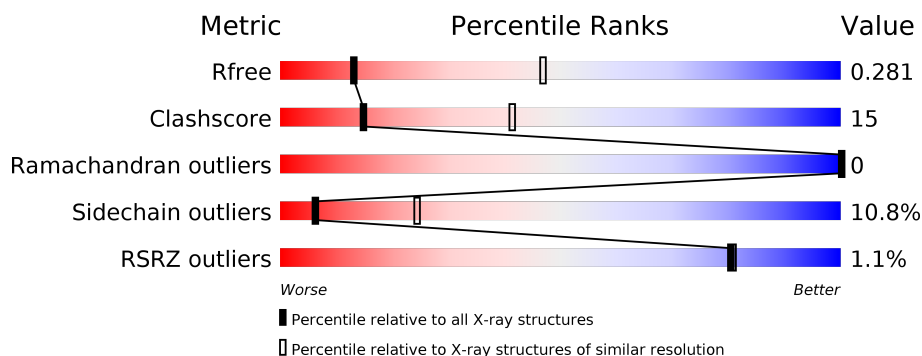
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	338	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	338	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	338	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>5%</div> <div>•</div> </div> </div>
1	D	338	<div> <div></div> <div> <div></div> <div>66%</div> <div>25%</div> <div>•</div> <div>7%</div> </div> </div>
2	E	21	<div> <div></div> <div> <div>19%</div> <div>43%</div> <div>19%</div> <div>19%</div> </div> </div>
2	F	21	<div> <div></div> <div> <div>14%</div> <div>43%</div> <div>10%</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	21	<div><div></div><div></div><div></div><div></div><div></div><div>29%</div><div>14%</div><div>19%</div><div>5%</div><div>33%</div></div>
2	H	21	<div><div></div><div></div><div></div><div></div><div></div><div>48%</div><div>19%</div><div>14%</div><div>19%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10427 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 Serine-aspartate repeat-containing protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	313	Total	C	N	O	S	0	0	0
			2447	1524	397	522	4			
1	A	313	Total	C	N	O	S	0	0	0
			2447	1524	397	522	4			
1	B	319	Total	C	N	O	S	0	0	0
			2491	1549	405	533	4			
1	C	323	Total	C	N	O	S	0	0	0
			2528	1575	410	539	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	489	MET	ILE	engineered mutation	UNP Q932F7
D	600	LEU	-	expression tag	UNP Q932F7
D	601	GLU	-	expression tag	UNP Q932F7
D	602	HIS	-	expression tag	UNP Q932F7
D	603	HIS	-	expression tag	UNP Q932F7
D	604	HIS	-	expression tag	UNP Q932F7
D	605	HIS	-	expression tag	UNP Q932F7
D	606	HIS	-	expression tag	UNP Q932F7
D	607	HIS	-	expression tag	UNP Q932F7
A	489	MET	ILE	engineered mutation	UNP Q932F7
A	600	LEU	-	expression tag	UNP Q932F7
A	601	GLU	-	expression tag	UNP Q932F7
A	602	HIS	-	expression tag	UNP Q932F7
A	603	HIS	-	expression tag	UNP Q932F7
A	604	HIS	-	expression tag	UNP Q932F7
A	605	HIS	-	expression tag	UNP Q932F7
A	606	HIS	-	expression tag	UNP Q932F7
A	607	HIS	-	expression tag	UNP Q932F7
B	489	MET	ILE	engineered mutation	UNP Q932F7
B	600	LEU	-	expression tag	UNP Q932F7
B	601	GLU	-	expression tag	UNP Q932F7

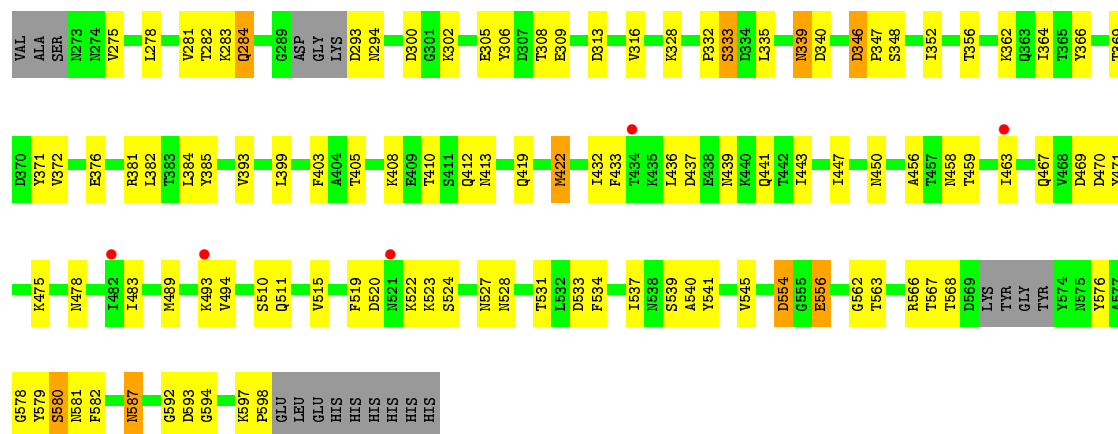
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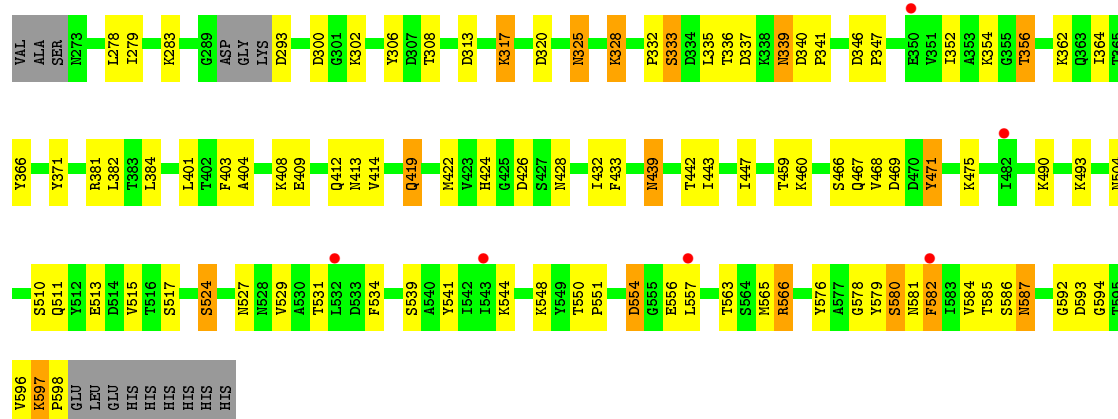
Chain	Residue	Modelled	Actual	Comment	Reference
B	602	HIS	-	expression tag	UNP Q932F7
B	603	HIS	-	expression tag	UNP Q932F7
B	604	HIS	-	expression tag	UNP Q932F7
B	605	HIS	-	expression tag	UNP Q932F7
B	606	HIS	-	expression tag	UNP Q932F7
B	607	HIS	-	expression tag	UNP Q932F7
C	489	MET	ILE	engineered mutation	UNP Q932F7
C	600	LEU	-	expression tag	UNP Q932F7
C	601	GLU	-	expression tag	UNP Q932F7
C	602	HIS	-	expression tag	UNP Q932F7
C	603	HIS	-	expression tag	UNP Q932F7
C	604	HIS	-	expression tag	UNP Q932F7
C	605	HIS	-	expression tag	UNP Q932F7
C	606	HIS	-	expression tag	UNP Q932F7
C	607	HIS	-	expression tag	UNP Q932F7

- Molecule 2 is a protein called Peptide from Complement factor H.

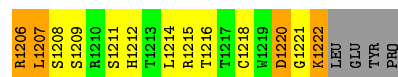
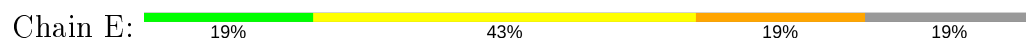
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	S	0	0	0
			139	83	30	25	1			
2	F	14	Total	C	N	O	S	0	0	0
			118	71	26	20	1			
2	G	14	Total	C	N	O	S	0	0	0
			118	71	26	20	1			
2	H	17	Total	C	N	O	S	0	0	0
			139	83	30	25	1			



• Molecule 1: Serine-aspartate repeat-containing protein E



• Molecule 2: Peptide from Complement factor H



• Molecule 2: Peptide from Complement factor H



• Molecule 2: Peptide from Complement factor H





● Molecule 2: Peptide from Complement factor H



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.50Å 117.50Å 154.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.30 49.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.79-3.30) 95.2 (49.75-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.222 , 0.281 0.223 , 0.281	Depositor DCC
R_{free} test set	1580 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	94.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.418 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10427	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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](#)

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	0.53	0/2485	0.71	1/3372 (0.0%)
1	B	0.50	0/2528	0.70	0/3431
1	C	0.51	0/2568	0.69	0/3486
1	D	0.54	0/2485	0.73	0/3372
2	E	0.54	0/141	0.92	0/188
2	F	0.62	0/120	0.93	0/161
2	G	0.62	0/120	1.02	1/161 (0.6%)
2	H	0.67	0/141	0.89	0/188
All	All	0.53	0/10588	0.72	2/14359 (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	426	ASP	CB-CG-OD2	5.19	122.97	118.30
2	G	1206	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	2447	0	2356	75	0
1	B	2491	0	2400	89	0
1	C	2528	0	2435	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2447	0	2356	65	0
2	E	139	0	138	24	0
2	F	118	0	118	17	0
2	G	118	0	118	13	0
2	H	139	0	138	13	0
All	All	10427	0	10059	312	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 15.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LYS:HG2	1:C:541:TYR:CE1	1.68	1.28
1:B:493:LYS:HG2	1:B:541:TYR:CE1	1.68	1.26
1:D:493:LYS:HG2	1:D:541:TYR:CE2	1.82	1.13
1:C:493:LYS:HG2	1:C:541:TYR:HE1	0.97	1.10
1:B:493:LYS:HG2	1:B:541:TYR:HE1	1.18	0.98
1:B:467:GLN:HG3	1:B:475:LYS:HB2	1.47	0.95
1:C:493:LYS:CG	1:C:541:TYR:HE1	1.79	0.94
1:C:467:GLN:OE1	1:C:475:LYS:HD3	1.73	0.89
1:B:469:ASP:OD1	1:B:475:LYS:CD	2.26	0.83
1:B:519:PHE:O	1:B:523:LYS:HG3	1.77	0.82
1:D:559:ILE:HB	1:D:583:ILE:HD13	1.58	0.82
1:A:318:LYS:HE2	1:C:550:THR:HG21	1.63	0.81
1:C:300:ASP:OD2	2:G:1215:ARG:HD3	1.83	0.79
1:A:318:LYS:HE2	1:C:550:THR:CG2	2.12	0.78
1:B:469:ASP:OD1	1:B:475:LYS:HD2	1.84	0.78
1:D:587:ASN:HA	2:H:1206:ARG:HG2	1.64	0.78
1:A:523:LYS:HG2	1:A:532:LEU:HD23	1.66	0.77
1:B:284:GLN:OE1	1:B:410:THR:HB	1.83	0.77
1:C:424:HIS:CD2	1:C:471:TYR:HE1	2.02	0.77
1:B:493:LYS:CG	1:B:541:TYR:HE1	1.96	0.75
1:B:376:GLU:HG2	1:B:597:LYS:HG2	1.69	0.74
1:D:493:LYS:HG2	1:D:541:TYR:HE2	1.51	0.74
1:B:433:PHE:HB2	2:F:1209:SER:HB3	1.71	0.72
1:D:433:PHE:HB2	2:H:1209:SER:HB3	1.71	0.72
1:B:587:ASN:HA	2:F:1206:ARG:HG3	1.71	0.71
1:A:439:ASN:O	1:C:356:THR:HB	1.90	0.70
1:A:544:LYS:HB3	1:A:544:LYS:HZ2	1.56	0.70
1:D:522:LYS:HD3	1:D:533:ASP:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ASP:OD1	1:B:475:LYS:HD3	1.90	0.70
1:A:354:LYS:HD2	1:C:551:PRO:HB3	1.73	0.70
1:B:419:GLN:NE2	2:F:1211:SER:OG	2.25	0.70
1:C:333:SER:HB2	1:C:339:ASN:HB3	1.75	0.68
1:B:597:LYS:HB3	1:B:598:PRO:HD2	1.76	0.67
1:C:424:HIS:CD2	1:C:471:TYR:CE1	2.82	0.67
1:B:300:ASP:OD2	2:F:1215:ARG:HD3	1.95	0.67
1:B:467:GLN:OE1	1:B:475:LYS:HE2	1.94	0.67
1:C:278:LEU:HD22	1:C:313:ASP:HB3	1.76	0.67
1:C:566:ARG:HG2	1:C:576:TYR:CE1	2.30	0.67
1:C:493:LYS:CG	1:C:541:TYR:CE1	2.60	0.66
1:B:328:LYS:O	1:B:362:LYS:NZ	2.28	0.66
1:B:459:THR:OG1	1:B:534:PHE:HB2	1.95	0.66
2:E:1220:ASP:HB3	2:F:1214:LEU:HA	1.77	0.66
1:A:436:LEU:HD22	2:E:1207:LEU:HD12	1.77	0.65
1:A:523:LYS:HG2	1:A:532:LEU:CD2	2.27	0.65
1:B:524:SER:HB2	1:B:531:THR:HB	1.79	0.65
1:D:435:LYS:HE3	1:D:505:ARG:HH21	1.62	0.64
1:C:566:ARG:HG2	1:C:576:TYR:CD1	2.32	0.64
1:B:456:ALA:HB1	1:B:567:THR:HG21	1.78	0.64
1:C:493:LYS:HD2	1:C:515:VAL:HG11	1.79	0.63
1:B:469:ASP:CG	1:B:475:LYS:HD2	2.19	0.63
1:C:328:LYS:O	1:C:362:LYS:NZ	2.32	0.63
1:A:335:LEU:HD12	2:E:1207:LEU:HB3	1.79	0.63
1:B:278:LEU:HD22	1:B:313:ASP:HB3	1.79	0.63
1:D:297:ALA:HB3	1:D:302:LYS:HD2	1.80	0.63
1:D:422:MET:HG2	2:H:1213:THR:HB	1.80	0.63
2:E:1214:LEU:HD13	2:F:1219:TRP:CZ3	2.34	0.63
1:A:364:ILE:HG21	1:A:366:TYR:CE2	2.34	0.62
1:B:493:LYS:CG	1:B:541:TYR:CE1	2.62	0.62
1:D:364:ILE:HG21	1:D:366:TYR:CE2	2.34	0.62
1:B:493:LYS:CD	1:B:515:VAL:HG11	2.29	0.62
1:C:493:LYS:CD	1:C:515:VAL:HG11	2.29	0.62
1:D:493:LYS:CG	1:D:541:TYR:CE2	2.72	0.62
2:E:1222:LYS:HB3	2:E:1222:LYS:HZ2	1.64	0.62
1:D:308:THR:HG21	1:D:405:THR:HG21	1.82	0.61
1:B:305:GLU:HG3	1:B:385:TYR:CE2	2.35	0.61
1:C:424:HIS:CG	1:C:471:TYR:HE1	2.18	0.61
1:A:574:TYR:CD2	2:F:1214:LEU:HD12	2.36	0.61
1:B:493:LYS:HD2	1:B:515:VAL:HG11	1.83	0.61
1:B:566:ARG:HG3	1:B:576:TYR:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HB	1:C:439:ASN:O	2.02	0.60
1:D:517:SER:O	1:D:520:ASP:HB2	2.01	0.60
1:C:279:ILE:O	1:C:408:LYS:NZ	2.36	0.59
1:C:584:VAL:N	2:G:1208:SER:O	2.33	0.59
1:A:519:PHE:HB3	1:A:523:LYS:HE3	1.84	0.59
1:B:306:TYR:CE1	1:B:403:PHE:HB3	2.38	0.59
1:D:335:LEU:CD1	2:H:1207:LEU:HB3	2.32	0.59
1:B:339:ASN:O	1:B:339:ASN:ND2	2.24	0.59
1:B:582:PHE:CD2	2:E:1222:LYS:HG3	2.37	0.59
1:B:493:LYS:HG2	1:B:541:TYR:CD1	2.33	0.59
1:C:317:LYS:HD2	1:C:320:ASP:OD1	2.03	0.59
1:A:585:THR:HG22	2:E:1207:LEU:CD2	2.32	0.59
1:B:308:THR:HG22	1:B:309:GLU:N	2.17	0.58
2:E:1214:LEU:HD13	2:F:1219:TRP:HZ3	1.68	0.58
1:A:278:LEU:HD22	1:A:313:ASP:HB3	1.86	0.58
1:B:470:ASP:O	1:B:578:GLY:N	2.28	0.58
1:C:325:ASN:ND2	1:C:404:ALA:HB3	2.18	0.58
2:E:1220:ASP:HB3	2:F:1214:LEU:HD23	1.85	0.58
1:B:519:PHE:HA	1:B:522:LYS:HB2	1.86	0.57
1:A:419:GLN:NE2	2:E:1211:SER:OG	2.37	0.57
1:A:492:TYR:CE2	1:A:509:PHE:CD2	2.93	0.57
1:D:297:ALA:H	1:D:302:LYS:HD2	1.68	0.57
1:D:335:LEU:HD12	2:H:1207:LEU:HB3	1.87	0.57
1:B:352:ILE:HG12	1:B:371:TYR:CD1	2.40	0.57
1:A:339:ASN:HA	2:E:1206:ARG:NH1	2.20	0.56
1:C:493:LYS:HB2	1:C:513:GLU:HB3	1.87	0.56
1:D:306:TYR:HH	1:D:405:THR:HG1	1.53	0.56
1:B:333:SER:HB2	1:B:339:ASN:HB3	1.87	0.56
1:C:332:PRO:HB2	2:G:1206:ARG:NH2	2.20	0.56
1:B:332:PRO:HB2	2:F:1206:ARG:NH2	2.20	0.56
1:A:433:PHE:HB2	2:E:1209:SER:HB3	1.87	0.56
1:A:343:ASP:N	1:A:343:ASP:OD1	2.38	0.56
1:D:433:PHE:HB2	2:H:1209:SER:CB	2.36	0.56
1:C:469:ASP:O	1:C:578:GLY:HA3	2.05	0.56
1:A:458:ASN:HB3	1:B:471:TYR:OH	2.05	0.56
1:C:510:SER:OG	1:C:511:GLN:N	2.38	0.56
1:D:278:LEU:HD22	1:D:313:ASP:HB3	1.88	0.55
1:A:544:LYS:HB3	1:A:544:LYS:NZ	2.19	0.55
1:A:587:ASN:HA	2:E:1206:ARG:HG3	1.88	0.55
1:B:281:VAL:HG11	1:B:284:GLN:HG2	1.86	0.55
1:B:459:THR:HG21	1:B:537:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:PHE:CE1	1:A:359:LYS:HA	2.42	0.55
1:A:588:ASP:OD2	2:E:1206:ARG:NH2	2.39	0.55
1:A:297:ALA:H	1:A:302:LYS:HD2	1.72	0.55
1:C:596:VAL:HG12	1:C:597:LYS:O	2.07	0.55
1:C:433:PHE:HB3	1:C:443:ILE:HD11	1.89	0.54
1:A:308:THR:HG21	1:A:405:THR:HG21	1.88	0.54
1:D:297:ALA:CB	1:D:302:LYS:HD2	2.38	0.54
1:B:469:ASP:OD2	1:B:475:LYS:HD2	2.08	0.54
1:C:467:GLN:HB3	1:C:475:LYS:HB3	1.89	0.54
1:A:355:GLY:HA2	1:A:366:TYR:HA	1.89	0.54
1:B:493:LYS:HG3	1:B:515:VAL:HG21	1.89	0.54
1:D:435:LYS:CE	1:D:505:ARG:HH21	2.21	0.54
1:D:435:LYS:CE	1:D:505:ARG:NH2	2.71	0.53
1:A:346:ASP:OD2	1:A:348:SER:OG	2.18	0.53
1:B:275:VAL:HG21	1:B:316:VAL:HG22	1.90	0.53
1:C:587:ASN:HA	2:G:1206:ARG:HG3	1.90	0.53
1:D:493:LYS:CD	1:D:515:VAL:HG11	2.38	0.53
1:D:524:SER:OG	1:D:531:THR:HB	2.08	0.53
1:D:312:ILE:HD13	1:D:368:PHE:HE2	1.73	0.53
1:A:335:LEU:CD1	2:E:1207:LEU:HB3	2.38	0.53
1:D:459:THR:HA	1:D:566:ARG:O	2.09	0.53
1:A:551:PRO:HB3	1:C:354:LYS:HD2	1.91	0.53
1:A:574:TYR:CE2	2:F:1214:LEU:HD12	2.43	0.53
1:C:593:ASP:OD1	1:C:594:GLY:N	2.42	0.53
1:C:332:PRO:HG2	1:C:339:ASN:HB2	1.91	0.52
1:A:422:MET:O	1:A:428:ASN:HA	2.09	0.52
1:D:493:LYS:CG	1:D:541:TYR:HE2	2.19	0.52
1:B:489:MET:HG2	1:B:545:VAL:HG22	1.89	0.52
1:A:418:TYR:CE2	1:A:503:SER:HA	2.44	0.52
1:A:312:ILE:HD13	1:A:368:PHE:HE2	1.75	0.52
1:C:293:ASP:OD2	1:C:302:LYS:NZ	2.43	0.52
1:C:447:ILE:HD13	1:C:563:THR:HG21	1.92	0.52
1:C:566:ARG:CG	1:C:576:TYR:HE1	2.22	0.52
1:C:585:THR:HG22	2:G:1207:LEU:CD2	2.40	0.51
1:B:300:ASP:OD2	2:F:1215:ARG:HB2	2.10	0.51
1:A:318:LYS:CE	1:C:550:THR:HG21	2.38	0.51
1:D:443:ILE:HD11	1:D:583:ILE:HD11	1.92	0.51
1:A:339:ASN:HA	2:E:1206:ARG:HH11	1.75	0.51
1:C:597:LYS:O	1:C:598:PRO:C	2.49	0.51
1:C:382:LEU:HD22	1:C:384:LEU:HD21	1.92	0.51
1:A:338:LYS:NZ	1:A:438:GLU:HB2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LYS:HG2	1:C:550:THR:HG21	1.93	0.51
1:B:364:ILE:HG21	1:B:366:TYR:CE1	2.46	0.51
1:D:435:LYS:HE3	1:D:505:ARG:NH2	2.24	0.51
1:C:278:LEU:HD22	1:C:313:ASP:CB	2.40	0.50
1:B:587:ASN:N	1:B:587:ASN:OD1	2.41	0.50
1:B:433:PHE:HB2	2:F:1209:SER:CB	2.39	0.50
1:D:447:ILE:HD13	1:D:563:THR:HG21	1.93	0.50
1:A:433:PHE:HB2	2:E:1209:SER:CB	2.40	0.50
1:D:430:GLN:HE21	1:D:504:ASN:ND2	2.10	0.50
2:G:1216:THR:C	2:G:1217:THR:HG22	2.32	0.50
1:B:447:ILE:HD13	1:B:563:THR:HG21	1.94	0.50
1:C:306:TYR:CE1	1:C:403:PHE:HB3	2.46	0.50
1:C:401:LEU:HG	1:C:414:VAL:HG22	1.93	0.49
1:B:332:PRO:HG2	1:B:339:ASN:HB2	1.93	0.49
1:D:493:LYS:HG3	1:D:515:VAL:HG21	1.93	0.49
1:D:351:VAL:HG12	1:D:369:THR:HG21	1.95	0.49
1:A:318:LYS:CE	1:C:550:THR:CG2	2.87	0.49
1:D:419:GLN:OE1	1:D:504:ASN:ND2	2.44	0.49
1:D:491:VAL:HG11	1:D:519:PHE:CE2	2.47	0.49
1:D:585:THR:HG22	2:H:1207:LEU:CD2	2.43	0.49
1:B:437:ASP:OD1	1:B:439:ASN:HB3	2.13	0.49
1:C:524:SER:HB2	1:C:531:THR:HB	1.94	0.49
1:A:299:HIS:CD2	1:A:432:ILE:HG21	2.48	0.48
1:A:447:ILE:HD13	1:A:563:THR:HG21	1.94	0.48
1:C:332:PRO:HB2	2:G:1206:ARG:HH22	1.78	0.48
1:C:493:LYS:HG2	1:C:541:TYR:CD1	2.38	0.48
1:D:552:THR:OG1	1:D:556:GLU:O	2.27	0.48
1:A:325:ASN:HB2	1:A:404:ALA:HB3	1.95	0.48
1:B:376:GLU:HB3	1:B:597:LYS:HD3	1.95	0.48
1:B:593:ASP:OD1	1:B:594:GLY:N	2.42	0.48
1:C:566:ARG:CG	1:C:576:TYR:CE1	2.96	0.48
1:B:278:LEU:HD22	1:B:313:ASP:CB	2.43	0.48
1:A:434:THR:O	1:A:505:ARG:NH1	2.47	0.48
1:B:467:GLN:OE1	1:B:475:LYS:CE	2.62	0.48
1:A:387:TYR:CE2	2:E:1208:SER:HB2	2.49	0.47
2:E:1222:LYS:CB	2:E:1222:LYS:HZ2	2.25	0.47
1:A:490:LYS:HD2	1:A:544:LYS:HZ3	1.79	0.47
1:B:346:ASP:HA	1:B:592:GLY:O	2.15	0.47
1:A:448:TYR:CE1	1:A:500:LEU:HD13	2.50	0.47
1:A:552:THR:HG21	1:A:554:ASP:OD2	2.15	0.47
1:B:432:ILE:HA	1:B:581:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ILE:HG21	1:C:366:TYR:CE1	2.49	0.47
1:C:447:ILE:CD1	1:C:563:THR:HG21	2.44	0.47
1:C:586:SER:O	2:G:1206:ARG:HG3	2.15	0.47
1:A:538:ASN:OD1	1:A:538:ASN:N	2.48	0.47
1:C:346:ASP:HA	1:C:592:GLY:O	2.15	0.47
1:D:493:LYS:HD2	1:D:515:VAL:HG11	1.96	0.47
1:A:465:GLY:O	1:A:466:SER:C	2.53	0.46
1:A:448:TYR:CD1	1:A:500:LEU:HD13	2.49	0.46
1:B:347:PRO:HD3	1:B:592:GLY:O	2.15	0.46
1:D:580:SER:O	2:H:1212:HIS:N	2.48	0.46
1:B:582:PHE:CE2	2:E:1222:LYS:HD3	2.51	0.46
1:A:310:PHE:CE1	1:A:380:ALA:HB3	2.51	0.46
1:A:391:GLN:HG3	1:A:507:TYR:CE2	2.51	0.46
1:A:463:ILE:HG13	1:A:563:THR:HG22	1.97	0.46
2:H:1211:SER:O	2:H:1212:HIS:ND1	2.44	0.46
1:A:491:VAL:HG11	1:A:519:PHE:CE2	2.49	0.46
1:B:467:GLN:CD	1:B:478:ASN:HD22	2.19	0.46
1:B:587:ASN:HA	2:F:1206:ARG:CG	2.41	0.46
1:D:557:LEU:HD12	2:H:1207:LEU:HD11	1.97	0.46
1:A:338:LYS:HZ2	1:A:438:GLU:HB2	1.81	0.46
1:C:347:PRO:HD3	1:C:592:GLY:O	2.15	0.46
1:C:597:LYS:HB3	1:C:598:PRO:HD2	1.98	0.45
1:D:564:SER:HA	1:D:578:GLY:HA2	1.98	0.45
1:A:391:GLN:HG3	1:A:507:TYR:CD2	2.51	0.45
1:B:293:ASP:OD2	1:B:302:LYS:NZ	2.48	0.45
1:B:545:VAL:HG12	1:B:545:VAL:O	2.15	0.45
1:A:562:GLY:HA2	1:A:580:SER:HA	1.98	0.45
1:C:527:ASN:O	1:C:529:VAL:HG23	2.15	0.45
1:D:434:THR:O	1:D:505:ARG:NH1	2.50	0.45
1:A:284:GLN:OE1	1:A:410:THR:HB	2.17	0.45
1:B:471:TYR:O	1:B:576:TYR:HB2	2.16	0.45
1:D:278:LEU:CD2	1:D:313:ASP:HB3	2.46	0.45
1:A:306:TYR:CE1	1:A:403:PHE:HB3	2.51	0.45
1:C:432:ILE:HG12	1:C:504:ASN:HB3	1.99	0.45
1:A:463:ILE:HD13	1:A:489:MET:CE	2.47	0.45
1:B:333:SER:CB	1:B:339:ASN:HB3	2.46	0.45
1:A:299:HIS:ND1	1:A:419:GLN:HG2	2.32	0.44
1:B:281:VAL:CG1	1:B:284:GLN:HG2	2.47	0.44
1:B:494:VAL:HB	1:B:540:ALA:HB3	1.99	0.44
1:A:298:ALA:HB3	1:A:418:TYR:HE1	1.82	0.44
1:A:392:ALA:C	1:A:394:PRO:HD3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLN:NE2	1:B:408:LYS:O	2.48	0.44
1:D:343:ASP:OD1	1:D:343:ASP:N	2.51	0.44
1:D:432:ILE:HG12	1:D:504:ASN:HB3	2.00	0.44
1:C:554:ASP:OD1	1:C:556:GLU:HB2	2.18	0.44
1:C:460:LYS:O	1:C:566:ARG:HB2	2.17	0.44
1:B:554:ASP:OD2	1:B:556:GLU:HB2	2.17	0.44
1:D:588:ASP:OD2	2:H:1206:ARG:NH2	2.50	0.44
1:C:332:PRO:O	2:G:1206:ARG:N	2.51	0.44
1:B:293:ASP:O	1:B:294:ASN:HB2	2.17	0.44
1:B:520:ASP:HA	1:B:523:LYS:HE3	2.00	0.44
1:C:534:PHE:HE2	1:C:541:TYR:CD2	2.35	0.44
1:C:582:PHE:CD1	1:C:582:PHE:N	2.86	0.43
2:E:1221:GLY:O	2:E:1222:LYS:CB	2.65	0.43
1:A:447:ILE:CD1	1:A:563:THR:HG21	2.47	0.43
1:B:382:LEU:HD22	1:B:384:LEU:HD11	2.01	0.43
1:D:481:THR:OG1	1:D:482:ILE:N	2.49	0.43
1:B:293:ASP:OD1	1:B:294:ASN:N	2.51	0.43
1:C:565:MET:O	1:C:576:TYR:HA	2.19	0.43
1:C:581:ASN:C	1:C:582:PHE:CD1	2.92	0.43
1:D:494:VAL:HG21	1:D:500:LEU:HD21	2.00	0.43
1:C:442:THR:HG22	1:C:548:LYS:HD3	2.00	0.43
1:B:493:LYS:HG3	1:B:515:VAL:CG2	2.49	0.43
1:D:395:ASN:O	1:D:397:THR:HG22	2.18	0.43
1:D:538:ASN:OD1	1:D:538:ASN:N	2.49	0.43
1:A:383:THR:HB	1:A:589:THR:HG23	2.00	0.43
1:B:483:ILE:HD12	1:B:528:ASN:O	2.19	0.43
1:C:490:LYS:HE2	1:C:544:LYS:HE2	2.00	0.43
1:B:493:LYS:CE	1:B:515:VAL:HG11	2.48	0.42
1:D:396:GLU:HG3	1:D:502:GLN:OE1	2.18	0.42
1:A:584:VAL:N	2:E:1208:SER:O	2.32	0.42
1:B:308:THR:HG21	1:B:405:THR:HG21	2.01	0.42
1:B:463:ILE:HG22	1:B:483:ILE:HD13	2.00	0.42
1:C:404:ALA:HB2	1:C:409:GLU:HG2	2.01	0.42
1:C:467:GLN:HB3	1:C:475:LYS:O	2.19	0.42
1:D:566:ARG:HD3	1:D:576:TYR:OH	2.19	0.42
1:B:562:GLY:HA2	1:B:580:SER:HA	2.01	0.42
2:E:1214:LEU:HB3	2:F:1219:TRP:HZ3	1.84	0.42
1:D:376:GLU:HG2	1:D:597:LYS:HG2	2.02	0.42
1:C:433:PHE:HB2	2:G:1209:SER:HB3	2.01	0.42
1:A:369:THR:O	1:A:372:VAL:HG22	2.19	0.42
1:D:484:ASP:O	1:D:485:GLN:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PRO:HG3	1:C:364:ILE:HG23	2.02	0.41
1:C:459:THR:HA	1:C:566:ARG:O	2.20	0.41
1:C:468:VAL:HG11	1:C:563:THR:O	2.20	0.41
1:A:293:ASP:OD1	1:A:293:ASP:N	2.53	0.41
1:C:468:VAL:O	1:C:580:SER:OG	2.39	0.41
1:D:280:THR:HA	1:B:282:THR:O	2.19	0.41
1:D:418:TYR:CE2	1:D:503:SER:HA	2.55	0.41
1:A:396:GLU:HG2	1:A:418:TYR:H	1.85	0.41
1:A:395:ASN:HA	1:A:502:GLN:HB2	2.02	0.41
1:D:493:LYS:HG3	1:D:515:VAL:HG11	2.01	0.41
1:A:306:TYR:CE2	1:A:308:THR:OG1	2.73	0.41
1:D:357:PHE:CE2	1:D:359:LYS:HA	2.55	0.41
1:D:582:PHE:HE2	2:H:1212:HIS:CD2	2.39	0.41
1:B:300:ASP:OD1	2:F:1210:ARG:NH2	2.53	0.41
1:B:458:ASN:HB3	1:B:568:THR:OG1	2.21	0.41
1:B:522:LYS:HD3	1:B:533:ASP:O	2.19	0.41
1:C:493:LYS:CE	1:C:515:VAL:HG11	2.51	0.41
1:C:352:ILE:HG12	1:C:371:TYR:CD2	2.56	0.41
1:C:550:THR:HA	1:C:551:PRO:HD3	1.97	0.41
1:D:325:ASN:OD1	1:D:404:ALA:HB3	2.20	0.41
1:D:398:SER:HA	1:D:415:SER:HA	2.03	0.41
1:D:435:LYS:HE2	1:D:505:ARG:NH2	2.35	0.41
2:E:1218:CYS:SG	2:F:1217:THR:HB	2.61	0.41
1:B:450:ASN:O	1:B:540:ALA:HA	2.21	0.41
1:B:510:SER:OG	1:B:511:GLN:N	2.54	0.41
1:C:585:THR:HG22	2:G:1207:LEU:HD22	2.02	0.41
1:D:422:MET:O	1:D:428:ASN:HA	2.21	0.41
1:A:278:LEU:HD21	1:A:315:LYS:HD2	2.02	0.41
1:B:306:TYR:CE2	1:B:308:THR:OG1	2.74	0.41
1:B:369:THR:O	1:B:372:VAL:HG22	2.21	0.41
1:B:422:MET:CE	1:B:470:ASP:HB3	2.51	0.41
2:H:1222:LYS:O	2:H:1222:LYS:HG3	2.21	0.41
1:A:525:PHE:CE1	1:A:530:ALA:HB2	2.56	0.40
2:G:1206:ARG:HE	2:G:1206:ARG:N	2.20	0.40
1:D:485:GLN:HA	1:D:525:PHE:CE2	2.56	0.40
1:D:447:ILE:CD1	1:D:563:THR:HG21	2.52	0.40
1:B:393:VAL:HG21	1:B:399:LEU:HD11	2.04	0.40
1:C:419:GLN:NE2	2:G:1211:SER:OG	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/338 (91%)	278 (91%)	29 (9%)	0	100	100
1	B	313/338 (93%)	285 (91%)	28 (9%)	0	100	100
1	C	319/338 (94%)	287 (90%)	32 (10%)	0	100	100
1	D	307/338 (91%)	275 (90%)	32 (10%)	0	100	100
2	E	15/21 (71%)	14 (93%)	1 (7%)	0	100	100
2	F	12/21 (57%)	10 (83%)	2 (17%)	0	100	100
2	G	12/21 (57%)	11 (92%)	1 (8%)	0	100	100
2	H	15/21 (71%)	15 (100%)	0	0	100	100
All	All	1300/1436 (90%)	1175 (90%)	125 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	279/301 (93%)	248 (89%)	31 (11%)	6	23
1	B	285/301 (95%)	262 (92%)	23 (8%)	11	36
1	C	288/301 (96%)	255 (88%)	33 (12%)	5	22
1	D	279/301 (93%)	257 (92%)	22 (8%)	12	37
2	E	16/20 (80%)	9 (56%)	7 (44%)	0	0
2	F	14/20 (70%)	9 (64%)	5 (36%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	14/20 (70%)	9 (64%)	5 (36%)	0	0
2	H	16/20 (80%)	13 (81%)	3 (19%)	1	6
All	All	1191/1284 (93%)	1062 (89%)	129 (11%)	6	24

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	277	ASP
1	D	278	LEU
1	D	283	LYS
1	D	335	LEU
1	D	337	ASP
1	D	339	ASN
1	D	381	ARG
1	D	384	LEU
1	D	386	SER
1	D	391	GLN
1	D	422	MET
1	D	428	ASN
1	D	436	LEU
1	D	466	SER
1	D	481	THR
1	D	524	SER
1	D	539	SER
1	D	554	ASP
1	D	579	TYR
1	D	580	SER
1	D	587	ASN
1	D	593	ASP
1	A	322	MET
1	A	335	LEU
1	A	337	ASP
1	A	339	ASN
1	A	340	ASP
1	A	343	ASP
1	A	356	THR
1	A	381	ARG
1	A	391	GLN
1	A	397	THR
1	A	410	THR
1	A	412	GLN

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Mol	Chain	Res	Type
1	A	413	ASN
1	A	420	ASP
1	A	428	ASN
1	A	436	LEU
1	A	439	ASN
1	A	489	MET
1	A	493	LYS
1	A	517	SER
1	A	518	GLN
1	A	533	ASP
1	A	539	SER
1	A	544	LYS
1	A	552	THR
1	A	579	TYR
1	A	584	VAL
1	A	587	ASN
1	A	589	THR
1	A	595	THR
1	A	596	VAL
1	B	283	LYS
1	B	284	GLN
1	B	333	SER
1	B	335	LEU
1	B	339	ASN
1	B	340	ASP
1	B	346	ASP
1	B	348	SER
1	B	356	THR
1	B	381	ARG
1	B	412	GLN
1	B	413	ASN
1	B	422	MET
1	B	436	LEU
1	B	441	GLN
1	B	443	ILE
1	B	527	ASN
1	B	539	SER
1	B	554	ASP
1	B	556	GLU
1	B	579	TYR
1	B	580	SER
1	B	587	ASN

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Mol	Chain	Res	Type
1	C	283	LYS
1	C	308	THR
1	C	317	LYS
1	C	325	ASN
1	C	328	LYS
1	C	333	SER
1	C	335	LEU
1	C	336	THR
1	C	337	ASP
1	C	339	ASN
1	C	340	ASP
1	C	356	THR
1	C	381	ARG
1	C	412	GLN
1	C	413	ASN
1	C	419	GLN
1	C	422	MET
1	C	426	ASP
1	C	428	ASN
1	C	439	ASN
1	C	466	SER
1	C	471	TYR
1	C	517	SER
1	C	524	SER
1	C	539	SER
1	C	554	ASP
1	C	557	LEU
1	C	566	ARG
1	C	579	TYR
1	C	580	SER
1	C	582	PHE
1	C	587	ASN
1	C	597	LYS
2	E	1206	ARG
2	E	1207	LEU
2	E	1212	HIS
2	E	1215	ARG
2	E	1216	THR
2	E	1220	ASP
2	E	1222	LYS
2	F	1206	ARG
2	F	1207	LEU

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Mol	Chain	Res	Type
2	F	1208	SER
2	F	1213	THR
2	F	1217	THR
2	G	1206	ARG
2	G	1207	LEU
2	G	1211	SER
2	G	1216	THR
2	G	1217	THR
2	H	1207	LEU
2	H	1212	HIS
2	H	1222	LYS

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

Mol	Chain	Res	Type
1	D	419	GLN
1	D	430	GLN
1	D	504	ASN
1	A	339	ASN
1	A	419	GLN
1	A	430	GLN
1	A	504	ASN
1	B	419	GLN
1	B	424	HIS
1	B	478	ASN
1	B	504	ASN
1	C	339	ASN
1	C	419	GLN
1	C	424	HIS
1	C	430	GLN
1	C	467	GLN
1	C	478	ASN
1	C	504	ASN
1	C	518	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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 ⓘ

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	313/338 (92%)	0.17	3 (0%) 82 82	62, 85, 109, 128	18 (5%)
1	B	319/338 (94%)	0.19	5 (1%) 72 70	63, 92, 128, 154	19 (5%)
1	C	323/338 (95%)	0.18	6 (1%) 66 65	63, 93, 122, 132	25 (7%)
1	D	313/338 (92%)	0.20	0 100 100	62, 85, 106, 126	20 (6%)
2	E	17/21 (80%)	0.04	0 100 100	66, 82, 98, 98	1 (5%)
2	F	14/21 (66%)	0.32	0 100 100	71, 87, 108, 120	2 (14%)
2	G	14/21 (66%)	0.23	0 100 100	67, 83, 92, 93	3 (21%)
2	H	17/21 (80%)	0.09	0 100 100	67, 81, 99, 104	1 (5%)
All	All	1330/1436 (92%)	0.18	14 (1%) 80 81	62, 88, 120, 154	89 (6%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	557	LEU	2.8
1	A	446	GLN	2.8
1	C	532	LEU	2.7
1	B	434	THR	2.6
1	A	436	LEU	2.6
1	B	482	ILE	2.4
1	A	543	ILE	2.3
1	B	463	ILE	2.2
1	C	350	GLU	2.2
1	C	482	ILE	2.2
1	C	582	PHE	2.1
1	B	521	ASN	2.1
1	B	493	LYS	2.1
1	C	543	ILE	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.