Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:50 pm BST

PDB ID	:	6GN0
Title	:	Exoenzyme S from Pseudomonas aeruginosa in complex with human 14-3-3 protein beta, tetrameric crystal form
Authors	:	Karlberg, T.; Pinto, A.F.; Hornyak, P.; Nareoja, K.; Schuler, H.
Deposited on	:	2018-05-29
Resolution	:	3.24 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:

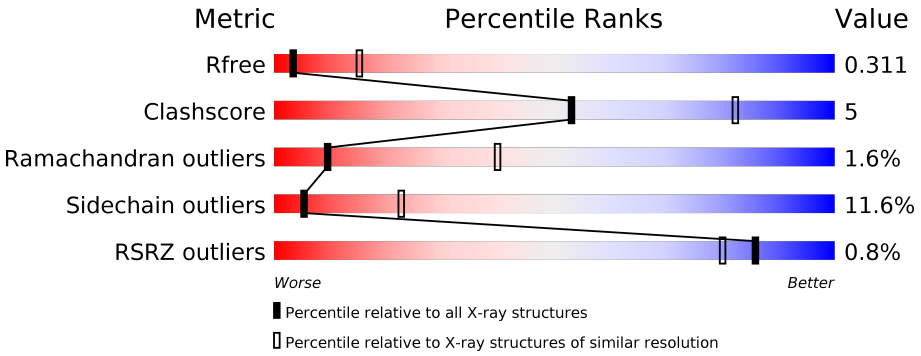
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	248	77% 17% • •
1	B	248	77% 15% • 6%
1	C	248	77% 16% • 5%
1	D	248	80% 15% • •
2	E	244	61% 15% • 20%
2	F	244	2% 55% 20% • 21%

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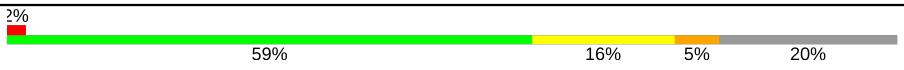
Mol	Chain	Length	Quality of chain
2	G	244	
2	H	244	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13303 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 14-3-3 protein beta/alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1919	1195	324	391	9			
1	B	233	Total	C	N	O	S	0	0	0
			1863	1164	312	378	9			
1	C	236	Total	C	N	O	S	0	0	0
			1895	1185	316	385	9			
1	D	237	Total	C	N	O	S	0	0	0
			1887	1178	315	385	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLU	-	expression tag	UNP P31946
A	241	ASN	-	expression tag	UNP P31946
A	242	LEU	-	expression tag	UNP P31946
A	243	TYR	-	expression tag	UNP P31946
A	244	PHE	-	expression tag	UNP P31946
A	245	GLN	-	expression tag	UNP P31946
A	246	SER	-	expression tag	UNP P31946
A	247	LEU	-	expression tag	UNP P31946
A	248	GLU	-	expression tag	UNP P31946
B	240	GLU	-	expression tag	UNP P31946
B	241	ASN	-	expression tag	UNP P31946
B	242	LEU	-	expression tag	UNP P31946
B	243	TYR	-	expression tag	UNP P31946
B	244	PHE	-	expression tag	UNP P31946
B	245	GLN	-	expression tag	UNP P31946
B	246	SER	-	expression tag	UNP P31946
B	247	LEU	-	expression tag	UNP P31946
B	248	GLU	-	expression tag	UNP P31946
C	240	GLU	-	expression tag	UNP P31946
C	241	ASN	-	expression tag	UNP P31946
C	242	LEU	-	expression tag	UNP P31946

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Chain	Residue	Modelled	Actual	Comment	Reference
C	243	TYR	-	expression tag	UNP P31946
C	244	PHE	-	expression tag	UNP P31946
C	245	GLN	-	expression tag	UNP P31946
C	246	SER	-	expression tag	UNP P31946
C	247	LEU	-	expression tag	UNP P31946
C	248	GLU	-	expression tag	UNP P31946
D	240	GLU	-	expression tag	UNP P31946
D	241	ASN	-	expression tag	UNP P31946
D	242	LEU	-	expression tag	UNP P31946
D	243	TYR	-	expression tag	UNP P31946
D	244	PHE	-	expression tag	UNP P31946
D	245	GLN	-	expression tag	UNP P31946
D	246	SER	-	expression tag	UNP P31946
D	247	LEU	-	expression tag	UNP P31946
D	248	GLU	-	expression tag	UNP P31946

- Molecule 2 is a protein called Exoenzyme S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	194	Total	C	N	O	S	0	0	0
			1438	887	256	292	3			
2	F	192	Total	C	N	O	S	0	0	0
			1423	876	256	288	3			
2	G	195	Total	C	N	O	S	0	0	0
			1446	892	258	293	3			
2	H	193	Total	C	N	O	S	0	0	0
			1432	882	258	289	3			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	210	MET	-	initiating methionine	UNP Q51451
E	211	GLY	-	expression tag	UNP Q51451
E	212	SER	-	expression tag	UNP Q51451
E	213	SER	-	expression tag	UNP Q51451
E	214	HIS	-	expression tag	UNP Q51451
E	215	HIS	-	expression tag	UNP Q51451
E	216	HIS	-	expression tag	UNP Q51451
E	217	HIS	-	expression tag	UNP Q51451
E	218	HIS	-	expression tag	UNP Q51451
E	219	HIS	-	expression tag	UNP Q51451
E	220	SER	-	expression tag	UNP Q51451

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Chain	Residue	Modelled	Actual	Comment	Reference
E	221	GLN	-	expression tag	UNP Q51451
E	222	ASP	-	expression tag	UNP Q51451
E	223	PRO	-	expression tag	UNP Q51451
E	224	ASN	-	expression tag	UNP Q51451
E	225	SER	-	expression tag	UNP Q51451
E	226	GLU	-	expression tag	UNP Q51451
E	227	ASN	-	expression tag	UNP Q51451
E	228	LEU	-	expression tag	UNP Q51451
E	229	TYR	-	expression tag	UNP Q51451
E	230	PHE	-	expression tag	UNP Q51451
E	231	GLN	-	expression tag	UNP Q51451
E	232	GLY	-	expression tag	UNP Q51451
E	233	ALA	-	expression tag	UNP Q51451
E	379	ALA	GLU	engineered mutation	UNP Q51451
E	381	ALA	GLU	engineered mutation	UNP Q51451
E	415	LEU	GLN	conflict	UNP Q51451
E	434	PRO	ARG	conflict	UNP Q51451
F	210	MET	-	initiating methionine	UNP Q51451
F	211	GLY	-	expression tag	UNP Q51451
F	212	SER	-	expression tag	UNP Q51451
F	213	SER	-	expression tag	UNP Q51451
F	214	HIS	-	expression tag	UNP Q51451
F	215	HIS	-	expression tag	UNP Q51451
F	216	HIS	-	expression tag	UNP Q51451
F	217	HIS	-	expression tag	UNP Q51451
F	218	HIS	-	expression tag	UNP Q51451
F	219	HIS	-	expression tag	UNP Q51451
F	220	SER	-	expression tag	UNP Q51451
F	221	GLN	-	expression tag	UNP Q51451
F	222	ASP	-	expression tag	UNP Q51451
F	223	PRO	-	expression tag	UNP Q51451
F	224	ASN	-	expression tag	UNP Q51451
F	225	SER	-	expression tag	UNP Q51451
F	226	GLU	-	expression tag	UNP Q51451
F	227	ASN	-	expression tag	UNP Q51451
F	228	LEU	-	expression tag	UNP Q51451
F	229	TYR	-	expression tag	UNP Q51451
F	230	PHE	-	expression tag	UNP Q51451
F	231	GLN	-	expression tag	UNP Q51451
F	232	GLY	-	expression tag	UNP Q51451
F	233	ALA	-	expression tag	UNP Q51451
F	379	ALA	GLU	engineered mutation	UNP Q51451

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Chain	Residue	Modelled	Actual	Comment	Reference
F	381	ALA	GLU	engineered mutation	UNP Q51451
F	415	LEU	GLN	conflict	UNP Q51451
F	434	PRO	ARG	conflict	UNP Q51451
G	210	MET	-	initiating methionine	UNP Q51451
G	211	GLY	-	expression tag	UNP Q51451
G	212	SER	-	expression tag	UNP Q51451
G	213	SER	-	expression tag	UNP Q51451
G	214	HIS	-	expression tag	UNP Q51451
G	215	HIS	-	expression tag	UNP Q51451
G	216	HIS	-	expression tag	UNP Q51451
G	217	HIS	-	expression tag	UNP Q51451
G	218	HIS	-	expression tag	UNP Q51451
G	219	HIS	-	expression tag	UNP Q51451
G	220	SER	-	expression tag	UNP Q51451
G	221	GLN	-	expression tag	UNP Q51451
G	222	ASP	-	expression tag	UNP Q51451
G	223	PRO	-	expression tag	UNP Q51451
G	224	ASN	-	expression tag	UNP Q51451
G	225	SER	-	expression tag	UNP Q51451
G	226	GLU	-	expression tag	UNP Q51451
G	227	ASN	-	expression tag	UNP Q51451
G	228	LEU	-	expression tag	UNP Q51451
G	229	TYR	-	expression tag	UNP Q51451
G	230	PHE	-	expression tag	UNP Q51451
G	231	GLN	-	expression tag	UNP Q51451
G	232	GLY	-	expression tag	UNP Q51451
G	233	ALA	-	expression tag	UNP Q51451
G	379	ALA	GLU	engineered mutation	UNP Q51451
G	381	ALA	GLU	engineered mutation	UNP Q51451
G	415	LEU	GLN	conflict	UNP Q51451
G	434	PRO	ARG	conflict	UNP Q51451
H	210	MET	-	initiating methionine	UNP Q51451
H	211	GLY	-	expression tag	UNP Q51451
H	212	SER	-	expression tag	UNP Q51451
H	213	SER	-	expression tag	UNP Q51451
H	214	HIS	-	expression tag	UNP Q51451
H	215	HIS	-	expression tag	UNP Q51451
H	216	HIS	-	expression tag	UNP Q51451
H	217	HIS	-	expression tag	UNP Q51451
H	218	HIS	-	expression tag	UNP Q51451
H	219	HIS	-	expression tag	UNP Q51451
H	220	SER	-	expression tag	UNP Q51451

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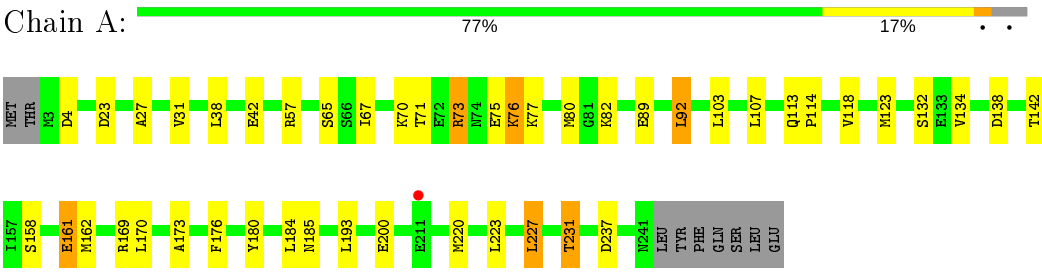
Chain	Residue	Modelled	Actual	Comment	Reference
H	221	GLN	-	expression tag	UNP Q51451
H	222	ASP	-	expression tag	UNP Q51451
H	223	PRO	-	expression tag	UNP Q51451
H	224	ASN	-	expression tag	UNP Q51451
H	225	SER	-	expression tag	UNP Q51451
H	226	GLU	-	expression tag	UNP Q51451
H	227	ASN	-	expression tag	UNP Q51451
H	228	LEU	-	expression tag	UNP Q51451
H	229	TYR	-	expression tag	UNP Q51451
H	230	PHE	-	expression tag	UNP Q51451
H	231	GLN	-	expression tag	UNP Q51451
H	232	GLY	-	expression tag	UNP Q51451
H	233	ALA	-	expression tag	UNP Q51451
H	379	ALA	GLU	engineered mutation	UNP Q51451
H	381	ALA	GLU	engineered mutation	UNP Q51451
H	415	LEU	GLN	conflict	UNP Q51451
H	434	PRO	ARG	conflict	UNP Q51451

3 Residue-property plots (i)

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.

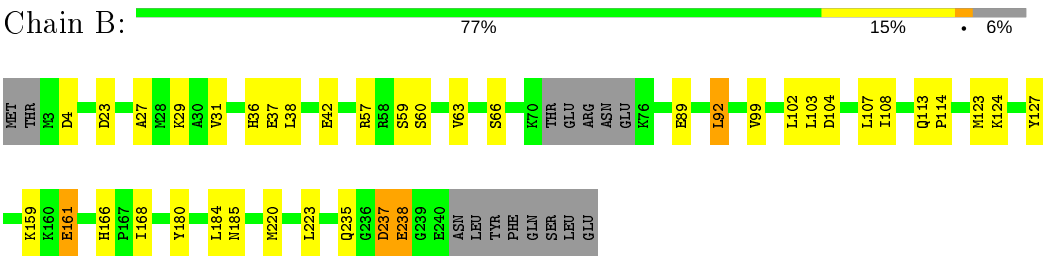
- Molecule 1: 14-3-3 protein beta/alpha

Chain A:



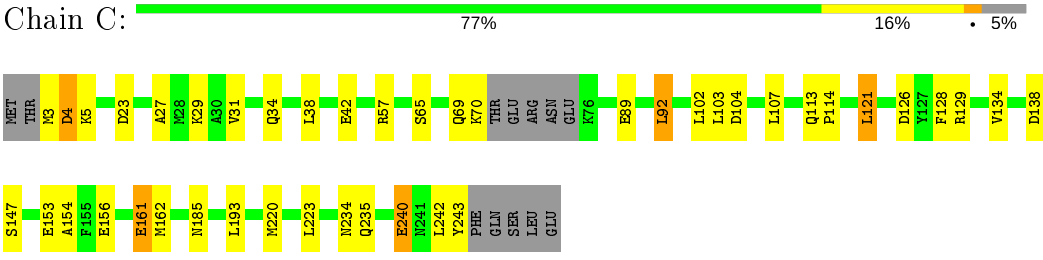
- Molecule 1: 14-3-3 protein beta/alpha

Chain B:



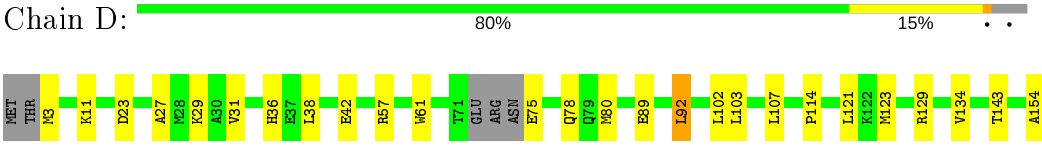
- Molecule 1: 14-3-3 protein beta/alpha

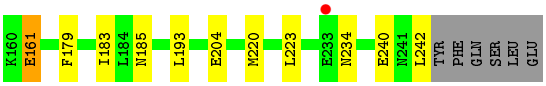
Chain C:



- Molecule 1: 14-3-3 protein beta/alpha

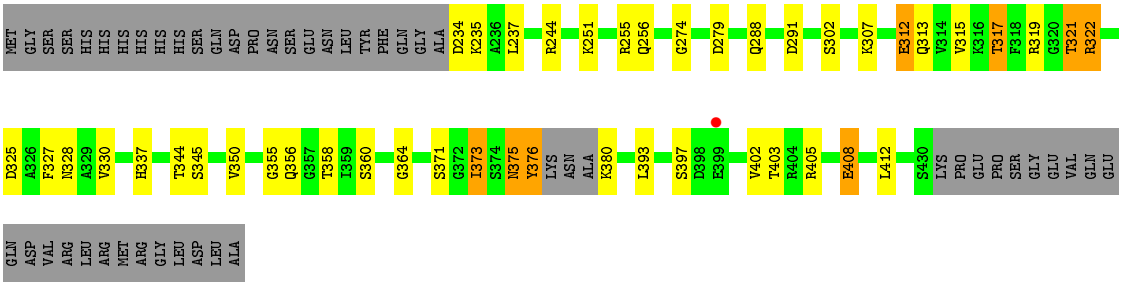
Chain D:





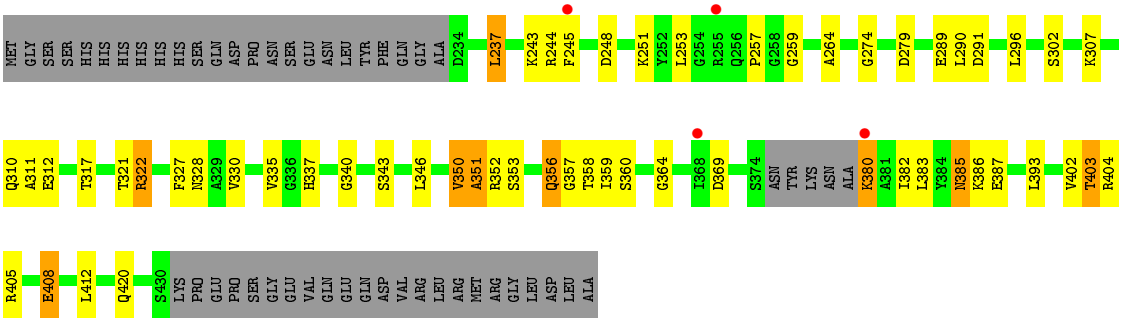
- Molecule 2: Exoenzyme S

Chain E:



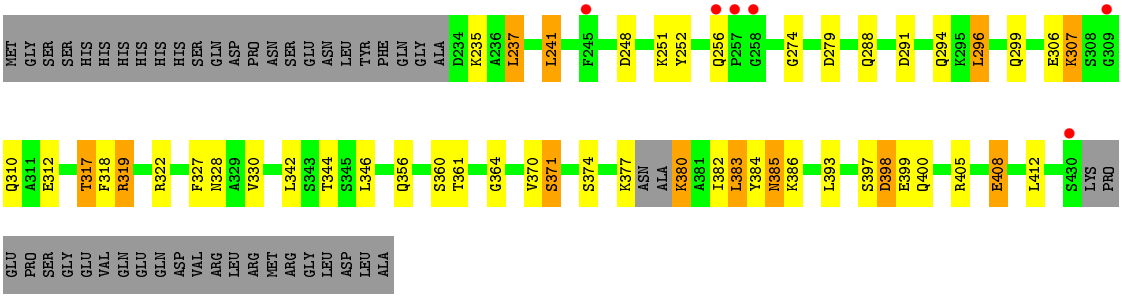
- Molecule 2: Exoenzyme S

Chain F:



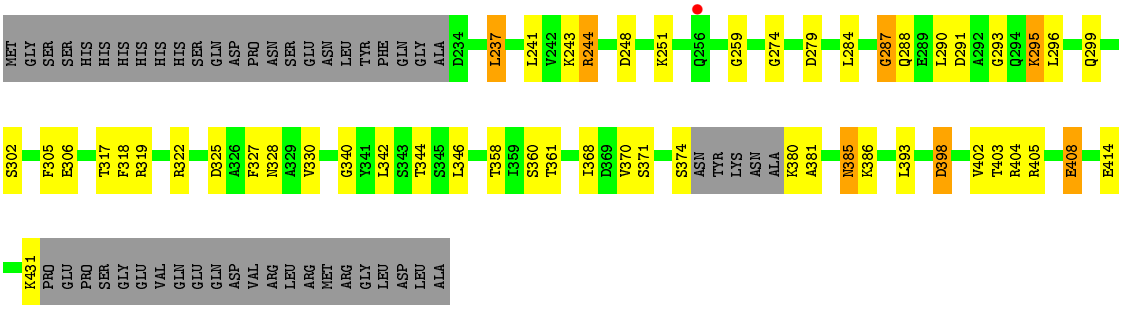
- Molecule 2: Exoenzyme S

Chain G:



- Molecule 2: Exoenzyme S

Chain H:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER GLN ASP PRO ASN SER GLU ASN LEU TYR PHE GLN GLY ALA D234 L237 L241 V242 K243 R244 D248 K251 Q256 G259 G274 D279 L284 G287 Q288 E289 L290 D291 A292 G293 Q294 K295 L296 Q299
S302 F305 E306 T317 F318 R319 R322 D325 A326 F327 N328 A329 V330 G340 Y341 L342 S343 T344 S345 L346 T358 I359 S360 T361 I368 D369 V370 S371 S374 ASN TYR LYS ASN ALA K380 A381 N385 K386 L393 D398 V402 T403 R404 R405 E408 E414
K431 PRO GLU PRO SER GLY GLU VAL GLN GLU GLN ASP VAL ARG LEU ARG MET ARG GLY LEU ASP LEU ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	165.20Å 168.76Å 82.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.05 – 3.24 118.05 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.0 (118.05-3.24) 98.9 (118.05-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.243 , 0.294 0.256 , 0.311	Depositor DCC
R_{free} test set	1830 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	13303	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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

5.1 Standard geometry

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	0/1946	0.67	0/2619
1	B	0.52	0/1889	0.65	0/2542
1	C	0.51	0/1922	0.66	1/2587 (0.0%)
1	D	0.50	0/1913	0.67	1/2577 (0.0%)
2	E	0.53	0/1454	0.79	0/1953
2	F	0.51	0/1438	0.79	1/1930 (0.1%)
2	G	0.54	0/1462	0.77	0/1963
2	H	0.51	0/1447	0.75	1/1941 (0.1%)
All	All	0.52	0/13471	0.71	4/18112 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	240	GLU	C-N-CA	8.85	143.83	121.70
1	C	240	GLU	C-N-CA	8.08	141.91	121.70
2	F	245	PHE	C-N-CA	5.99	134.88	122.30
2	H	287	GLY	C-N-CA	5.29	134.92	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	240	GLU	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	1919	0	1879	16	0
1	B	1863	0	1823	17	0
1	C	1895	0	1853	15	0
1	D	1887	0	1836	16	0
2	E	1438	0	1401	17	0
2	F	1423	0	1395	26	0
2	G	1446	0	1412	19	0
2	H	1432	0	1408	20	0
All	All	13303	0	13007	142	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 5.

All (142) 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:237:ASP:HB2	1:B:238:GLU:HB3	1.55	0.86
1:D:204:GLU:HG2	2:F:352:ARG:NH1	1.91	0.85
1:C:4:ASP:HA	1:C:34:GLN:HE22	1.42	0.83
1:D:204:GLU:HG2	2:F:352:ARG:HH12	1.45	0.81
2:H:385:ASN:HD22	2:H:386:LYS:H	1.31	0.79
2:F:385:ASN:HD22	2:F:386:LYS:H	1.31	0.76
2:G:385:ASN:HD22	2:G:386:LYS:H	1.33	0.72
1:B:237:ASP:HB2	1:B:238:GLU:CB	2.22	0.70
2:E:322:ARG:HE	2:E:322:ARG:HA	1.55	0.70
2:H:319:ARG:HB2	2:H:344:THR:HG22	1.75	0.68
1:B:114:PRO:HG3	1:B:161:GLU:HG2	1.75	0.67
2:E:371:SER:OG	2:E:380:LYS:HA	1.95	0.66
2:F:351:ALA:HA	2:F:359:ILE:HG21	1.78	0.66
2:E:317:THR:HB	2:E:344:THR:HB	1.79	0.64
2:G:393:LEU:HD21	2:G:408:GLU:HG2	1.79	0.63
1:A:76:LYS:O	1:A:80:MET:HG2	1.99	0.63
2:F:350:VAL:HA	2:F:353:SER:HB2	1.81	0.63
1:A:227:LEU:O	1:A:231:THR:HB	1.99	0.62
1:A:114:PRO:HG3	1:A:161:GLU:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:PRO:HG3	1:D:161:GLU:HG2	1.80	0.62
2:E:321:THR:HG21	2:E:325:ASP:HB2	1.82	0.62
2:E:393:LEU:HD21	2:E:408:GLU:HG2	1.82	0.61
1:C:121:LEU:HB3	1:C:154:ALA:HB2	1.82	0.61
2:H:241:LEU:HD12	2:H:296:LEU:HD23	1.83	0.61
2:G:371:SER:HG	2:G:380:LYS:N	1.99	0.60
2:E:321:THR:HB	2:E:358:THR:OG1	2.02	0.58
2:G:319:ARG:HB3	2:G:344:THR:HG22	1.84	0.58
2:H:393:LEU:HD21	2:H:408:GLU:HG2	1.85	0.56
2:F:393:LEU:HD21	2:F:408:GLU:HG2	1.88	0.55
1:D:121:LEU:HB2	1:D:154:ALA:HB2	1.89	0.55
1:B:237:ASP:HB2	1:B:238:GLU:CA	2.37	0.54
2:E:397:SER:HB3	2:E:403:THR:HA	1.88	0.54
1:D:38:LEU:HD22	1:D:42:GLU:HB3	1.90	0.54
2:H:346:LEU:HB2	2:H:380:LYS:HB3	1.89	0.54
1:D:103:LEU:HA	1:D:107:LEU:HB2	1.90	0.54
1:C:38:LEU:HD22	1:C:42:GLU:HB3	1.90	0.54
2:G:370:VAL:HG11	2:G:383:LEU:HD23	1.90	0.54
2:G:397:SER:O	2:G:398:ASP:O	2.26	0.53
2:F:289:GLU:HB3	2:F:290:LEU:HB2	1.89	0.53
1:A:158:SER:HA	1:A:162:MET:HE3	1.91	0.53
1:A:170:LEU:O	1:A:173:ALA:HB3	2.09	0.52
2:E:322:ARG:NE	2:E:322:ARG:HA	2.21	0.52
1:C:114:PRO:HG3	1:C:161:GLU:HG3	1.91	0.52
1:B:103:LEU:HA	1:B:107:LEU:HB2	1.90	0.52
2:H:327:PHE:HA	2:H:330:VAL:HG23	1.92	0.52
1:A:38:LEU:HD22	1:A:42:GLU:HB3	1.92	0.52
1:B:99:VAL:HG11	1:B:127:TYR:CD2	2.45	0.52
2:H:328:ASN:HA	2:H:405:ARG:NH2	2.25	0.52
2:G:364:GLY:HA2	2:G:412:LEU:HD11	1.91	0.51
2:G:317:THR:HG21	2:G:382:ILE:HB	1.92	0.51
2:E:345:SER:HB3	2:E:350:VAL:HG21	1.92	0.51
1:A:89:GLU:HG2	1:A:134:VAL:HB	1.93	0.51
1:D:204:GLU:CG	2:F:352:ARG:HH12	2.20	0.51
2:H:237:LEU:HD11	2:H:299:GLN:HB3	1.91	0.51
1:C:103:LEU:HA	1:C:107:LEU:HB2	1.93	0.50
2:F:385:ASN:HD22	2:F:386:LYS:N	2.05	0.50
2:H:325:ASP:H	2:H:328:ASN:ND2	2.09	0.50
2:F:322:ARG:HG2	2:F:357:GLY:H	1.77	0.50
2:G:291:ASP:HB2	2:G:294:GLN:HG3	1.93	0.50
2:F:337:HIS:CD2	2:F:387:GLU:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:358:THR:HG22	2:F:403:THR:HG23	1.93	0.49
2:G:241:LEU:HD13	2:G:296:LEU:HD12	1.95	0.49
1:C:89:GLU:HG2	1:C:134:VAL:HB	1.94	0.49
2:G:385:ASN:HD22	2:G:386:LYS:N	2.05	0.49
1:C:126:ASP:O	1:C:129:ARG:HB3	2.12	0.49
2:F:237:LEU:HD12	2:F:264:ALA:HB1	1.95	0.49
2:H:385:ASN:HD22	2:H:386:LYS:N	2.05	0.48
1:A:220:MET:HA	1:A:223:LEU:HD12	1.94	0.48
1:A:103:LEU:HA	1:A:107:LEU:HB2	1.93	0.48
1:D:129:ARG:HD3	1:D:179:PHE:HB2	1.95	0.48
1:B:108:ILE:CD1	1:B:124:LYS:HE2	2.44	0.48
1:B:220:MET:HA	1:B:223:LEU:HD12	1.96	0.48
2:F:328:ASN:HA	2:F:405:ARG:NH2	2.29	0.48
2:F:408:GLU:O	2:F:408:GLU:HG3	2.13	0.48
2:E:319:ARG:HB2	2:E:344:THR:HG22	1.95	0.48
1:B:89:GLU:HG2	1:B:134:VAL:HB	1.95	0.48
2:F:322:ARG:HE	2:F:322:ARG:HA	1.78	0.47
2:G:237:LEU:HD11	2:G:299:GLN:HG3	1.96	0.47
1:D:61:TRP:CE2	1:D:134:VAL:HG12	2.49	0.47
2:G:237:LEU:HD23	2:G:241:LEU:HD22	1.96	0.47
2:H:371:SER:HB3	2:H:380:LYS:HA	1.95	0.47
1:D:121:LEU:CB	1:D:154:ALA:HB2	2.45	0.47
1:B:38:LEU:HD22	1:B:42:GLU:HB3	1.96	0.46
2:G:252:TYR:HE1	2:G:374:SER:HB3	1.79	0.46
1:C:220:MET:HA	1:C:223:LEU:HD12	1.97	0.46
2:E:356:GLN:O	2:E:402:VAL:HB	2.16	0.46
2:E:375:ASN:HB2	2:E:376:TYR:CD2	2.50	0.46
1:A:67:ILE:HA	1:A:70:LYS:HE2	1.98	0.46
1:D:220:MET:HA	1:D:223:LEU:HD12	1.97	0.45
2:H:358:THR:HG22	2:H:403:THR:HB	1.96	0.45
2:H:290:LEU:HD23	2:H:295:LYS:HA	1.98	0.45
2:F:346:LEU:HB2	2:F:380:LYS:HB2	1.99	0.45
1:C:121:LEU:HD22	1:C:153:GLU:HB3	1.99	0.45
1:A:27:ALA:O	1:A:31:VAL:HG23	2.17	0.45
2:F:364:GLY:HA2	2:F:412:LEU:HD11	1.99	0.45
2:E:364:GLY:HA2	2:E:412:LEU:HD11	1.99	0.45
2:E:328:ASN:HA	2:E:405:ARG:NH2	2.31	0.45
2:F:322:ARG:HG2	2:F:357:GLY:N	2.33	0.44
1:D:129:ARG:HG3	1:D:183:ILE:HG13	1.98	0.44
2:E:327:PHE:HA	2:E:330:VAL:HG23	1.99	0.44
2:F:369:ASP:HA	2:F:382:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:328:ASN:HA	2:G:405:ARG:NH2	2.33	0.44
1:D:89:GLU:HG2	1:D:134:VAL:HB	2.00	0.44
2:F:327:PHE:HA	2:F:330:VAL:HG23	2.00	0.44
2:H:398:ASP:HB2	2:H:402:VAL:H	1.82	0.44
1:C:57:ARG:HB3	1:C:92:LEU:HD12	2.00	0.43
2:F:351:ALA:HA	2:F:359:ILE:CG2	2.45	0.43
2:G:346:LEU:HB2	2:G:380:LYS:HB3	1.99	0.43
2:H:284:LEU:HD13	2:H:340:GLY:HA2	2.00	0.43
2:H:305:PHE:HA	2:H:368:ILE:HD11	2.01	0.43
1:C:27:ALA:O	1:C:31:VAL:HG23	2.19	0.43
2:G:342:LEU:HB3	2:G:384:TYR:HB2	2.00	0.43
1:D:27:ALA:O	1:D:31:VAL:HG23	2.19	0.43
2:E:322:ARG:HD2	2:E:355:GLY:O	2.18	0.43
2:G:318:PHE:HD1	2:G:361:THR:HG22	1.82	0.43
2:H:325:ASP:OD2	2:H:327:PHE:HB2	2.18	0.43
1:A:142:THR:HG22	1:A:146:ASN:HD21	1.83	0.42
1:B:27:ALA:O	1:B:31:VAL:HG23	2.18	0.42
1:A:158:SER:HB2	1:A:169:ARG:HG3	2.01	0.42
2:H:244:ARG:HD2	2:H:293:GLY:HA3	2.01	0.42
1:C:29:LYS:HG3	1:C:102:LEU:HD11	2.02	0.42
1:A:57:ARG:HB3	1:A:92:LEU:HD12	2.01	0.42
1:B:57:ARG:HB3	1:B:92:LEU:HD12	2.01	0.42
2:F:340:GLY:O	2:F:386:LYS:HA	2.19	0.41
2:H:318:PHE:CD1	2:H:361:THR:HG22	2.55	0.41
1:B:36:HIS:CE1	1:C:3:MET:HA	2.55	0.41
1:B:166:HIS:HE1	1:B:168:ILE:HD12	1.85	0.41
2:F:322:ARG:HA	2:F:322:ARG:NE	2.35	0.41
2:H:370:VAL:HG23	2:H:381:ALA:HB3	2.03	0.41
2:F:343:SER:HA	2:F:383:LEU:HD23	2.02	0.41
1:A:180:TYR:CD1	1:A:184:LEU:HD12	2.56	0.41
1:B:29:LYS:HG3	1:B:102:LEU:HD11	2.02	0.41
1:D:57:ARG:HB3	1:D:92:LEU:HD12	2.02	0.41
2:F:356:GLN:HE21	2:F:356:GLN:HA	1.85	0.41
1:B:180:TYR:CD1	1:B:184:LEU:HD12	2.56	0.41
1:D:29:LYS:HG3	1:D:102:LEU:HD11	2.02	0.40
2:G:327:PHE:HA	2:G:330:VAL:HG23	2.02	0.40
1:A:118:VAL:HG21	1:A:162:MET:HE3	2.03	0.40
1:B:59:SER:O	1:B:63:VAL:HG23	2.21	0.40
1:C:142:THR:HG22	1:C:146:ASN:HD21	1.86	0.40
1:C:128:PHE:HB3	1:C:147:SER:HB2	2.03	0.40
2:E:376:TYR:CD1	2:E:376:TYR:N	2.90	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	237/248 (96%)	221 (93%)	15 (6%)	1 (0%)	34	68
1	B	229/248 (92%)	214 (93%)	13 (6%)	2 (1%)	17	52
1	C	232/248 (94%)	219 (94%)	12 (5%)	1 (0%)	34	68
1	D	233/248 (94%)	222 (95%)	11 (5%)	0	100	100
2	E	190/244 (78%)	161 (85%)	22 (12%)	7 (4%)	3	20
2	F	188/244 (77%)	164 (87%)	17 (9%)	7 (4%)	3	20
2	G	191/244 (78%)	171 (90%)	15 (8%)	5 (3%)	5	28
2	H	189/244 (78%)	163 (86%)	22 (12%)	4 (2%)	7	33
All	All	1689/1968 (86%)	1535 (91%)	127 (8%)	27 (2%)	9	40

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	5	LYS
2	E	256	GLN
2	F	257	PRO
2	G	398	ASP
2	H	288	GLN
2	E	375	ASN
2	F	259	GLY
2	F	310	GLN
2	F	351	ALA
2	G	312	GLU
2	H	287	GLY
1	B	37	GLU
1	B	235	GLN
2	E	255	ARG

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Mol	Chain	Res	Type
2	E	312	GLU
2	H	274	GLY
1	A	73	ARG
2	E	288	GLN
2	F	311	ALA
2	F	420	GLN
2	G	307	LYS
2	G	399	GLU
2	H	259	GLY
2	E	274	GLY
2	E	373	ILE
2	F	274	GLY
2	G	274	GLY

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	210/220 (96%)	187 (89%)	23 (11%)	6 25
1	B	203/220 (92%)	189 (93%)	14 (7%)	15 46
1	C	207/220 (94%)	188 (91%)	19 (9%)	9 32
1	D	205/220 (93%)	188 (92%)	17 (8%)	11 38
2	E	145/189 (77%)	125 (86%)	20 (14%)	3 15
2	F	144/189 (76%)	119 (83%)	25 (17%)	2 9
2	G	146/189 (77%)	122 (84%)	24 (16%)	2 10
2	H	145/189 (77%)	124 (86%)	21 (14%)	3 14
All	All	1405/1636 (86%)	1242 (88%)	163 (12%)	5 23

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	23	ASP

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Mol	Chain	Res	Type
1	A	65	SER
1	A	71	THR
1	A	73	ARG
1	A	75	GLU
1	A	76	LYS
1	A	77	LYS
1	A	82	LYS
1	A	92	LEU
1	A	113	GLN
1	A	123	MET
1	A	132	SER
1	A	138	ASP
1	A	156	GLU
1	A	161	GLU
1	A	176	PHE
1	A	185	ASN
1	A	193	LEU
1	A	200	GLU
1	A	227	LEU
1	A	231	THR
1	A	237	ASP
1	B	4	ASP
1	B	23	ASP
1	B	60	SER
1	B	66	SER
1	B	92	LEU
1	B	104	ASP
1	B	113	GLN
1	B	123	MET
1	B	156	GLU
1	B	159	LYS
1	B	161	GLU
1	B	185	ASN
1	B	237	ASP
1	B	238	GLU
1	C	4	ASP
1	C	23	ASP
1	C	65	SER
1	C	69	GLN
1	C	70	LYS
1	C	92	LEU
1	C	104	ASP

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Mol	Chain	Res	Type
1	C	113	GLN
1	C	121	LEU
1	C	138	ASP
1	C	156	GLU
1	C	161	GLU
1	C	162	MET
1	C	185	ASN
1	C	193	LEU
1	C	234	ASN
1	C	235	GLN
1	C	242	LEU
1	C	243	TYR
1	D	3	MET
1	D	11	LYS
1	D	23	ASP
1	D	36	HIS
1	D	75	GLU
1	D	78	GLN
1	D	80	MET
1	D	92	LEU
1	D	123	MET
1	D	143	THR
1	D	156	GLU
1	D	159	LYS
1	D	161	GLU
1	D	185	ASN
1	D	193	LEU
1	D	234	ASN
1	D	242	LEU
2	E	234	ASP
2	E	235	LYS
2	E	237	LEU
2	E	244	ARG
2	E	251	LYS
2	E	279	ASP
2	E	291	ASP
2	E	302	SER
2	E	307	LYS
2	E	312	GLU
2	E	313	GLN
2	E	315	VAL
2	E	317	THR

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Mol	Chain	Res	Type
2	E	321	THR
2	E	322	ARG
2	E	337	HIS
2	E	360	SER
2	E	373	ILE
2	E	376	TYR
2	E	408	GLU
2	F	237	LEU
2	F	243	LYS
2	F	244	ARG
2	F	248	ASP
2	F	251	LYS
2	F	253	LEU
2	F	279	ASP
2	F	291	ASP
2	F	296	LEU
2	F	302	SER
2	F	307	LYS
2	F	312	GLU
2	F	317	THR
2	F	321	THR
2	F	322	ARG
2	F	335	VAL
2	F	350	VAL
2	F	356	GLN
2	F	360	SER
2	F	380	LYS
2	F	385	ASN
2	F	402	VAL
2	F	403	THR
2	F	404	ARG
2	F	408	GLU
2	G	235	LYS
2	G	237	LEU
2	G	241	LEU
2	G	248	ASP
2	G	251	LYS
2	G	256	GLN
2	G	279	ASP
2	G	288	GLN
2	G	296	LEU
2	G	306	GLU

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Mol	Chain	Res	Type
2	G	307	LYS
2	G	310	GLN
2	G	317	THR
2	G	319	ARG
2	G	322	ARG
2	G	356	GLN
2	G	360	SER
2	G	371	SER
2	G	377	LYS
2	G	380	LYS
2	G	383	LEU
2	G	385	ASN
2	G	400	GLN
2	G	408	GLU
2	H	237	LEU
2	H	243	LYS
2	H	244	ARG
2	H	248	ASP
2	H	251	LYS
2	H	279	ASP
2	H	291	ASP
2	H	295	LYS
2	H	302	SER
2	H	306	GLU
2	H	317	THR
2	H	322	ARG
2	H	342	LEU
2	H	360	SER
2	H	374	SER
2	H	385	ASN
2	H	398	ASP
2	H	404	ARG
2	H	408	GLU
2	H	414	GLU
2	H	431	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	B	79	GLN
1	B	146	ASN

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Mol	Chain	Res	Type
1	B	234	ASN
1	C	34	GLN
1	C	146	ASN
1	D	221	GLN
1	D	235	GLN
2	E	286	GLN
2	F	385	ASN
2	G	356	GLN
2	G	375	ASN
2	G	385	ASN
2	H	294	GLN
2	H	310	GLN
2	H	385	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	239/248 (96%)	-0.29	1 (0%) 92 90	18, 38, 74, 101	0
1	B	233/248 (93%)	-0.01	0 100 100	15, 37, 66, 104	0
1	C	236/248 (95%)	0.03	0 100 100	33, 57, 84, 100	0
1	D	237/248 (95%)	0.04	1 (0%) 92 90	25, 54, 91, 115	0
2	E	194/244 (79%)	0.13	1 (0%) 91 87	23, 55, 90, 98	0
2	F	192/244 (78%)	0.21	4 (2%) 63 53	28, 61, 101, 122	0
2	G	195/244 (79%)	0.09	6 (3%) 49 37	15, 53, 95, 110	0
2	H	193/244 (79%)	-0.15	1 (0%) 91 87	35, 59, 90, 123	0
All	All	1719/1968 (87%)	-0.00	14 (0%) 86 80	15, 52, 90, 123	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	258	GLY	3.5
2	G	256	GLN	3.3
2	G	257	PRO	2.8
2	E	399	GLU	2.7
2	F	380	LYS	2.7
2	F	245	PHE	2.6
2	G	245	PHE	2.5
2	H	256	GLN	2.2
2	G	309	GLY	2.2
2	F	368	ILE	2.2
2	G	430	SER	2.2
1	D	233	GLU	2.2
2	F	255	ARG	2.1
1	A	211	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.