



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:09 AM GMT

PDB ID : 2PNJ
Title : Crystal structure of human ferrochelatase mutant with Phe 337 replaced by Ala
Authors : Dailey, H.A.; Wu, C.-K.; Horanyi, P.; Medlock, A.E.; Najahi-Missaoui, W.; Burden, A.E.; Dailey, T.A.; Rose, J.P.
Deposited on : 2007-04-24
Resolution : 2.35 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

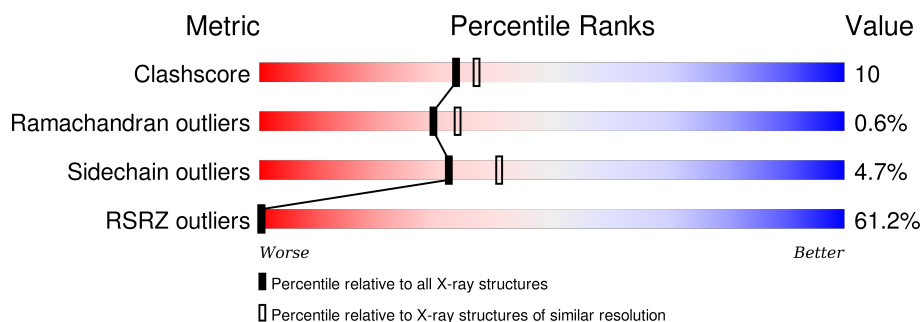
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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	359	<div> <div>36%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
1	B	359	<div> <div>85%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CHD	B	501	-	-	-	X
3	CHD	B	502	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CHD	B	503	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6166 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.

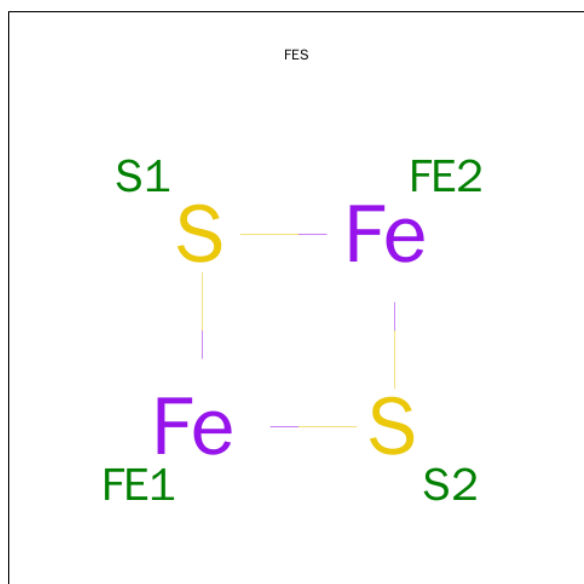
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2815	1794	481	522	18			
1	B	356	Total	C	N	O	S	0	0	0
			2827	1803	484	522	18			

There are 4 discrepancies between the modelled and reference sequences:

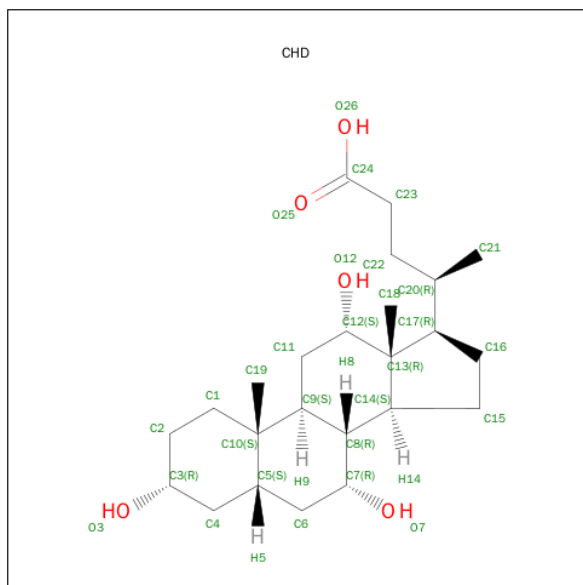
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	ENGINEERED	UNP P22830
A	337	ALA	PHE	ENGINEERED	UNP P22830
B	115	LEU	ARG	ENGINEERED	UNP P22830
B	337	ALA	PHE	ENGINEERED	UNP P22830

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0

- Molecule 3 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0

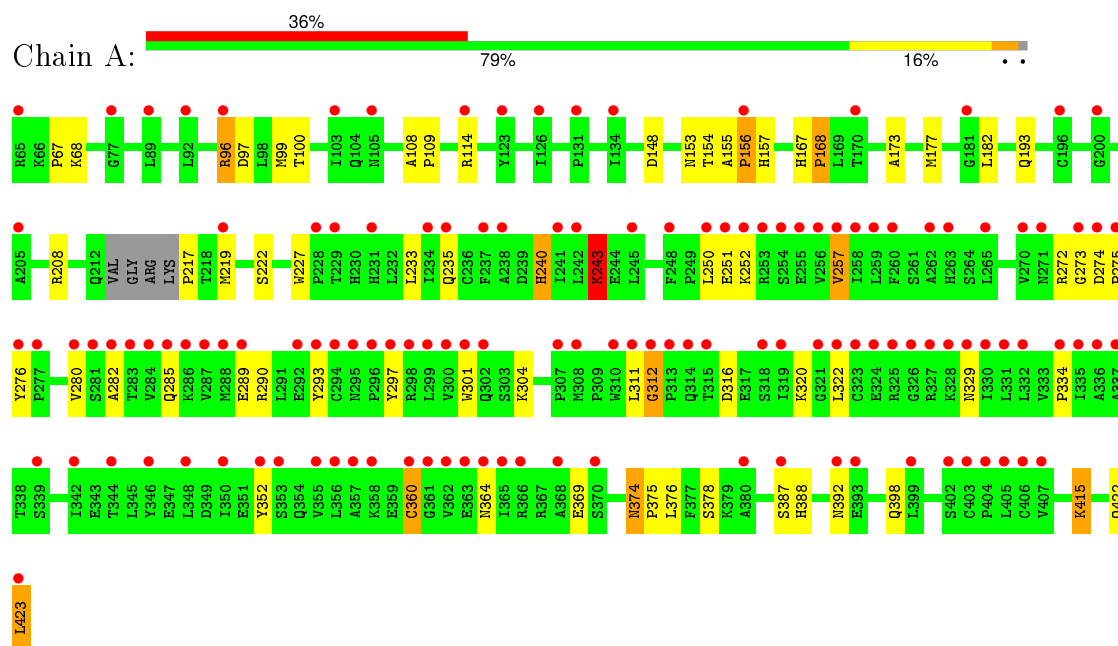
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	172	Total O 172 172	0	0
4	B	170	Total O 170 170	0	0

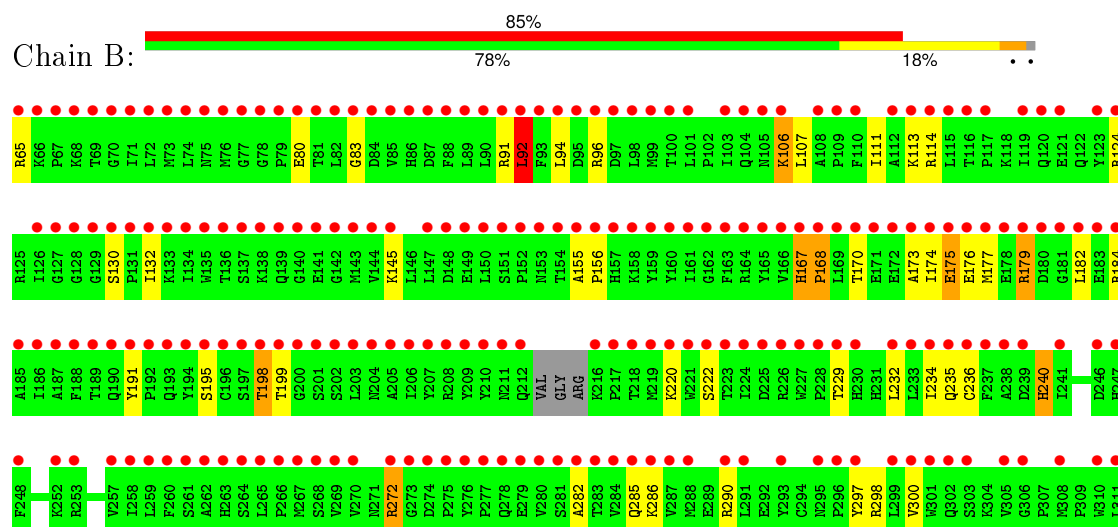
3 Residue-property plots

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



• Molecule 1: Ferrochelatase, mitochondrial



G312	P313	Q314	T315	S318	I319	K320	C323	E324	N329	I330	L331	L332	V333	P334	I335	A336	A337	T338	S339	D340	H341	I342	T343	T344	L345	Y346	E347	L348	D349	I350	E351	Y352	S353	Q354	V355	L356	A357	K358	E359	C360	G361	V362	E363	N364	I365	R366	R367	A368	E369	S370	L371	N372	G373	N374	P375	L376
F377	S378	K379	A380	I381	A382	D383	L384	Y385	H386	S387	H388	I389	Q390	S391	N392	E393	I394	C395	S396	K397	Q398	L399	T400	I401	S402	C403	P404	L405	C406	V407	M408	P409	V410	C411	R412	E413	T414	R415	S416	F417	F418	T419	S420	Q421	Q422	L423										

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.69Å 94.05Å 113.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 2.35 48.52 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.44-2.35) 80.5 (48.52-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.192 , 0.253 0.401 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 58876 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	6166	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.66 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5280e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHD, FES

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	0.76	1/2883 (0.0%)	0.78	2/3916 (0.1%)
1	B	0.77	0/2895	0.81	4/3931 (0.1%)
All	All	0.76	1/5778 (0.0%)	0.80	6/7847 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	GLY	CA-C	-5.00	1.43	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	HIS	C-N-CD	-9.73	99.19	120.60
1	B	92	LEU	CA-CB-CG	7.40	132.33	115.30
1	A	312	GLY	N-CA-C	-6.72	96.29	113.10
1	B	91	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	243	LYS	CD-CE-NZ	5.49	124.32	111.70
1	B	167	HIS	C-N-CA	5.03	143.13	122.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ALA	Peptide
1	A	167	HIS	Mainchain,Peptide
1	A	311	LEU	Peptide
1	B	155	ALA	Mainchain,Peptide
1	B	167	HIS	Peptide
1	B	312	GLY	Mainchain,Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2815	0	2769	56	8
1	B	2827	0	2790	64	5
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	87	0	117	2	0
3	B	87	0	117	4	0
4	A	172	0	0	13	2
4	B	170	0	0	19	7
All	All	6166	0	5793	118	11

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 10.

All (118) 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:243:LYS:HD2	4:A:616:HOH:O	1.28	1.31
1:B:410:VAL:HB	4:B:633:HOH:O	1.43	1.18
1:B:323:CYS:HB3	4:B:602:HOH:O	1.47	1.13
1:A:398:GLN:HE22	1:B:297:TYR:H	1.15	0.94
1:B:272:ARG:NH1	4:B:673:HOH:O	2.01	0.93
1:B:323:CYS:CB	4:B:602:HOH:O	2.09	0.86
1:A:240:HIS:O	1:A:243:LYS:HE3	1.75	0.85
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:CYS:SG	4:B:602:HOH:O	2.35	0.83
1:B:198:THR:HG22	1:B:199:THR:H	1.42	0.83
1:A:67:PRO:HA	1:A:156:PRO:HB2	1.60	0.82
1:A:388:HIS:HD2	4:A:561:HOH:O	1.69	0.76
1:B:300:VAL:HG12	1:B:313:PRO:HG2	1.70	0.74
1:B:198:THR:HG21	4:B:517:HOH:O	1.87	0.74
1:B:176:GLU:HG3	4:B:609:HOH:O	1.87	0.73
1:A:297:TYR:H	1:B:398:GLN:HE22	1.33	0.73
1:B:334:PRO:CG	4:B:564:HOH:O	2.37	0.72
1:A:222:SER:OG	1:A:388:HIS:HE1	1.73	0.71
1:A:217:PRO:N	4:A:504:HOH:O	2.23	0.70
1:B:334:PRO:HG3	4:B:564:HOH:O	1.90	0.70
1:B:222:SER:OG	1:B:388:HIS:HE1	1.75	0.70
1:B:402:SER:CB	4:B:551:HOH:O	2.40	0.70
1:A:392:ASN:ND2	4:A:605:HOH:O	2.26	0.68
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.59	0.67
1:B:298:ARG:HG2	4:B:565:HOH:O	1.95	0.65
1:A:240:HIS:HD2	1:A:369:GLU:O	1.79	0.64
1:B:422:GLN:O	1:B:423:LEU:HB2	1.98	0.64
1:B:402:SER:HB3	4:B:551:HOH:O	1.98	0.63
1:A:329:ASN:ND2	1:A:364:ASN:HB2	2.12	0.63
1:B:175:GLU:O	1:B:179:ARG:HG2	1.99	0.62
1:B:240:HIS:HD2	1:B:369:GLU:O	1.83	0.61
1:A:114:ARG:HG3	4:A:585:HOH:O	2.00	0.61
1:A:422:GLN:O	1:A:423:LEU:HB2	2.01	0.61
1:A:398:GLN:HE22	1:B:297:TYR:N	1.93	0.60
1:B:168:PRO:HD3	4:B:639:HOH:O	2.00	0.60
1:B:198:THR:CG2	1:B:199:THR:H	2.16	0.58
1:B:388:HIS:HD2	1:B:393:GLU:OE1	1.86	0.58
1:B:386:HIS:O	1:B:390:GLN:HG3	2.04	0.57
1:B:191:TYR:CD1	1:B:198:THR:HG23	2.40	0.57
1:A:273:GLY:O	1:B:298:ARG:HD3	2.04	0.57
1:B:402:SER:HB2	4:B:551:HOH:O	2.04	0.56
1:A:240:HIS:HA	1:A:243:LYS:HE3	1.87	0.56
1:B:195:SER:HB3	1:B:198:THR:HB	1.87	0.56
1:B:229:THR:HB	1:B:286:LYS:HE2	1.87	0.55
1:A:334:PRO:HG2	4:A:578:HOH:O	2.05	0.54
1:B:173:ALA:O	1:B:177:MET:HG3	2.08	0.54
1:A:97:ASP:CG	1:A:208:ARG:HH22	2.11	0.53
1:A:97:ASP:OD1	1:A:208:ARG:NH2	2.41	0.53
1:A:243:LYS:CD	4:A:616:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:SER:OG	1:B:388:HIS:CE1	2.60	0.52
1:A:168:PRO:HD3	4:A:626:HOH:O	2.08	0.52
1:A:68:LYS:NZ	1:A:153:ASN:O	2.41	0.52
1:A:240:HIS:HA	1:A:243:LYS:CE	2.40	0.52
1:B:392:ASN:HB2	4:B:660:HOH:O	2.09	0.52
1:B:232:LEU:HD22	1:B:376:LEU:HD11	1.92	0.52
1:B:229:THR:HB	1:B:286:LYS:CE	2.40	0.51
1:A:154:THR:OG1	1:A:157:HIS:HE1	1.94	0.51
1:B:106:LYS:HB2	1:B:106:LYS:NZ	2.26	0.51
1:A:374:ASN:HD22	1:A:375:PRO:N	2.09	0.50
1:B:416:SER:O	1:B:420:SER:HB2	2.10	0.50
1:B:235:GLN:HG3	1:B:290:ARG:CZ	2.42	0.49
1:A:243:LYS:CE	4:A:616:HOH:O	2.50	0.49
1:B:198:THR:HG22	1:B:199:THR:N	2.19	0.49
1:B:92:LEU:HD11	3:B:501:CHD:H62	1.95	0.49
1:A:240:HIS:CA	1:A:243:LYS:HE3	2.42	0.49
1:B:320:LYS:O	1:B:324:GLU:HG3	2.13	0.49
1:A:148:ASP:OD1	1:A:157:HIS:HD2	1.94	0.49
1:B:94:LEU:O	1:B:96:ARG:NH1	2.44	0.48
1:A:374:ASN:ND2	1:A:376:LEU:H	2.11	0.48
1:A:222:SER:OG	1:A:388:HIS:CE1	2.61	0.48
1:A:374:ASN:HD22	1:A:374:ASN:C	2.16	0.48
1:B:198:THR:CG2	1:B:199:THR:N	2.74	0.47
1:A:320:LYS:HG3	1:A:360:CYS:SG	2.53	0.47
1:A:154:THR:OG1	1:A:157:HIS:CE1	2.68	0.47
1:A:240:HIS:C	1:A:243:LYS:HE3	2.34	0.47
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.95	0.47
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.48	0.47
1:A:301:TRP:CD1	1:A:312:GLY:HA3	2.50	0.47
1:B:130:SER:OG	1:B:132:ILE:HG13	2.16	0.46
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.77	0.46
1:A:97:ASP:HB2	4:A:665:HOH:O	2.15	0.46
1:B:235:GLN:HG3	1:B:290:ARG:NH1	2.30	0.46
1:B:65:ARG:N	4:B:601:HOH:O	2.49	0.46
1:B:113:LYS:HG2	4:B:661:HOH:O	2.15	0.46
1:A:285:GLN:HG2	1:B:282:ALA:HB1	1.98	0.46
1:B:334:PRO:HG2	4:B:564:HOH:O	2.07	0.46
1:A:415:LYS:CE	4:A:563:HOH:O	2.64	0.45
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.17	0.45
1:A:257:VAL:HG21	1:A:322:LEU:HD13	1.99	0.45
1:B:398:GLN:NE2	1:B:398:GLN:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:HG2	1:A:280:VAL:HA	1.99	0.43
1:A:173:ALA:O	1:A:177:MET:HG3	2.17	0.43
1:B:234:ILE:HG13	1:B:286:LYS:HE3	2.00	0.43
1:A:282:ALA:HB1	1:B:285:GLN:HG2	1.99	0.42
1:B:374:ASN:HD22	1:B:376:LEU:H	1.67	0.42
3:A:501:CHD:H222	3:A:501:CHD:C18	2.50	0.42
1:B:329:ASN:ND2	1:B:364:ASN:HB2	2.30	0.42
3:B:501:CHD:H12	3:B:501:CHD:H212	2.01	0.42
1:A:285:GLN:O	1:A:289:GLU:HG3	2.20	0.42
1:A:177:MET:HB3	1:A:182:LEU:HD12	2.01	0.42
1:B:170:THR:O	1:B:174:ILE:HG13	2.20	0.42
1:A:374:ASN:HD22	1:A:376:LEU:H	1.67	0.42
1:A:304:LYS:HE2	4:A:635:HOH:O	2.19	0.42
1:A:227:TRP:CZ3	1:A:233:LEU:HD13	2.55	0.41
1:A:96:ARG:HA	1:A:99:MET:O	2.19	0.41
1:B:412:ARG:HG2	1:B:412:ARG:HH11	1.85	0.41
3:B:501:CHD:H20	3:B:501:CHD:H183	1.92	0.41
1:A:276:TYR:O	1:A:280:VAL:HG23	2.20	0.41
1:A:235:GLN:HG3	1:A:290:ARG:CZ	2.51	0.41
3:B:503:CHD:H162	3:B:503:CHD:H222	1.79	0.41
1:B:107:LEU:O	1:B:111:ILE:HG13	2.20	0.41
1:B:145:LYS:HB3	1:B:145:LYS:NZ	2.36	0.41
1:B:357:ALA:HB1	1:B:362:VAL:HG11	2.03	0.40
1:B:236:CYS:HB3	1:B:371:LEU:HD22	2.03	0.40
4:A:624:HOH:O	1:B:286:LYS:HD3	2.20	0.40
1:B:341:HIS:HE1	4:B:563:HOH:O	2.03	0.40
3:A:502:CHD:H12A	3:A:502:CHD:H112	1.90	0.40
1:A:273:GLY:HA2	1:B:313:PRO:HG3	2.04	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:645:HOH:O	4:B:628:HOH:O[3_655]	0.89	1.31
1:B:80:GLU:OE1	4:A:620:HOH:O[3_645]	1.08	1.12
1:A:252:LYS:CE	4:B:599:HOH:O[3_655]	1.09	1.11
1:A:252:LYS:CD	4:B:599:HOH:O[3_655]	1.66	0.54
1:A:251:GLU:CB	1:B:83:GLY:O[3_655]	1.75	0.45
1:B:124:ARG:O	4:B:521:HOH:O[3_645]	1.79	0.41
1:A:251:GLU:CA	1:B:83:GLY:O[3_655]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:OE1	4:B:567:HOH:O[3_655]	2.00	0.20
1:A:251:GLU:CG	4:B:567:HOH:O[3_655]	2.01	0.19
1:A:251:GLU:O	1:B:83:GLY:CA[3_655]	2.03	0.17
1:A:251:GLU:CD	4:B:567:HOH:O[3_655]	2.05	0.15

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	351/359 (98%)	338 (96%)	11 (3%)	2 (1%)	30	34
1	B	352/359 (98%)	340 (97%)	10 (3%)	2 (1%)	30	34
All	All	703/718 (98%)	678 (96%)	21 (3%)	4 (1%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	B	168	PRO
1	A	168	PRO
1	B	156	PRO

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	310/323 (96%)	296 (96%)	14 (4%)	34	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	311/323 (96%)	296 (95%)	15 (5%)	31	40
All	All	621/646 (96%)	592 (95%)	29 (5%)	32	41

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	100	THR
1	A	219	MET
1	A	240	HIS
1	A	243	LYS
1	A	250	LEU
1	A	257	VAL
1	A	272	ARG
1	A	360	CYS
1	A	374	ASN
1	A	378	SER
1	A	387	SER
1	A	415	LYS
1	A	423	LEU
1	B	92	LEU
1	B	106	LYS
1	B	114	ARG
1	B	175	GLU
1	B	179	ARG
1	B	182	LEU
1	B	184	ARG
1	B	198	THR
1	B	220	LYS
1	B	240	HIS
1	B	272	ARG
1	B	341	HIS
1	B	362	VAL
1	B	374	ASN
1	B	423	LEU

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

Mol	Chain	Res	Type
1	A	157	HIS
1	A	235	GLN

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Mol	Chain	Res	Type
1	A	240	HIS
1	A	314	GLN
1	A	329	ASN
1	A	341	HIS
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	388	HIS
1	A	390	GLN
1	A	392	ASN
1	A	398	GLN
1	A	421	GLN
1	B	167	HIS
1	B	235	GLN
1	B	240	HIS
1	B	314	GLN
1	B	329	ASN
1	B	341	HIS
1	B	374	ASN
1	B	388	HIS
1	B	398	GLN
1	B	421	GLN

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 ⓘ

8 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	FES	A	499	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CHD	A	501	-	29,32,32	0.57	0	48,51,51	1.80	14 (29%)
3	CHD	A	502	-	29,32,32	0.52	0	48,51,51	1.83	15 (31%)
3	CHD	A	503	-	29,32,32	0.54	0	48,51,51	1.42	8 (16%)
2	FES	B	499	1	0,4,4	0.00	-	0,4,4	0.00	-
3	CHD	B	501	-	29,32,32	0.68	0	48,51,51	2.07	11 (22%)
3	CHD	B	502	-	29,32,32	0.44	0	48,51,51	1.81	10 (20%)
3	CHD	B	503	-	29,32,32	0.51	0	48,51,51	1.50	10 (20%)

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	FES	A	499	1	-	0/0/4/4	0/1/1/1
3	CHD	A	501	-	-	0/7/74/74	0/4/4/4
3	CHD	A	502	-	-	0/7/74/74	0/4/4/4
3	CHD	A	503	-	-	0/7/74/74	0/4/4/4
2	FES	B	499	1	-	0/0/4/4	0/1/1/1
3	CHD	B	501	-	-	0/7/74/74	0/4/4/4
3	CHD	B	502	-	-	0/7/74/74	0/4/4/4
3	CHD	B	503	-	-	0/7/74/74	0/4/4/4

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CHD	C23-C22-C20	-7.18	106.29	114.75
3	B	501	CHD	C13-C17-C20	-4.61	113.89	119.50
3	A	501	CHD	C6-C5-C4	-4.60	105.91	111.05
3	A	502	CHD	C6-C5-C4	-4.47	106.05	111.05
3	B	501	CHD	C6-C5-C4	-4.44	106.08	111.05
3	B	502	CHD	C17-C13-C14	-4.35	95.65	100.05
3	B	502	CHD	C6-C5-C4	-3.49	107.15	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CHD	C11-C9-C10	-3.32	110.34	113.79
3	A	502	CHD	C17-C13-C14	-3.18	96.84	100.05
3	B	502	CHD	C19-C10-C5	-3.09	104.80	110.25
3	A	501	CHD	C13-C17-C20	-3.08	115.75	119.50
3	B	502	CHD	C22-C20-C17	-3.05	103.84	110.24
3	A	501	CHD	C9-C8-C7	-2.94	108.45	111.92
3	A	501	CHD	C21-C20-C17	-2.72	108.42	112.96
3	B	501	CHD	C17-C13-C12	-2.70	115.29	117.68
3	A	502	CHD	C22-C20-C17	-2.69	104.59	110.24
3	A	503	CHD	C14-C8-C9	-2.48	106.21	109.62
3	B	501	CHD	O3-C3-C4	-2.47	104.96	109.86
3	B	503	CHD	C17-C13-C14	-2.45	97.58	100.05
3	A	502	CHD	C19-C10-C1	-2.37	104.21	108.20
3	A	501	CHD	C22-C23-C24	-2.35	103.42	113.02
3	B	503	CHD	C14-C8-C9	-2.24	106.55	109.62
3	A	501	CHD	C17-C13-C14	-2.21	97.82	100.05
3	A	502	CHD	C21-C20-C22	-2.19	106.69	110.35
3	A	501	CHD	C23-C22-C20	-2.17	112.19	114.75
3	B	501	CHD	C13-C14-C8	-2.08	112.06	114.75
3	B	502	CHD	C16-C15-C14	-2.05	101.00	105.12
3	A	502	CHD	C23-C22-C20	-2.02	112.37	114.75
3	B	503	CHD	C10-C9-C8	2.06	114.14	111.88
3	A	502	CHD	C5-C4-C3	2.08	116.01	112.91
3	A	501	CHD	C11-C12-C13	2.13	113.37	111.20
3	A	503	CHD	C9-C8-C7	2.14	114.45	111.92
3	A	502	CHD	C11-C9-C8	2.23	113.89	110.73
3	B	503	CHD	C11-C9-C8	2.23	113.89	110.73
3	B	503	CHD	C14-C13-C12	2.27	109.42	107.39
3	A	503	CHD	C14-C8-C7	2.30	114.93	111.74
3	A	503	CHD	C4-C5-C10	2.30	115.19	112.66
3	A	501	CHD	C16-C17-C13	2.42	106.00	103.60
3	B	502	CHD	C21-C20-C17	2.42	116.99	112.96
3	A	502	CHD	C15-C14-C13	2.42	106.01	103.60
3	A	503	CHD	C9-C10-C5	2.44	112.29	108.67
3	B	501	CHD	C18-C13-C12	2.47	111.50	109.09
3	A	502	CHD	C1-C10-C5	2.49	111.89	107.81
3	A	502	CHD	C6-C5-C10	2.57	115.48	112.66
3	A	502	CHD	C2-C1-C10	2.57	117.43	112.84
3	B	502	CHD	C11-C9-C8	2.59	114.41	110.73
3	B	503	CHD	C11-C12-C13	2.70	113.94	111.20
3	B	501	CHD	C11-C9-C8	2.84	114.76	110.73
3	B	503	CHD	C4-C5-C10	2.86	115.81	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	CHD	C15-C14-C13	2.87	106.45	103.60
3	A	503	CHD	C10-C9-C8	2.88	115.05	111.88
3	A	503	CHD	C6-C7-C8	2.96	114.61	111.47
3	A	501	CHD	C11-C9-C8	2.98	114.96	110.73
3	A	501	CHD	C9-C11-C12	3.01	118.16	114.36
3	B	503	CHD	C9-C10-C5	3.02	113.14	108.67
3	A	502	CHD	C9-C10-C5	3.02	113.14	108.67
3	B	502	CHD	C1-C10-C5	3.18	113.03	107.81
3	B	503	CHD	C16-C17-C13	3.20	106.78	103.60
3	B	502	CHD	C13-C17-C20	3.29	123.50	119.50
3	A	502	CHD	C21-C20-C17	3.31	118.46	112.96
3	A	502	CHD	C13-C17-C20	3.36	123.59	119.50
3	B	501	CHD	C16-C17-C20	3.40	118.12	112.05
3	B	503	CHD	C15-C14-C13	3.41	106.99	103.60
3	A	501	CHD	C14-C13-C12	3.68	110.69	107.39
3	B	501	CHD	C14-C13-C12	3.69	110.69	107.39
3	A	503	CHD	C15-C14-C13	3.94	107.52	103.60
3	A	501	CHD	C16-C17-C20	3.99	119.16	112.05
3	B	502	CHD	C15-C14-C13	4.29	107.87	103.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	CHD	1	0
3	A	502	CHD	1	0
3	B	501	CHD	3	0
3	B	503	CHD	1	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

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	355/359 (98%)	1.86	131 (36%) 0 0	14, 23, 40, 50	0
1	B	356/359 (99%)	4.05	304 (85%) 0 0	13, 23, 41, 48	0
All	All	711/718 (99%)	2.95	435 (61%) 0 0	13, 23, 41, 50	0

All (435) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	ILE	11.4
1	B	169	LEU	10.9
1	B	206	ILE	10.6
1	B	410	VAL	9.9
1	B	83	GLY	9.7
1	B	418	PHE	9.5
1	B	101	LEU	9.3
1	B	168	PRO	9.0
1	B	342	ILE	8.9
1	B	382	ALA	8.7
1	B	134	ILE	8.4
1	B	218	THR	8.4
1	B	210	TYR	8.3
1	B	163	PHE	8.3
1	B	106	LYS	8.2
1	B	132	ILE	8.2
1	B	136	THR	8.1
1	B	345	LEU	7.9
1	B	109	PRO	7.7
1	B	207	TYR	7.7
1	B	71	ILE	7.6
1	B	414	THR	7.4
1	B	181	GLY	7.4
1	B	94	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	156	PRO	7.3
1	B	276	TYR	7.3
1	B	73	MET	7.2
1	B	135	TRP	7.2
1	B	346	TYR	7.1
1	B	128	GLY	7.1
1	B	110	PHE	7.0
1	B	209	TYR	7.0
1	B	159	TYR	6.9
1	B	305	VAL	6.9
1	A	326	GLY	6.9
1	B	76	MET	6.8
1	B	81	THR	6.7
1	B	227	TRP	6.7
1	B	90	LEU	6.7
1	B	123	TYR	6.7
1	B	420	SER	6.6
1	B	185	ALA	6.6
1	B	196	CYS	6.5
1	B	112	ALA	6.5
1	B	188	PHE	6.4
1	B	99	MET	6.3
1	B	103	ILE	6.3
1	B	77	GLY	6.2
1	A	297	TYR	6.2
1	A	357	ALA	6.2
1	B	65	ARG	6.1
1	A	293	TYR	6.0
1	B	195	SER	6.0
1	B	205	ALA	6.0
1	B	221	TRP	6.0
1	B	394	LEU	6.0
1	B	411	CYS	5.9
1	B	378	SER	5.9
1	B	406	CYS	5.9
1	B	224	ILE	5.8
1	B	219	MET	5.8
1	B	353	SER	5.8
1	B	273	GLY	5.8
1	B	372	ASN	5.7
1	B	392	ASN	5.7
1	B	86	HIS	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	5.6
1	B	117	PRO	5.6
1	B	130	SER	5.6
1	B	116	THR	5.6
1	B	167	HIS	5.6
1	B	82	LEU	5.6
1	B	155	ALA	5.6
1	B	381	LEU	5.6
1	B	311	LEU	5.5
1	B	340	ASP	5.5
1	B	131	PRO	5.5
1	B	72	LEU	5.5
1	B	191	TYR	5.5
1	B	375	PRO	5.5
1	B	137	SER	5.4
1	B	93	PHE	5.4
1	A	322	LEU	5.4
1	B	423	LEU	5.4
1	B	385	VAL	5.4
1	B	140	GLY	5.3
1	B	108	ALA	5.3
1	B	183	GLU	5.3
1	B	164	ARG	5.3
1	B	142	GLY	5.2
1	B	153	ASN	5.2
1	B	257	VAL	5.2
1	B	70	GLY	5.1
1	B	395	CYS	5.1
1	B	352	TYR	5.1
1	B	384	LEU	5.1
1	B	409	PRO	5.1
1	B	308	MET	5.0
1	B	362	VAL	5.0
1	B	98	LEU	5.0
1	B	144	VAL	5.0
1	A	299	LEU	5.0
1	B	194	TYR	5.0
1	B	389	ILE	4.9
1	B	126	ILE	4.9
1	B	176	GLU	4.9
1	B	403	CYS	4.9
1	B	365	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	250	LEU	4.8
1	B	74	LEU	4.8
1	B	145	LYS	4.8
1	B	283	THR	4.8
1	A	325	ARG	4.8
1	B	393	GLU	4.8
1	B	105	ASN	4.8
1	B	79	PRO	4.8
1	B	129	GLY	4.8
1	B	172	GLU	4.8
1	B	201	SER	4.7
1	B	199	THR	4.7
1	B	269	VAL	4.7
1	A	254	SER	4.7
1	B	189	THR	4.7
1	B	165	TYR	4.7
1	B	407	VAL	4.7
1	A	335	ILE	4.7
1	B	173	ALA	4.7
1	A	360	CYS	4.6
1	B	293	TYR	4.6
1	A	238	ALA	4.6
1	B	180	ASP	4.6
1	B	143	MET	4.6
1	B	175	GLU	4.6
1	B	386	HIS	4.5
1	B	333	VAL	4.5
1	B	162	GLY	4.5
1	B	306	GLY	4.5
1	B	319	ILE	4.5
1	B	211	ASN	4.5
1	A	323	CYS	4.5
1	B	417	PHE	4.5
1	B	190	GLN	4.5
1	B	69	THR	4.5
1	A	258	ILE	4.5
1	B	334	PRO	4.5
1	B	148	ASP	4.4
1	A	296	PRO	4.4
1	B	198	THR	4.4
1	B	216	LYS	4.4
1	B	339	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	388	HIS	4.4
1	A	294	CYS	4.4
1	A	252	LYS	4.4
1	B	287	VAL	4.4
1	B	259	LEU	4.3
1	A	237	PHE	4.3
1	B	370	SER	4.3
1	B	275	PRO	4.3
1	B	166	VAL	4.3
1	B	187	ALA	4.3
1	B	338	THR	4.3
1	B	120	GLN	4.3
1	B	192	PRO	4.2
1	B	233	LEU	4.2
1	A	329	ASN	4.2
1	A	265	LEU	4.2
1	B	237	PHE	4.2
1	B	178	GLU	4.2
1	A	103	ILE	4.2
1	A	315	THR	4.1
1	B	280	VAL	4.1
1	A	321	GLY	4.1
1	B	278	GLN	4.1
1	B	297	TYR	4.1
1	B	413	GLU	4.1
1	B	197	SER	4.1
1	B	202	SER	4.1
1	B	68	LYS	4.0
1	B	300	VAL	4.0
1	A	318	SER	4.0
1	B	341	HIS	4.0
1	B	265	LEU	4.0
1	B	158	LYS	4.0
1	B	405	LEU	4.0
1	B	377	PHE	4.0
1	A	288	MET	4.0
1	B	154	THR	3.9
1	B	179	ARG	3.9
1	B	66	LYS	3.9
1	B	230	HIS	3.9
1	A	352	TYR	3.9
1	B	91	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	184	ARG	3.9
1	B	171	GLU	3.9
1	B	75	ASN	3.9
1	B	315	THR	3.8
1	A	276	TYR	3.8
1	A	280	VAL	3.8
1	B	360	CYS	3.8
1	B	299	LEU	3.8
1	B	235	GLN	3.8
1	B	400	THR	3.8
1	A	314	GLN	3.8
1	B	124	ARG	3.8
1	B	263	HIS	3.8
1	A	356	LEU	3.8
1	B	182	LEU	3.8
1	B	408	ASN	3.8
1	A	282	ALA	3.7
1	B	186	ILE	3.7
1	A	270	VAL	3.7
1	A	362	VAL	3.7
1	B	80	GLU	3.7
1	B	415	LYS	3.7
1	B	119	ILE	3.7
1	A	281	SER	3.7
1	B	85	VAL	3.7
1	B	160	TYR	3.7
1	A	311	LEU	3.7
1	A	284	VAL	3.7
1	B	373	GLY	3.7
1	B	270	VAL	3.6
1	B	323	CYS	3.6
1	B	268	SER	3.6
1	B	282	ALA	3.6
1	B	401	LEU	3.6
1	B	170	THR	3.6
1	B	422	GLN	3.6
1	B	104	GLN	3.6
1	B	354	GLN	3.6
1	A	353	SER	3.6
1	B	412	ARG	3.6
1	A	361	GLY	3.6
1	B	133	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	84	ASP	3.5
1	A	241	ILE	3.5
1	B	310	TRP	3.5
1	B	95	ASP	3.5
1	B	152	PRO	3.5
1	B	204	ASN	3.5
1	A	328	LYS	3.5
1	B	89	LEU	3.5
1	B	303	SER	3.4
1	B	419	THR	3.4
1	B	138	LYS	3.4
1	B	262	ALA	3.4
1	B	335	ILE	3.4
1	B	350	ILE	3.4
1	B	220	LYS	3.4
1	A	332	LEU	3.4
1	B	277	PRO	3.4
1	B	174	ILE	3.4
1	B	78	GLY	3.4
1	A	251	GLU	3.4
1	B	232	LEU	3.4
1	B	348	LEU	3.3
1	B	349	ASP	3.3
1	B	147	LEU	3.3
1	B	288	MET	3.3
1	B	331	LEU	3.3
1	B	399	LEU	3.3
1	B	344	THR	3.3
1	B	258	ILE	3.3
1	A	380	ALA	3.3
1	A	275	PRO	3.3
1	B	253	ARG	3.2
1	B	318	SER	3.2
1	A	292	GLU	3.2
1	B	336	ALA	3.2
1	B	337	ALA	3.2
1	A	301	TRP	3.2
1	A	423	LEU	3.2
1	A	337	ALA	3.2
1	B	67	PRO	3.2
1	A	257	VAL	3.2
1	B	358	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	264	SER	3.2
1	A	245	LEU	3.2
1	B	228	PRO	3.2
1	A	300	VAL	3.2
1	B	236	CYS	3.1
1	A	319	ILE	3.1
1	B	223	THR	3.1
1	B	193	GLN	3.1
1	B	208	ARG	3.1
1	B	295	ASN	3.1
1	A	350	ILE	3.1
1	B	200	GLY	3.1
1	A	205	ALA	3.1
1	A	255	GLU	3.1
1	B	367	ARG	3.1
1	B	279	GLU	3.0
1	A	366	ARG	3.0
1	B	88	PHE	3.0
1	A	77	GLY	3.0
1	A	253	ARG	3.0
1	A	242	LEU	3.0
1	B	92	LEU	3.0
1	B	397	LYS	3.0
1	B	301	TRP	3.0
1	A	277	PRO	3.0
1	B	272	ARG	3.0
1	B	260	PHE	3.0
1	B	177	MET	3.0
1	B	157	HIS	3.0
1	B	96	ARG	3.0
1	B	416	SER	3.0
1	A	273	GLY	2.9
1	A	336	ALA	2.9
1	B	225	ASP	2.9
1	A	235	GLN	2.9
1	A	123	TYR	2.9
1	A	196	CYS	2.9
1	B	267	MET	2.9
1	A	344	THR	2.9
1	B	266	PRO	2.9
1	B	261	SER	2.9
1	B	286	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	346	TYR	2.9
1	B	248	PHE	2.9
1	A	295	ASN	2.8
1	B	113	LYS	2.8
1	B	291	LEU	2.8
1	A	339	SER	2.8
1	B	330	ILE	2.8
1	A	283	THR	2.8
1	B	366	ARG	2.8
1	B	100	THR	2.8
1	B	421	GLN	2.7
1	B	290	ARG	2.7
1	A	365	ILE	2.7
1	A	260	PHE	2.7
1	A	307	PRO	2.7
1	A	256	VAL	2.7
1	A	287	VAL	2.7
1	B	97	ASP	2.7
1	A	263	HIS	2.7
1	A	285	GLN	2.7
1	A	289	GLU	2.7
1	A	342	ILE	2.7
1	B	114	ARG	2.6
1	B	404	PRO	2.6
1	B	151	SER	2.6
1	A	89	LEU	2.6
1	A	313	PRO	2.6
1	A	92	LEU	2.6
1	B	281	SER	2.6
1	A	286	LYS	2.6
1	A	399	LEU	2.6
1	A	170	THR	2.6
1	A	403	CYS	2.6
1	B	234	ILE	2.5
1	A	200	GLY	2.5
1	B	141	GLU	2.5
1	B	284	VAL	2.5
1	A	387	SER	2.5
1	B	149	GLU	2.5
1	B	274	ASP	2.5
1	B	379	LYS	2.5
1	A	259	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	121	GLU	2.5
1	B	313	PRO	2.5
1	A	358	LYS	2.5
1	A	406	CYS	2.5
1	A	368	ALA	2.5
1	B	355	VAL	2.5
1	B	87	ASP	2.5
1	B	343	GLU	2.5
1	A	231	HIS	2.5
1	A	310	TRP	2.5
1	B	222	SER	2.5
1	A	331	LEU	2.5
1	A	363	GLU	2.5
1	A	402	SER	2.4
1	A	348	LEU	2.4
1	A	96	ARG	2.4
1	B	391	SER	2.4
1	B	229	THR	2.4
1	B	226	ARG	2.4
1	B	241	ILE	2.4
1	B	369	GLU	2.4
1	A	308	MET	2.4
1	A	271	ASN	2.4
1	A	392	ASN	2.4
1	B	238	ALA	2.4
1	A	156	PRO	2.4
1	A	134	ILE	2.4
1	A	181	GLY	2.4
1	B	252	LYS	2.4
1	A	312	GLY	2.4
1	B	368	ALA	2.4
1	B	312	GLY	2.3
1	B	356	LEU	2.3
1	A	114	ARG	2.3
1	A	302	GLN	2.3
1	A	274	ASP	2.3
1	B	139	GLN	2.3
1	B	239	ASP	2.3
1	B	296	PRO	2.3
1	B	383	ASP	2.3
1	A	364	ASN	2.3
1	A	405	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	246	ASP	2.2
1	A	327	ARG	2.2
1	B	115	LEU	2.2
1	A	228	PRO	2.2
1	B	127	GLY	2.2
1	A	370	SER	2.2
1	B	314	GLN	2.2
1	B	398	GLN	2.2
1	B	150	LEU	2.2
1	A	334	PRO	2.2
1	B	285	GLN	2.2
1	A	234	ILE	2.2
1	A	407	VAL	2.2
1	B	212	GLN	2.2
1	A	324	GLU	2.2
1	B	247	HIS	2.2
1	A	229	THR	2.2
1	A	330	ILE	2.1
1	A	355	VAL	2.1
1	A	393	GLU	2.1
1	A	105	ASN	2.1
1	B	396	SER	2.1
1	B	302	GLN	2.1
1	A	219	MET	2.1
1	A	126	ILE	2.1
1	A	65	ARG	2.1
1	A	404	PRO	2.1
1	B	217	PRO	2.1
1	B	390	GLN	2.1
1	A	248	PHE	2.1
1	A	262	ALA	2.1
1	A	298	ARG	2.0
1	A	131	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CHD	A	501	29/29	0.74	0.28	1.08	26,31,47,48	0
3	CHD	B	503	29/29	0.59	0.45	1.02	45,48,63,64	0
3	CHD	B	501	29/29	0.64	0.42	0.89	28,29,41,45	0
3	CHD	A	502	29/29	0.66	0.26	0.88	37,41,49,51	0
3	CHD	B	502	29/29	0.51	0.44	0.65	34,38,51,53	0
3	CHD	A	503	29/29	0.54	0.31	-0.09	43,47,50,51	0
2	FES	B	499	4/4	0.51	0.25	-2.14	20,20,22,23	0
2	FES	A	499	4/4	0.88	0.12	-3.50	16,17,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.