



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:53 PM GMT

PDB ID : 1HRK
Title : CRYSTAL STRUCTURE OF HUMAN FERROCHELATASE
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Deposited on : 2000-12-21
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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

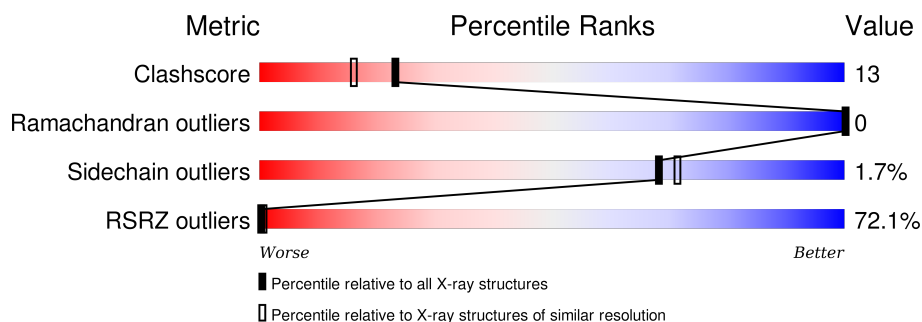
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	359	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6486 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.

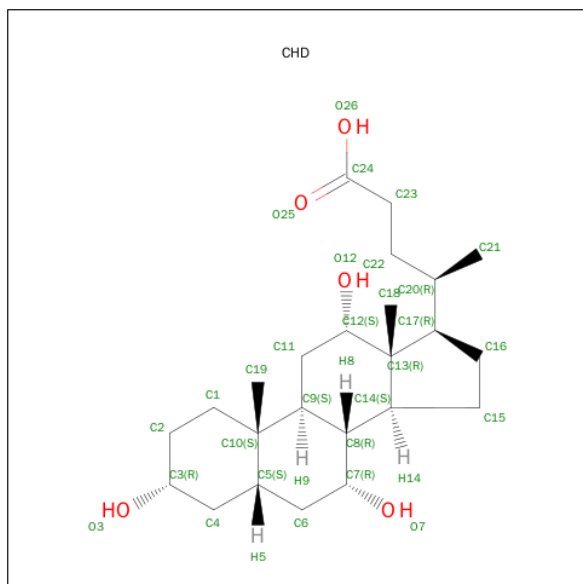
- Molecule 1 is a protein called FERROCHELATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2854	1819	491	526	18			
1	B	359	Total	C	N	O	S	0	0	0
			2854	1819	491	526	18			

There are 4 discrepancies between the modelled and reference sequences:

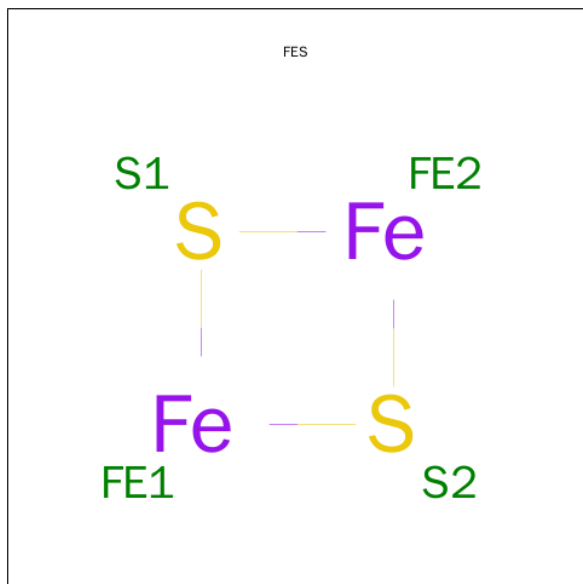
Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ARG	GLN	ENGINEERED	UNP P22830
A	115	LEU	ARG	ENGINEERED	UNP P22830
B	96	ARG	GLN	ENGINEERED	UNP P22830
B	115	LEU	ARG	ENGINEERED	UNP P22830

- Molecule 2 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	291	Total	O	0	0
			291	291		
4	B	305	Total	O	0	0
			305	305		

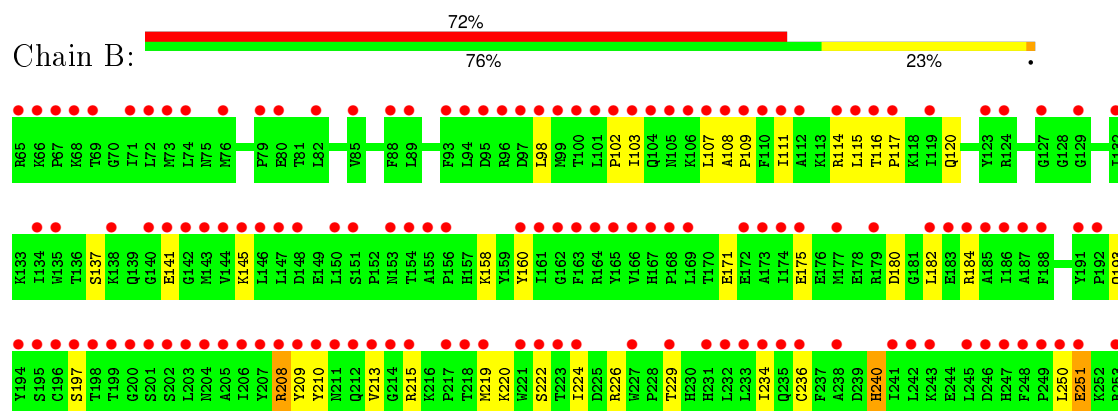
3 Residue-property plots

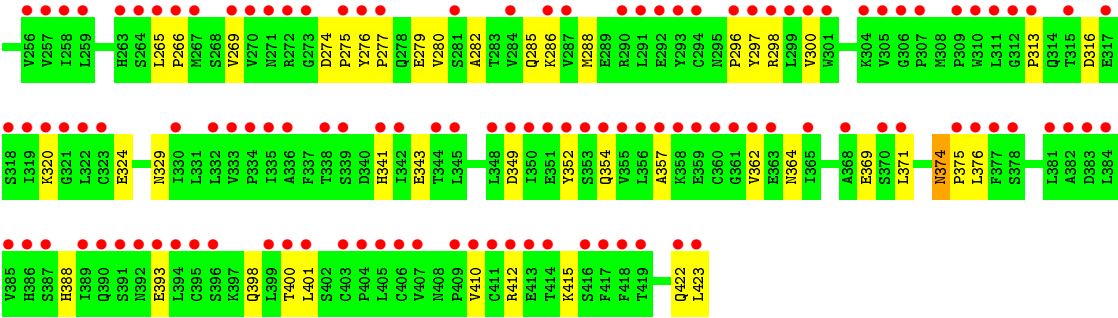
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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



• Molecule 1: FERROCHELATASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.43 Å 87.57 Å 109.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.00 19.87 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.87-2.00) 94.6 (19.87-1.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 1.84 Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.202 , 0.226 0.306 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 73.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 75224 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	6486	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 43.66 % 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 1.7074e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/2924	0.58	1/3971 (0.0%)
1	B	0.31	0/2924	0.58	1/3971 (0.0%)
All	All	0.31	0/5848	0.58	2/7942 (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	B	224	ILE	N-CA-C	-5.73	95.52	111.00
1	A	224	ILE	N-CA-C	-5.53	96.07	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2854	0	2821	78	0
1	B	2854	0	2821	79	0
2	A	87	0	117	12	0
2	B	87	0	117	12	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	291	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	305	0	0	6	0
All	All	6486	0	5876	158	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 13.

All (158) 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:297:TYR:H	1:B:398:GLN:HE22	1.13	0.96
1:A:208:ARG:NH2	1:A:410:VAL:HG21	1.81	0.96
1:A:398:GLN:HE22	1:B:297:TYR:H	1.15	0.93
1:B:250:LEU:H	1:B:250:LEU:HD12	1.34	0.91
1:B:208:ARG:NH2	1:B:410:VAL:HG21	1.88	0.87
1:A:250:LEU:H	1:A:250:LEU:HD12	1.40	0.85
1:A:422:GLN:O	1:A:423:LEU:HB2	1.79	0.82
1:B:422:GLN:O	1:B:423:LEU:HB2	1.79	0.81
1:A:229:THR:HB	1:A:286:LYS:HE2	1.62	0.80
1:A:300:VAL:HG12	1:A:313:PRO:HG2	1.65	0.78
1:B:300:VAL:HG12	1:B:313:PRO:HG2	1.67	0.74
1:A:269:VAL:O	1:A:272:ARG:HG2	1.87	0.74
2:B:2501:CHD:H12	2:B:2501:CHD:H212	1.70	0.74
1:B:208:ARG:HH21	1:B:410:VAL:HG21	1.49	0.74
1:A:234:ILE:HG13	1:A:286:LYS:HE3	1.69	0.74
1:B:171:GLU:O	1:B:175:GLU:HG3	1.88	0.73
1:B:98:LEU:HD11	2:B:2501:CHD:H162	1.70	0.73
1:B:229:THR:HB	1:B:286:LYS:HE2	1.70	0.73
1:B:234:ILE:HG13	1:B:286:LYS:HE3	1.70	0.72
1:B:265:LEU:HD22	2:B:2501:CHD:O26	1.91	0.71
1:B:250:LEU:H	1:B:250:LEU:CD1	2.05	0.70
1:A:222:SER:OG	1:A:388:HIS:HE1	1.75	0.70
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.73	0.69
1:A:197:SER:HB3	2:A:1501:CHD:O25	1.92	0.69
2:A:1501:CHD:H12	2:A:1501:CHD:H212	1.75	0.68
1:B:222:SER:OG	1:B:388:HIS:HE1	1.76	0.68
1:A:265:LEU:HD22	2:A:1501:CHD:O26	1.93	0.68
1:B:357:ALA:HB1	1:B:362:VAL:HG11	1.74	0.67
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.77	0.67
1:B:298:ARG:HD3	4:B:3003:HOH:O	1.94	0.66
1:B:250:LEU:HD12	1:B:250:LEU:N	2.09	0.65
1:A:115:LEU:HD21	2:A:1502:CHD:H231	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LYS:HD3	1:B:423:LEU:HG	1.79	0.63
1:B:210:TYR:HA	1:B:213:VAL:HG12	1.79	0.63
1:B:374:ASN:HD22	1:B:375:PRO:N	1.97	0.63
1:A:220:LYS:HD2	1:A:423:LEU:HG	1.80	0.62
1:A:297:TYR:N	1:B:398:GLN:HE22	1.90	0.62
1:B:374:ASN:HD22	1:B:374:ASN:C	2.02	0.62
1:B:240:HIS:HD2	1:B:369:GLU:O	1.82	0.62
1:A:415:LYS:HB3	1:A:415:LYS:HZ3	1.65	0.61
1:A:398:GLN:HE22	1:B:297:TYR:N	1.91	0.61
1:A:250:LEU:CD1	1:A:250:LEU:H	2.13	0.61
1:A:114:ARG:HD3	2:A:1502:CHD:O26	2.00	0.60
1:A:357:ALA:HB1	1:A:362:VAL:HG11	1.83	0.60
1:A:208:ARG:HH21	1:A:410:VAL:HG21	1.61	0.60
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.83	0.60
1:B:197:SER:HB3	2:B:2501:CHD:O25	2.01	0.60
1:A:282:ALA:HB1	1:B:285:GLN:HG2	1.83	0.60
1:B:400:THR:HA	1:B:415:LYS:HD2	1.84	0.60
1:A:374:ASN:HD22	1:A:374:ASN:C	2.05	0.59
1:B:374:ASN:ND2	1:B:376:LEU:H	1.99	0.59
1:A:374:ASN:HD22	1:A:375:PRO:N	1.99	0.59
1:A:349:ASP:O	1:A:354:GLN:HG3	2.02	0.59
1:A:240:HIS:HD2	1:A:369:GLU:O	1.85	0.59
1:A:415:LYS:HB3	1:A:415:LYS:NZ	2.18	0.58
1:A:320:LYS:O	1:A:324:GLU:HG3	2.03	0.58
1:A:285:GLN:HG2	1:B:282:ALA:HB1	1.85	0.58
1:A:400:THR:HA	1:A:415:LYS:HD2	1.85	0.57
1:A:208:ARG:HH11	1:A:208:ARG:HG3	1.70	0.57
2:B:2502:CHD:H213	4:B:3264:HOH:O	2.04	0.57
1:B:213:VAL:CG2	1:B:215:ARG:HH21	2.18	0.56
1:A:374:ASN:ND2	1:A:376:LEU:H	2.04	0.56
1:B:415:LYS:NZ	1:B:415:LYS:HB3	2.21	0.56
1:A:184:ARG:NH2	4:A:1553:HOH:O	2.35	0.55
1:B:115:LEU:HD21	2:B:2502:CHD:H231	1.87	0.55
1:B:111:ILE:HA	1:B:114:ARG:HG2	1.89	0.54
1:A:250:LEU:N	1:A:250:LEU:HD12	2.17	0.54
1:B:251:GLU:H	1:B:251:GLU:CD	2.10	0.54
1:B:320:LYS:O	1:B:324:GLU:HG3	2.08	0.53
1:A:296:PRO:HB2	1:B:401:LEU:HB2	1.91	0.52
1:A:341:HIS:HE1	4:A:1651:HOH:O	1.92	0.52
1:A:145:LYS:NZ	1:A:145:LYS:HB3	2.24	0.52
1:B:349:ASP:O	1:B:354:GLN:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1503:CHD:H12	2:A:1503:CHD:H212	1.90	0.52
1:A:135:TRP:CE3	1:A:372:ASN:HB3	2.45	0.52
1:A:145:LYS:HZ3	1:A:145:LYS:HB3	1.75	0.52
1:B:341:HIS:HE1	4:B:3148:HOH:O	1.93	0.51
1:A:98:LEU:HD11	2:A:1501:CHD:H162	1.92	0.51
1:B:145:LYS:HB3	1:B:145:LYS:HZ3	1.76	0.51
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.76	0.51
1:B:412:ARG:HG3	1:B:415:LYS:HZ1	1.75	0.50
1:B:415:LYS:HB3	1:B:415:LYS:HZ3	1.76	0.50
2:B:2503:CHD:H12	2:B:2503:CHD:H212	1.93	0.50
1:B:269:VAL:HG21	2:B:2501:CHD:C24	2.42	0.49
1:A:135:TRP:CZ3	1:A:372:ASN:HB3	2.48	0.49
1:B:208:ARG:HG3	1:B:208:ARG:HH11	1.76	0.49
1:A:341:HIS:HD2	4:A:1650:HOH:O	1.95	0.49
1:A:379:LYS:HE3	4:A:1620:HOH:O	2.12	0.49
1:B:213:VAL:HG21	1:B:215:ARG:HH21	1.77	0.49
1:B:145:LYS:HB3	1:B:145:LYS:NZ	2.28	0.49
1:A:422:GLN:HG2	1:A:423:LEU:HD23	1.95	0.48
1:B:213:VAL:HG22	1:B:215:ARG:HE	1.78	0.48
1:B:175:GLU:HG2	1:B:209:TYR:OH	2.15	0.47
1:B:103:ILE:HG13	1:B:107:LEU:HG	1.97	0.47
1:A:177:MET:HB3	1:A:182:LEU:HD12	1.96	0.47
1:A:173:ALA:O	1:A:177:MET:HG3	2.15	0.47
1:A:103:ILE:HG13	1:A:107:LEU:HG	1.95	0.47
1:A:273:GLY:O	1:B:298:ARG:HD2	2.15	0.47
1:B:357:ALA:HB1	1:B:362:VAL:CG1	2.45	0.46
2:B:2502:CHD:H12	2:B:2502:CHD:H212	1.97	0.46
1:B:102:PRO:O	1:B:103:ILE:C	2.53	0.46
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.50	0.46
1:B:236:CYS:HB3	1:B:371:LEU:HD22	1.97	0.46
1:B:341:HIS:CE1	1:B:343:GLU:HB2	2.51	0.46
1:B:102:PRO:O	1:B:107:LEU:HD12	2.15	0.46
1:B:193:GLN:HG2	1:B:280:VAL:HA	1.97	0.45
1:B:388:HIS:HD2	1:B:393:GLU:CD	2.19	0.45
1:B:116:THR:HB	1:B:117:PRO:HD3	1.99	0.45
1:A:116:THR:HB	1:A:117:PRO:HD3	1.98	0.45
1:A:111:ILE:HA	1:A:114:ARG:HG2	1.99	0.45
1:B:374:ASN:HD22	1:B:376:LEU:H	1.65	0.45
1:A:417:PHE:O	1:A:421:GLN:HG2	2.15	0.45
1:B:341:HIS:HD2	4:B:3150:HOH:O	2.00	0.45
1:A:296:PRO:HA	1:B:398:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB1	1:A:156:PRO:HA	1.99	0.45
2:A:1501:CHD:H212	2:A:1502:CHD:H193	1.99	0.45
1:A:298:ARG:HD3	4:A:1512:HOH:O	2.16	0.45
1:A:102:PRO:O	1:A:103:ILE:C	2.56	0.44
1:A:193:GLN:HG2	1:A:280:VAL:HA	1.99	0.44
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.52	0.44
1:A:96:ARG:C	1:A:98:LEU:H	2.20	0.44
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.81	0.44
1:B:220:LYS:HD2	4:B:3267:HOH:O	2.16	0.44
2:B:2501:CHD:H212	2:B:2502:CHD:H193	1.99	0.44
1:B:288:MET:HG3	1:B:297:TYR:CD2	2.53	0.43
1:A:269:VAL:HG21	2:A:1501:CHD:C24	2.47	0.43
1:B:226:ARG:HD3	1:B:279:GLU:OE1	2.19	0.43
1:A:101:LEU:HB2	1:A:104:GLN:HG3	2.00	0.43
1:A:412:ARG:HH11	1:A:412:ARG:HG2	1.82	0.43
1:A:97:ASP:OD2	1:A:208:ARG:NH1	2.34	0.43
1:A:236:CYS:HB3	1:A:371:LEU:HD22	1.99	0.43
1:A:208:ARG:NH1	1:A:208:ARG:HG3	2.32	0.43
2:A:1501:CHD:H211	2:A:1501:CHD:H232	1.75	0.43
1:A:164:ARG:HD2	1:A:201:SER:OG	2.18	0.43
2:A:1502:CHD:H213	4:A:1713:HOH:O	2.18	0.43
1:A:388:HIS:HD2	1:A:393:GLU:CD	2.21	0.43
1:B:266:PRO:HG2	2:B:2502:CHD:H11	1.99	0.43
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.53	0.43
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.84	0.43
4:A:1618:HOH:O	1:B:286:LYS:HD3	2.19	0.42
2:A:1502:CHD:H212	2:A:1502:CHD:H12	2.00	0.42
1:B:266:PRO:CG	2:B:2502:CHD:H11	2.49	0.42
1:B:180:ASP:HB2	1:B:182:LEU:HD13	2.01	0.42
1:B:116:THR:O	1:B:120:GLN:HG3	2.20	0.42
1:A:230:HIS:CE1	1:A:232:LEU:HB2	2.55	0.42
1:A:226:ARG:HD3	1:A:279:GLU:OE1	2.19	0.41
1:A:74:LEU:HD13	1:A:202:SER:HB3	2.01	0.41
1:A:171:GLU:H	1:A:171:GLU:CD	2.23	0.41
1:B:158:LYS:HD3	1:B:160:TYR:OH	2.20	0.41
1:A:134:ILE:HG13	4:A:1586:HOH:O	2.21	0.41
1:A:96:ARG:NH2	4:A:1691:HOH:O	2.53	0.41
1:A:398:GLN:NE2	1:B:296:PRO:HA	2.36	0.41
1:B:422:GLN:O	1:B:423:LEU:CB	2.58	0.41
1:A:111:ILE:O	1:A:114:ARG:HG3	2.21	0.41
1:B:208:ARG:NH1	1:B:208:ARG:HG3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:NH2	4:B:3056:HOH:O	2.50	0.40
1:A:108:ALA:HB3	1:A:109:PRO:CD	2.51	0.40
1:B:137:SER:O	1:B:141:GLU:HG3	2.22	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	357/359 (99%)	346 (97%)	11 (3%)	0	100	100
1	B	357/359 (99%)	348 (98%)	9 (2%)	0	100	100
All	All	714/718 (99%)	694 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	316/324 (98%)	310 (98%)	6 (2%)	65	67
1	B	316/324 (98%)	311 (98%)	5 (2%)	70	73
All	All	632/648 (98%)	621 (98%)	11 (2%)	68	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	A	208	ARG
1	A	213	VAL
1	A	240	HIS
1	A	298	ARG
1	A	374	ASN
1	B	208	ARG
1	B	219	MET
1	B	240	HIS
1	B	251	GLU
1	B	374	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	235	GLN
1	A	240	HIS
1	A	247	HIS
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	398	GLN
1	A	421	GLN
1	B	235	GLN
1	B	240	HIS
1	B	329	ASN
1	B	341	HIS
1	B	354	GLN
1	B	364	ASN
1	B	374	ASN
1	B	388	HIS
1	B	390	GLN
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	$\# Z > 2$
3	FES	A	1499	1	0,4,4	0.00	-	0,4,4	0.00	-
2	CHD	A	1501	-	29,32,32	0.79	0	48,51,51	1.69	7 (14%)
2	CHD	A	1502	-	29,32,32	0.80	2 (6%)	48,51,51	1.12	3 (6%)
2	CHD	A	1503	-	29,32,32	0.79	0	48,51,51	1.14	4 (8%)
2	CHD	B	2501	-	29,32,32	0.77	0	48,51,51	1.79	8 (16%)
2	CHD	B	2502	-	29,32,32	0.79	1 (3%)	48,51,51	1.10	2 (4%)
2	CHD	B	2503	-	29,32,32	0.79	2 (6%)	48,51,51	1.17	3 (6%)
3	FES	B	2999	1	0,4,4	0.00	-	0,4,4	0.00	-

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
3	FES	A	1499	1	-	0/0/4/4	0/1/1/1
2	CHD	A	1501	-	-	0/7/74/74	0/4/4/4
2	CHD	A	1502	-	-	0/7/74/74	0/4/4/4
2	CHD	A	1503	-	-	0/7/74/74	0/4/4/4
2	CHD	B	2501	-	-	0/7/74/74	0/4/4/4
2	CHD	B	2502	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHD	B	2503	-	-	0/7/74/74	0/4/4/4
3	FES	B	2999	1	-	0/0/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2502	CHD	O12-C12	-2.32	1.39	1.43
2	B	2503	CHD	O12-C12	-2.15	1.40	1.43
2	A	1502	CHD	O12-C12	-2.02	1.40	1.43
2	B	2503	CHD	C11-C12	2.05	1.57	1.53
2	A	1502	CHD	C11-C12	2.12	1.57	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2501	CHD	C13-C17-C20	-6.19	111.96	119.50
2	B	2501	CHD	C23-C22-C20	-5.50	108.27	114.75
2	A	1501	CHD	C13-C17-C20	-5.44	112.88	119.50
2	A	1501	CHD	C23-C22-C20	-4.86	109.03	114.75
2	A	1501	CHD	C11-C12-C13	-3.19	107.96	111.20
2	B	2501	CHD	C11-C12-C13	-3.15	108.00	111.20
2	A	1503	CHD	C4-C5-C10	-3.07	109.27	112.66
2	B	2501	CHD	C21-C20-C22	-3.00	105.34	110.35
2	A	1501	CHD	C21-C20-C22	-2.75	105.76	110.35
2	B	2501	CHD	C4-C5-C10	-2.60	109.79	112.66
2	B	2503	CHD	C4-C5-C10	-2.56	109.83	112.66
2	B	2503	CHD	C13-C17-C20	-2.52	116.43	119.50
2	B	2502	CHD	C4-C5-C10	-2.44	109.97	112.66
2	B	2503	CHD	C11-C12-C13	-2.41	108.76	111.20
2	A	1501	CHD	C1-C2-C3	-2.36	106.61	110.43
2	A	1502	CHD	C4-C5-C10	-2.31	110.11	112.66
2	A	1503	CHD	C13-C17-C20	-2.27	116.73	119.50
2	A	1501	CHD	C4-C5-C10	-2.26	110.17	112.66
2	B	2501	CHD	C11-C9-C10	-2.22	111.48	113.79
2	B	2501	CHD	C13-C14-C8	-2.20	111.91	114.75
2	A	1503	CHD	C11-C12-C13	-2.09	109.07	111.20
2	A	1502	CHD	C11-C12-C13	-2.08	109.08	111.20
2	B	2502	CHD	C11-C12-C13	-2.04	109.12	111.20
2	A	1503	CHD	C11-C9-C10	-2.03	111.68	113.79
2	A	1502	CHD	C11-C9-C10	-2.02	111.69	113.79
2	B	2501	CHD	C1-C2-C3	-2.00	107.19	110.43
2	A	1501	CHD	C6-C5-C4	2.34	113.66	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	CHD	7	0
2	A	1502	CHD	5	0
2	A	1503	CHD	1	0
2	B	2501	CHD	6	0
2	B	2502	CHD	6	0
2	B	2503	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	359/359 (100%)	2.69	260 (72%) 0 1	7, 17, 28, 33	0
1	B	359/359 (100%)	2.70	258 (71%) 0 1	8, 17, 28, 34	0
All	All	718/718 (100%)	2.70	518 (72%) 0 1	7, 17, 28, 34	0

All (518) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	VAL	11.7
1	B	213	VAL	10.1
1	B	214	GLY	9.4
1	B	423	LEU	7.8
1	A	423	LEU	7.1
1	B	182	LEU	7.0
1	B	215	ARG	6.9
1	A	360	CYS	6.8
1	A	212	GLN	6.7
1	B	250	LEU	6.4
1	B	66	LYS	6.3
1	A	96	ARG	6.1
1	B	168	PRO	6.0
1	A	355	VAL	6.0
1	B	104	GLN	5.9
1	B	361	GLY	5.9
1	B	174	ILE	5.8
1	A	250	LEU	5.8
1	A	214	GLY	5.8
1	A	132	ILE	5.7
1	B	134	ILE	5.7
1	A	144	VAL	5.6
1	B	212	GLN	5.4
1	A	185	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	150	LEU	5.4
1	B	257	VAL	5.4
1	B	358	LYS	5.4
1	B	360	CYS	5.3
1	B	132	ILE	5.3
1	B	394	LEU	5.2
1	A	319	ILE	5.1
1	A	153	ASN	5.1
1	A	155	ALA	5.1
1	B	115	LEU	5.1
1	A	134	ILE	5.0
1	A	211	ASN	5.0
1	B	405	LEU	4.9
1	B	101	LEU	4.9
1	B	112	ALA	4.8
1	A	307	PRO	4.8
1	B	209	TYR	4.8
1	B	390	GLN	4.7
1	B	144	VAL	4.7
1	B	102	PRO	4.7
1	A	306	GLY	4.7
1	B	351	GLU	4.6
1	A	115	LEU	4.6
1	A	217	PRO	4.6
1	A	215	ARG	4.5
1	A	206	ILE	4.5
1	B	100	THR	4.5
1	A	362	VAL	4.5
1	A	407	VAL	4.5
1	A	247	HIS	4.4
1	B	221	TRP	4.4
1	A	200	GLY	4.4
1	A	65	ARG	4.4
1	A	105	ASN	4.4
1	A	277	PRO	4.4
1	A	249	PRO	4.3
1	B	69	THR	4.3
1	B	175	GLU	4.3
1	B	173	ALA	4.3
1	B	146	LEU	4.3
1	A	270	VAL	4.3
1	A	219	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	4.3
1	B	393	GLU	4.3
1	B	98	LEU	4.2
1	A	305	VAL	4.2
1	B	270	VAL	4.2
1	B	105	ASN	4.2
1	B	410	VAL	4.2
1	B	422	GLN	4.2
1	B	200	GLY	4.2
1	B	249	PRO	4.2
1	B	352	TYR	4.2
1	A	284	VAL	4.1
1	A	344	THR	4.1
1	B	322	LEU	4.1
1	A	207	TYR	4.1
1	B	234	ILE	4.1
1	A	174	ILE	4.1
1	B	247	HIS	4.1
1	B	307	PRO	4.1
1	A	100	THR	4.1
1	A	150	LEU	4.1
1	A	293	TYR	4.1
1	A	351	GLU	4.1
1	B	355	VAL	4.1
1	B	210	TYR	4.1
1	B	357	ALA	4.1
1	A	210	TYR	4.0
1	B	305	VAL	4.0
1	A	103	ILE	4.0
1	A	202	SER	4.0
1	A	173	ALA	4.0
1	A	209	TYR	4.0
1	B	378	SER	4.0
1	A	221	TRP	4.0
1	A	410	VAL	4.0
1	B	310	TRP	3.9
1	A	66	LYS	3.9
1	A	418	PHE	3.9
1	B	145	LYS	3.9
1	A	315	THR	3.9
1	A	384	LEU	3.9
1	B	284	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	3.9
1	A	375	PRO	3.8
1	A	409	PRO	3.8
1	B	321	GLY	3.8
1	A	392	ASN	3.8
1	B	153	ASN	3.8
1	B	217	PRO	3.8
1	A	368	ALA	3.8
1	A	203	LEU	3.8
1	A	356	LEU	3.8
1	A	378	SER	3.8
1	B	404	PRO	3.8
1	A	98	LEU	3.8
1	A	146	LEU	3.8
1	A	358	LYS	3.8
1	A	114	ARG	3.8
1	A	352	TYR	3.8
1	B	313	PRO	3.8
1	A	141	GLU	3.8
1	A	365	ILE	3.7
1	A	183	GLU	3.7
1	B	108	ALA	3.7
1	A	166	VAL	3.7
1	A	99	MET	3.7
1	B	375	PRO	3.7
1	B	111	ILE	3.7
1	A	187	ALA	3.7
1	A	257	VAL	3.7
1	A	403	CYS	3.7
1	B	107	LEU	3.7
1	B	348	LEU	3.6
1	A	111	ILE	3.6
1	B	293	TYR	3.6
1	B	409	PRO	3.6
1	B	251	GLU	3.6
1	A	101	LEU	3.6
1	A	97	ASP	3.6
1	A	74	LEU	3.6
1	A	401	LEU	3.6
1	B	94	LEU	3.5
1	A	145	LYS	3.5
1	A	94	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	3.5
1	A	297	TYR	3.5
1	B	344	THR	3.5
1	A	82	LEU	3.5
1	A	218	THR	3.5
1	B	301	TRP	3.5
1	B	306	GLY	3.5
1	B	154	THR	3.5
1	A	390	GLN	3.5
1	B	287	VAL	3.4
1	A	381	LEU	3.4
1	B	85	VAL	3.4
1	A	235	GLN	3.4
1	B	363	GLU	3.4
1	B	103	ILE	3.4
1	B	236	CYS	3.4
1	B	116	THR	3.4
1	B	232	LEU	3.4
1	B	67	PRO	3.4
1	B	403	CYS	3.4
1	A	182	LEU	3.4
1	B	233	LEU	3.4
1	B	165	TYR	3.4
1	B	317	GLU	3.4
1	A	414	THR	3.3
1	B	386	HIS	3.3
1	B	248	PHE	3.3
1	A	160	TYR	3.3
1	B	127	GLY	3.3
1	A	151	SER	3.3
1	A	287	VAL	3.3
1	B	205	ALA	3.3
1	A	258	ILE	3.3
1	A	123	TYR	3.3
1	A	310	TRP	3.3
1	B	245	LEU	3.3
1	B	406	CYS	3.3
1	B	277	PRO	3.3
1	B	155	ALA	3.3
1	B	418	PHE	3.3
1	A	346	TYR	3.2
1	A	104	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	233	LEU	3.2
1	A	119	ILE	3.2
1	A	245	LEU	3.2
1	A	194	TYR	3.2
1	B	96	ARG	3.2
1	B	350	ILE	3.2
1	A	189	THR	3.2
1	B	407	VAL	3.2
1	A	223	THR	3.2
1	A	363	GLU	3.2
1	A	224	ILE	3.1
1	B	291	LEU	3.1
1	B	401	LEU	3.1
1	A	361	GLY	3.1
1	B	266	PRO	3.1
1	B	65	ARG	3.1
1	A	102	PRO	3.1
1	B	231	HIS	3.1
1	A	147	LEU	3.1
1	B	315	THR	3.1
1	B	297	TYR	3.1
1	A	301	TRP	3.1
1	A	348	LEU	3.1
1	B	319	ILE	3.1
1	A	313	PRO	3.1
1	A	322	LEU	3.0
1	B	183	GLU	3.0
1	B	299	LEU	3.0
1	B	323	CYS	3.0
1	A	168	PRO	3.0
1	A	334	PRO	3.0
1	A	161	ILE	3.0
1	B	119	ILE	3.0
1	B	292	GLU	3.0
1	A	159	TYR	3.0
1	A	260	PHE	3.0
1	A	417	PHE	3.0
1	A	116	THR	3.0
1	A	269	VAL	3.0
1	A	330	ILE	3.0
1	B	186	ILE	3.0
1	B	389	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLY	3.0
1	B	123	TYR	3.0
1	A	79	PRO	3.0
1	A	253	ARG	3.0
1	A	164	ARG	3.0
1	A	259	LEU	3.0
1	B	169	LEU	3.0
1	B	265	LEU	3.0
1	B	356	LEU	3.0
1	B	336	ALA	3.0
1	B	114	ARG	2.9
1	A	152	PRO	2.9
1	A	232	LEU	2.9
1	A	165	TYR	2.9
1	A	88	PHE	2.9
1	A	110	PHE	2.9
1	B	163	PHE	2.9
1	B	253	ARG	2.9
1	B	311	LEU	2.9
1	B	141	GLU	2.9
1	B	68	LYS	2.9
1	B	82	LEU	2.9
1	B	259	LEU	2.9
1	B	194	TYR	2.9
1	A	163	PHE	2.9
1	A	241	ILE	2.9
1	B	224	ILE	2.9
1	B	219	MET	2.9
1	A	135	TRP	2.9
1	B	359	GLU	2.9
1	B	365	ILE	2.9
1	A	413	GLU	2.9
1	B	258	ILE	2.8
1	A	357	ALA	2.8
1	B	167	HIS	2.8
1	A	191	TYR	2.8
1	A	68	LYS	2.8
1	B	241	ILE	2.8
1	A	376	LEU	2.8
1	A	380	ALA	2.8
1	A	389	ILE	2.8
1	B	99	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	267	MET	2.8
1	B	354	GLN	2.8
1	A	248	PHE	2.8
1	B	417	PHE	2.8
1	A	184	ARG	2.8
1	B	272	ARG	2.8
1	B	294	CYS	2.8
1	A	387	SER	2.8
1	B	160	TYR	2.8
1	B	223	THR	2.8
1	A	106	LYS	2.7
1	B	95	ASP	2.7
1	B	164	ARG	2.7
1	B	395	CYS	2.7
1	A	89	LEU	2.7
1	A	107	LEU	2.7
1	A	309	PRO	2.7
1	A	385	VAL	2.7
1	B	166	VAL	2.7
1	B	177	MET	2.7
1	B	385	VAL	2.7
1	A	175	GLU	2.7
1	B	276	TYR	2.7
1	A	345	LEU	2.7
1	B	384	LEU	2.7
1	B	416	SER	2.7
1	B	235	GLN	2.7
1	A	90	LEU	2.7
1	A	371	LEU	2.7
1	A	422	GLN	2.7
1	A	169	LEU	2.7
1	A	300	VAL	2.7
1	A	354	GLN	2.7
1	A	236	CYS	2.7
1	B	135	TRP	2.7
1	B	229	THR	2.7
1	B	207	TYR	2.7
1	A	242	LEU	2.6
1	B	147	LEU	2.6
1	A	399	LEU	2.6
1	A	192	PRO	2.6
1	A	420	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	77	GLY	2.6
1	B	377	PHE	2.6
1	A	265	LEU	2.6
1	A	296	PRO	2.6
1	A	140	GLY	2.6
1	B	191	TYR	2.6
1	A	377	PHE	2.6
1	B	383	ASP	2.6
1	B	391	SER	2.6
1	B	286	LYS	2.6
1	B	188	PHE	2.6
1	A	271	ASN	2.5
1	B	198	THR	2.5
1	A	412	ARG	2.5
1	A	109	PRO	2.5
1	A	127	GLY	2.5
1	B	371	LEU	2.5
1	A	186	ILE	2.5
1	B	335	ILE	2.5
1	B	370	SER	2.5
1	A	272	ARG	2.5
1	A	298	ARG	2.5
1	B	275	PRO	2.5
1	A	108	ALA	2.5
1	B	411	CYS	2.5
1	B	179	ARG	2.5
1	B	263	HIS	2.5
1	A	154	THR	2.5
1	B	368	ALA	2.5
1	B	110	PHE	2.5
1	B	197	SER	2.5
1	B	192	PRO	2.5
1	A	71	ILE	2.5
1	B	333	VAL	2.5
1	A	302	GLN	2.5
1	A	237	PHE	2.5
1	A	396	SER	2.5
1	B	387	SER	2.5
1	B	381	LEU	2.5
1	B	97	ASP	2.5
1	A	342	ILE	2.5
1	B	413	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	408	ASN	2.4
1	B	273	GLY	2.4
1	B	88	PHE	2.4
1	A	177	MET	2.4
1	B	256	VAL	2.4
1	B	161	ILE	2.4
1	B	342	ILE	2.4
1	B	172	GLU	2.4
1	B	298	ARG	2.4
1	B	196	CYS	2.4
1	B	117	PRO	2.4
1	B	296	PRO	2.4
1	B	201	SER	2.4
1	A	231	HIS	2.4
1	B	309	PRO	2.4
1	B	399	LEU	2.4
1	B	419	THR	2.4
1	A	112	ALA	2.4
1	A	131	PRO	2.4
1	A	404	PRO	2.4
1	B	109	PRO	2.4
1	A	294	CYS	2.4
1	A	72	LEU	2.4
1	B	89	LEU	2.4
1	A	262	ALA	2.3
1	A	180	ASP	2.3
1	B	148	ASP	2.3
1	A	335	ILE	2.3
1	B	281	SER	2.3
1	B	304	LYS	2.3
1	A	81	THR	2.3
1	B	218	THR	2.3
1	A	394	LEU	2.3
1	A	117	PRO	2.3
1	B	334	PRO	2.3
1	A	179	ARG	2.3
1	A	138	LYS	2.3
1	A	176	GLU	2.3
1	B	271	ASN	2.3
1	B	392	ASN	2.3
1	B	79	PRO	2.3
1	B	376	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	PHE	2.3
1	A	251	GLU	2.3
1	A	227	TRP	2.3
1	B	227	TRP	2.3
1	A	201	SER	2.3
1	B	206	ILE	2.3
1	A	288	MET	2.3
1	A	170	THR	2.3
1	A	379	LYS	2.3
1	A	332	LEU	2.3
1	B	72	LEU	2.3
1	A	93	PHE	2.3
1	B	93	PHE	2.3
1	B	382	ALA	2.3
1	A	411	CYS	2.3
1	A	181	GLY	2.3
1	B	222	SER	2.3
1	A	292	GLU	2.3
1	B	269	VAL	2.3
1	A	311	LEU	2.3
1	B	74	LEU	2.3
1	B	80	GLU	2.3
1	A	197	SER	2.3
1	B	202	SER	2.3
1	A	196	CYS	2.3
1	A	333	VAL	2.3
1	A	67	PRO	2.3
1	A	156	PRO	2.2
1	B	71	ILE	2.2
1	A	129	GLY	2.2
1	B	238	ALA	2.2
1	A	291	LEU	2.2
1	B	332	LEU	2.2
1	A	243	LYS	2.2
1	A	276	TYR	2.2
1	B	243	LYS	2.2
1	A	308	MET	2.2
1	B	349	ASP	2.2
1	B	211	ASN	2.2
1	A	406	CYS	2.2
1	A	222	SER	2.2
1	A	205	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	359	GLU	2.2
1	B	138	LYS	2.2
1	A	274	ASP	2.2
1	A	199	THR	2.2
1	A	369	GLU	2.2
1	A	393	GLU	2.2
1	A	402	SER	2.2
1	B	195	SER	2.2
1	B	312	GLY	2.2
1	A	421	GLN	2.2
1	B	124	ARG	2.2
1	A	349	ASP	2.2
1	A	92	LEU	2.2
1	A	143	MET	2.2
1	B	76	MET	2.2
1	A	317	GLU	2.2
1	A	229	THR	2.2
1	B	264	SER	2.2
1	B	199	THR	2.2
1	B	338	THR	2.2
1	A	266	PRO	2.2
1	B	156	PRO	2.2
1	A	299	LEU	2.1
1	A	331	LEU	2.1
1	A	405	LEU	2.1
1	B	242	LEU	2.1
1	B	345	LEU	2.1
1	A	70	GLY	2.1
1	A	289	GLU	2.1
1	B	318	SER	2.1
1	B	320	LYS	2.1
1	B	187	ALA	2.1
1	A	388	HIS	2.1
1	B	341	HIS	2.1
1	A	264	SER	2.1
1	B	414	THR	2.1
1	A	323	CYS	2.1
1	B	412	ARG	2.1
1	A	171	GLU	2.1
1	A	172	GLU	2.1
1	A	316	ASP	2.1
1	B	246	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	142	GLY	2.1
1	B	162	GLY	2.1
1	B	330	ILE	2.1
1	B	204	ASN	2.1
1	A	290	ARG	2.1
1	A	282	ALA	2.1
1	B	362	VAL	2.1
1	A	386	HIS	2.1
1	A	382	ALA	2.1
1	B	129	GLY	2.1
1	A	137	SER	2.1
1	B	143	MET	2.1
1	B	396	SER	2.1
1	B	184	ARG	2.1
1	A	273	GLY	2.1
1	B	73	MET	2.1
1	B	106	LYS	2.0
1	B	151	SER	2.0
1	B	300	VAL	2.0
1	B	290	ARG	2.0
1	A	122	GLN	2.0
1	A	364	ASN	2.0
1	A	128	GLY	2.0
1	A	162	GLY	2.0
1	A	370	SER	2.0
1	A	267	MET	2.0
1	B	208	ARG	2.0
1	B	400	THR	2.0
1	A	195	SER	2.0
1	A	339	SER	2.0
1	B	339	SER	2.0
1	B	353	SER	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

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
2	CHD	A	1503	29/29	0.53	0.35	1.27	32,33,39,40	0
2	CHD	B	2503	29/29	0.50	0.37	1.25	33,35,42,43	0
2	CHD	B	2501	29/29	0.65	0.32	1.22	18,19,35,37	0
2	CHD	A	1501	29/29	0.72	0.30	1.02	16,18,36,39	0
2	CHD	B	2502	29/29	0.57	0.30	0.10	24,25,33,35	0
2	CHD	A	1502	29/29	0.55	0.30	-0.02	24,24,33,34	0
3	FES	B	2999	4/4	0.92	0.15	-2.33	14,15,15,15	0
3	FES	A	1499	4/4	0.96	0.11	-3.10	13,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.