



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:05 PM UTC

PDB ID : 1S9K / pdb_00001s9k
Title : Crystal Structure of Human NFAT1 and Fos-Jun on the IL-2 ARRE1 Site
Authors : Wang, D.; Stroud, J.C.; Chen, L.
Deposited on : 2004-02-04
Resolution : 3.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

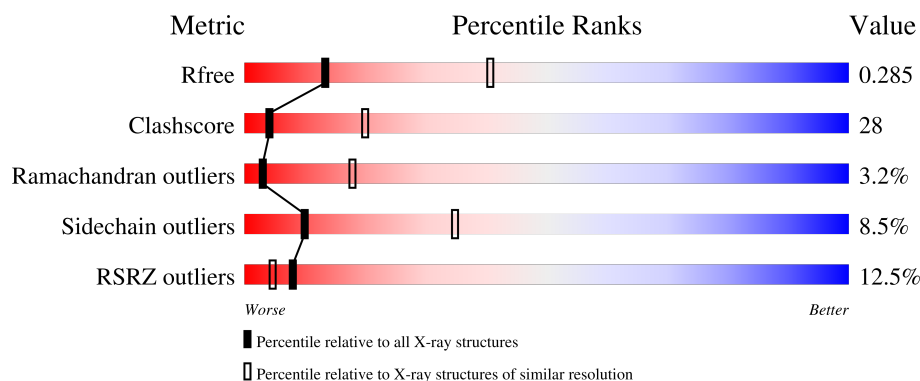
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	20	10% 90%
2	B	20	5% 5% 80% 15%
3	C	280	12% 44% 47% 8% .
4	D	53	9% 49% 45% . .
5	E	52	23% 54% 44% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3887 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 DNA chain called Human IL-2 ARRE1 Promoter Element, Plus Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	P	0	0	0
			413	200	76	118	19			

- Molecule 2 is a DNA chain called Human IL-2 ARRE1 Promoter Element, Minus Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			401	196	68	118	19			

- Molecule 3 is a protein called Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	280	Total	C	N	O	S	0	0	0
			2204	1383	404	408	9			

- Molecule 4 is a protein called Proto-oncogene protein c-fos.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	53	Total	C	N	O	S	0	0	0
			443	262	92	87	2			

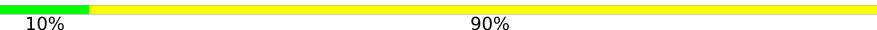
- Molecule 5 is a protein called Transcription factor AP-1.

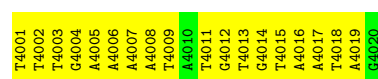
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	52	Total	C	N	O	S	0	0	0
			426	257	92	74	3			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Human IL-2 ARRE1 Promoter Element, Plus Strand

Chain A: 

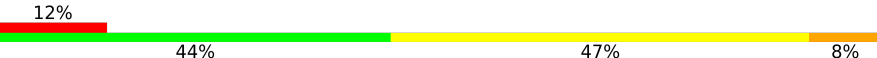


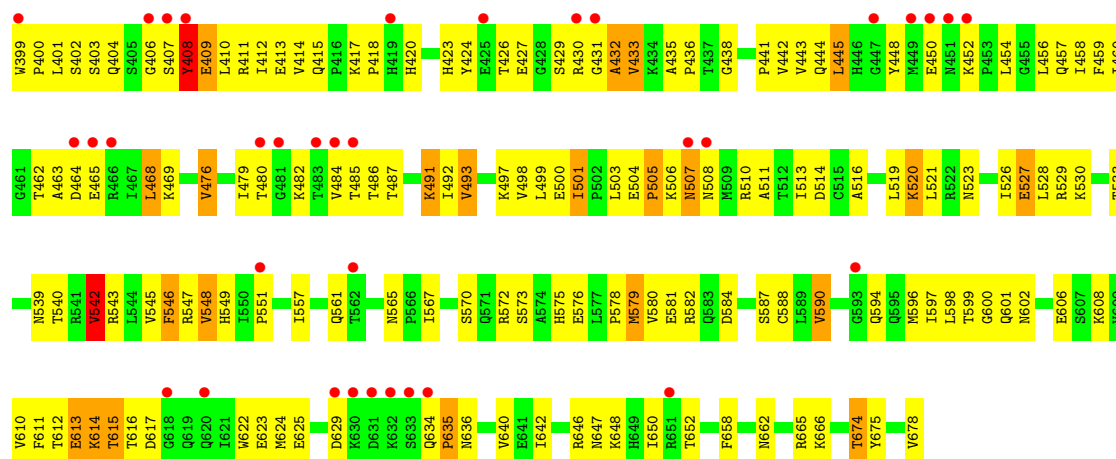
- Molecule 2: Human IL-2 ARRE1 Promoter Element, Minus Strand

Chain B: 



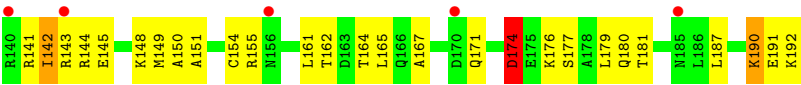
- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

Chain C: 



- Molecule 4: Proto-oncogene protein c-fos

Chain D: 



● Molecule 5: Transcription factor AP-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.77Å 86.26Å 84.04Å 90.00° 111.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.10) 97.3 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.05Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.275 0.250 , 0.285	Depositor DCC
R_{free} test set	1578 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.934	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.37	0/464	0.86	1/716 (0.1%)
2	B	0.42	0/448	0.87	0/688
3	C	0.59	1/2253 (0.0%)	1.15	15/3050 (0.5%)
4	D	0.74	1/442 (0.2%)	1.08	3/583 (0.5%)
5	E	0.82	1/425 (0.2%)	1.00	1/558 (0.2%)
All	All	0.60	3/4032 (0.1%)	1.06	20/5595 (0.4%)

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
2	B	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	279	CYS	CB-SG	-12.08	1.41	1.81
4	D	154	CYS	CB-SG	-11.58	1.43	1.81
3	C	432	ALA	CA-CB	-6.35	1.42	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	141	ARG	N-CA-C	-9.17	102.22	113.50
3	C	400	PRO	N-CA-C	-8.61	102.57	114.80
3	C	406	GLY	N-CA-C	7.50	122.68	112.17
3	C	616	THR	N-CA-C	-7.25	104.17	112.87
3	C	408	TYR	N-CA-C	-6.88	96.15	110.80
3	C	606	GLU	N-CA-C	-6.84	104.97	113.38
3	C	431	GLY	N-CA-C	-6.79	103.85	112.54
3	C	493	VAL	N-CA-C	6.63	123.14	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	404	GLN	N-CA-C	6.34	118.18	109.18
3	C	542	VAL	N-CA-C	6.15	117.03	108.23
5	E	268	LYS	N-CA-C	6.02	123.63	110.80
3	C	438	GLY	N-CA-C	-5.94	107.62	114.69
4	D	142	ILE	N-CA-C	-5.65	104.86	110.62
1	A	4011	DT	N1-C1'-C2'	5.56	121.84	113.50
3	C	612	THR	N-CA-C	5.53	118.08	109.52
4	D	174	ASP	N-CA-C	-5.40	105.09	110.97
3	C	433	VAL	N-CA-C	5.28	120.31	109.34
3	C	505	PRO	N-CA-C	-5.24	106.25	113.53
3	C	590	VAL	N-CA-C	5.16	120.08	109.34
3	C	407	SER	N-CA-C	-5.01	107.16	113.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	5009	DC	Sidechain
2	B	5014	DA	Sidechain
2	B	5016	DT	Sidechain

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	413	0	230	26	0
2	B	401	0	230	23	0
3	C	2204	0	2168	138	0
4	D	443	0	461	17	0
5	E	426	0	472	28	0
All	All	3887	0	3561	205	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 28.

All (205) 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)
3:C:613:GLU:HB2	3:C:622:TRP:HB3	1.36	1.04
2:B:5005:DA:H1'	2:B:5006:DT:H5'	1.51	0.92
5:E:310:MET:HE2	5:E:314:GLN:HE21	1.38	0.87
3:C:441:PRO:HG2	3:C:513:ILE:HB	1.60	0.82
3:C:521:LEU:HD12	3:C:521:LEU:N	1.95	0.81
4:D:162:THR:HG22	5:E:287:ILE:HG12	1.65	0.78
3:C:501:ILE:H	3:C:501:ILE:HD13	1.47	0.78
1:A:4003:DT:H1'	1:A:4004:DG:H5'	1.66	0.76
3:C:444:GLN:HE21	3:C:510:ARG:HB2	1.50	0.76
3:C:587:SER:HB3	3:C:674:THR:HG23	1.67	0.76
3:C:410:LEU:HD22	3:C:548:VAL:HG22	1.66	0.76
3:C:570:SER:HB3	3:C:573:SER:HB2	1.69	0.74
4:D:177:SER:O	4:D:181:THR:HG23	1.87	0.74
3:C:547:ARG:HG2	3:C:561:GLN:HB2	1.69	0.73
1:A:4001:DT:H2'	1:A:4002:DT:C7	2.17	0.73
2:B:5009:DC:P	5:E:273:ARG:HE	2.13	0.72
3:C:578:PRO:HA	3:C:602:ASN:HB2	1.70	0.71
1:A:4018:DT:H2''	1:A:4019:DA:OP2	1.91	0.71
3:C:596:MET:HE3	3:C:598:LEU:HD13	1.73	0.70
4:D:171:GLN:O	4:D:174:ASP:HB2	1.92	0.70
3:C:456:LEU:HD11	3:C:546:PHE:HB3	1.73	0.69
3:C:647:ASN:O	3:C:650:ILE:HG23	1.91	0.69
3:C:458:ILE:HG22	3:C:546:PHE:HD2	1.57	0.69
2:B:5003:DC:H2''	2:B:5004:DT:OP2	1.92	0.68
3:C:482:LYS:N	3:C:482:LYS:HD2	2.08	0.68
3:C:458:ILE:HG22	3:C:546:PHE:CD2	2.28	0.68
1:A:4003:DT:H71	3:C:430:ARG:NH1	2.09	0.67
2:B:5002:DA:H2''	2:B:5003:DC:OP2	1.94	0.67
3:C:457:GLN:HB3	3:C:500:GLU:HG2	1.78	0.66
1:A:4003:DT:C7	3:C:430:ARG:HH12	2.09	0.66
1:A:4004:DG:H1'	1:A:4005:DA:H5''	1.79	0.65
3:C:542:VAL:CG1	3:C:543:ARG:N	2.60	0.65
1:A:4003:DT:C7	3:C:430:ARG:NH1	2.59	0.65
1:A:4008:DA:H1'	1:A:4009:DT:H5''	1.78	0.65
3:C:584:ASP:CB	3:C:597:ILE:H	2.10	0.64
2:B:5009:DC:OP1	5:E:273:ARG:NE	2.31	0.63
2:B:5010:DA:H3'	5:E:269:ARG:NE	2.13	0.63
1:A:4014:DG:H1'	1:A:4015:DT:H5''	1.79	0.62
3:C:634:GLN:CB	3:C:635:PRO:HD2	2.28	0.62
1:A:4002:DT:H1'	1:A:4003:DT:H5'	1.82	0.62
1:A:4001:DT:H2''	1:A:4002:DT:O5'	2.00	0.61
3:C:551:PRO:HA	3:C:557:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:444:GLN:NE2	3:C:510:ARG:HB2	2.15	0.61
1:A:4001:DT:H2'	1:A:4002:DT:H72	1.83	0.60
3:C:412:ILE:HA	3:C:443:VAL:HG22	1.84	0.60
3:C:575:HIS:O	3:C:602:ASN:ND2	2.35	0.59
3:C:456:LEU:O	3:C:501:ILE:HD13	2.03	0.59
3:C:526:ILE:C	3:C:528:LEU:H	2.11	0.59
3:C:614:LYS:HB2	3:C:614:LYS:NZ	2.18	0.59
5:E:290:LEU:O	5:E:294:VAL:HG23	2.01	0.59
3:C:520:LYS:HD3	3:C:521:LEU:N	2.18	0.59
3:C:399:TRP:HB2	3:C:547:ARG:HH22	1.67	0.58
1:A:4001:DT:H2'	1:A:4002:DT:H73	1.86	0.58
3:C:584:ASP:HB3	3:C:597:ILE:H	1.69	0.57
3:C:542:VAL:HG13	3:C:543:ARG:N	2.20	0.57
3:C:587:SER:CB	3:C:674:THR:HG23	2.33	0.57
3:C:435:ALA:HB1	3:C:436:PRO:HD2	1.85	0.57
3:C:507:ASN:O	3:C:508:ASN:HB3	2.04	0.57
1:A:4003:DT:H71	3:C:430:ARG:HH12	1.69	0.57
2:B:5012:DA:H1'	2:B:5013:DT:H5''	1.86	0.57
4:D:151:ALA:O	4:D:155:ARG:HG3	2.03	0.57
3:C:521:LEU:N	3:C:521:LEU:CD1	2.68	0.57
3:C:572:ARG:HG2	3:C:576:GLU:HG3	1.87	0.57
3:C:526:ILE:O	3:C:528:LEU:N	2.37	0.56
1:A:4005:DA:H2''	1:A:4006:DA:C8	2.40	0.56
3:C:460:ILE:HG23	3:C:542:VAL:CG1	2.36	0.56
3:C:457:GLN:HA	3:C:499:LEU:O	2.06	0.56
3:C:601:GLN:O	3:C:602:ASN:HB2	2.05	0.55
3:C:423:HIS:O	3:C:519:LEU:HD12	2.07	0.55
3:C:462:THR:HG22	3:C:463:ALA:N	2.21	0.55
3:C:526:ILE:C	3:C:528:LEU:N	2.64	0.55
3:C:584:ASP:HB2	3:C:597:ILE:HB	1.89	0.55
1:A:4004:DG:H1'	1:A:4005:DA:C5'	2.36	0.55
2:B:5003:DC:C6	2:B:5004:DT:H72	2.41	0.55
3:C:408:TYR:O	3:C:409:GLU:HB2	2.06	0.55
3:C:460:ILE:HG12	3:C:476:VAL:HG13	1.88	0.55
3:C:482:LYS:HD3	3:C:486:THR:H	1.73	0.54
3:C:579:MET:HE1	3:C:581:GLU:HB3	1.89	0.54
3:C:579:MET:O	3:C:579:MET:HG3	2.06	0.54
5:E:280:ARG:O	5:E:281:LYS:C	2.50	0.54
3:C:610:VAL:O	3:C:658:PHE:HA	2.08	0.54
2:B:5015:DT:H1'	2:B:5016:DT:H5'	1.89	0.53
3:C:501:ILE:H	3:C:501:ILE:CD1	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5010:DA:H3'	5:E:269:ARG:CZ	2.38	0.53
3:C:412:ILE:HG12	3:C:443:VAL:HG22	1.91	0.53
3:C:549:HIS:O	3:C:551:PRO:HD3	2.09	0.53
3:C:608:LYS:HD2	3:C:625:GLU:OE2	2.08	0.53
3:C:468:LEU:HD13	3:C:469:LYS:N	2.23	0.53
3:C:615:THR:C	3:C:617:ASP:N	2.67	0.53
3:C:420:HIS:CD2	3:C:433:VAL:HA	2.44	0.53
3:C:444:GLN:CB	3:C:510:ARG:HA	2.38	0.53
3:C:646:ARG:HG3	3:C:647:ASN:H	1.74	0.52
2:B:5008:DA:H2'	5:E:280:ARG:HH22	1.74	0.52
3:C:420:HIS:CD2	3:C:433:VAL:HG22	2.45	0.52
3:C:482:LYS:HD2	3:C:482:LYS:H	1.72	0.52
3:C:581:GLU:HG2	3:C:600:GLY:HA2	1.90	0.52
3:C:530:LYS:HA	5:E:289:ARG:NH2	2.25	0.52
1:A:4012:DG:H5''	3:C:665:ARG:HH22	1.74	0.52
1:A:4017:DA:H1'	1:A:4018:DT:H5'	1.92	0.51
2:B:5007:DT:H2''	2:B:5008:DA:OP2	2.10	0.51
2:B:5009:DC:OP2	5:E:273:ARG:HG3	2.10	0.51
4:D:176:LYS:HA	4:D:179:LEU:HD12	1.92	0.51
3:C:414:VAL:HG23	3:C:442:VAL:HB	1.92	0.51
1:A:4012:DG:C5'	3:C:665:ARG:HH22	2.23	0.51
1:A:4007:DA:H2''	1:A:4008:DA:OP2	2.11	0.51
2:B:5017:DT:H2''	2:B:5018:DT:OP2	2.09	0.51
1:A:4003:DT:OP2	3:C:430:ARG:NH2	2.44	0.50
3:C:462:THR:CG2	3:C:463:ALA:N	2.74	0.50
3:C:520:LYS:C	3:C:521:LEU:HD12	2.35	0.50
3:C:432:ALA:HB2	3:C:479:ILE:CB	2.41	0.50
3:C:526:ILE:O	3:C:529:ARG:HG2	2.11	0.50
3:C:417:LYS:HG2	3:C:418:PRO:HD2	1.92	0.50
3:C:588:CYS:O	3:C:675:TYR:HA	2.12	0.50
3:C:662:ASN:O	3:C:666:LYS:HB2	2.12	0.50
3:C:600:GLY:O	3:C:636:ASN:HB2	2.12	0.50
5:E:312:ARG:HG2	5:E:312:ARG:NH1	2.27	0.49
1:A:4003:DT:H72	3:C:430:ARG:HH12	1.76	0.49
2:B:5018:DT:H72	3:C:427:GLU:OE2	2.12	0.49
3:C:587:SER:HB2	3:C:674:THR:O	2.12	0.49
3:C:658:PHE:C	3:C:658:PHE:CD1	2.90	0.49
5:E:276:ALA:HB1	5:E:280:ARG:NH1	2.27	0.48
3:C:444:GLN:HB3	3:C:510:ARG:HA	1.94	0.48
3:C:540:THR:HG21	3:C:570:SER:HB2	1.95	0.48
3:C:482:LYS:HG2	3:C:514:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5018:DT:H1'	2:B:5019:DC:H5''	1.94	0.48
5:E:309:ASN:O	5:E:312:ARG:HB2	2.12	0.47
3:C:615:THR:C	3:C:617:ASP:H	2.20	0.47
5:E:272:ASN:O	5:E:273:ARG:C	2.57	0.47
2:B:5001:DA:H2''	2:B:5002:DA:O5'	2.14	0.47
3:C:520:LYS:HD3	3:C:520:LYS:C	2.40	0.47
3:C:678:VAL:OXT	3:C:678:VAL:HG13	2.13	0.47
5:E:312:ARG:HG2	5:E:312:ARG:HH11	1.79	0.47
3:C:411:ARG:O	3:C:443:VAL:HG13	2.14	0.46
3:C:458:ILE:CG1	3:C:499:LEU:HB2	2.45	0.46
2:B:5010:DA:OP1	5:E:269:ARG:HD3	2.15	0.46
3:C:460:ILE:HG23	3:C:542:VAL:HG13	1.96	0.46
3:C:456:LEU:HG	3:C:501:ILE:HD11	1.97	0.46
3:C:401:LEU:CD2	4:D:180:GLN:HE22	2.29	0.46
1:A:4013:DT:H2''	1:A:4014:DG:OP2	2.15	0.46
3:C:458:ILE:HA	3:C:545:VAL:O	2.16	0.46
4:D:142:ILE:O	4:D:143:ARG:C	2.60	0.45
4:D:162:THR:CG2	5:E:287:ILE:HG12	2.43	0.45
3:C:582:ARG:HB2	3:C:599:THR:HB	1.97	0.45
4:D:190:LYS:O	4:D:192:LYS:N	2.50	0.45
5:E:287:ILE:O	5:E:291:GLU:HG3	2.17	0.45
5:E:314:GLN:O	5:E:318:LEU:HG	2.17	0.45
3:C:413:GLU:N	3:C:442:VAL:O	2.50	0.44
3:C:460:ILE:HG23	3:C:542:VAL:HG11	1.98	0.44
3:C:539:ASN:ND2	3:C:539:ASN:C	2.75	0.44
3:C:579:MET:HE3	3:C:580:VAL:C	2.41	0.44
1:A:4005:DA:H2''	1:A:4006:DA:N7	2.32	0.44
2:B:5014:DA:H1'	2:B:5015:DT:H5''	1.99	0.44
3:C:634:GLN:CB	3:C:635:PRO:CD	2.94	0.44
2:B:5017:DT:H2'	3:C:424:TYR:CE2	2.52	0.44
4:D:149:MET:O	4:D:150:ALA:C	2.60	0.44
3:C:410:LEU:HD22	3:C:548:VAL:CG2	2.43	0.44
3:C:546:PHE:O	3:C:561:GLN:HA	2.18	0.44
3:C:542:VAL:HG13	3:C:543:ARG:H	1.82	0.44
4:D:164:THR:O	4:D:167:ALA:HB3	2.17	0.44
3:C:433:VAL:HG23	3:C:516:ALA:O	2.18	0.44
3:C:458:ILE:HG12	3:C:499:LEU:HB2	1.99	0.44
3:C:456:LEU:HD12	3:C:457:GLN:N	2.33	0.44
3:C:507:ASN:O	3:C:508:ASN:CB	2.66	0.43
3:C:579:MET:CE	3:C:581:GLU:HB3	2.47	0.43
3:C:611:PHE:O	3:C:623:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:297:LEU:O	5:E:298:LYS:C	2.62	0.43
1:A:4003:DT:H72	3:C:430:ARG:NH1	2.32	0.43
3:C:409:GLU:O	3:C:445:LEU:HD23	2.18	0.43
3:C:635:PRO:HG2	3:C:636:ASN:H	1.82	0.43
3:C:452:LYS:HD3	3:C:452:LYS:HA	1.69	0.43
3:C:542:VAL:O	3:C:567:ILE:N	2.52	0.43
3:C:456:LEU:HD12	3:C:547:ARG:O	2.19	0.43
3:C:415:GLN:HG3	3:C:565:ASN:ND2	2.33	0.43
5:E:276:ALA:O	5:E:277:SER:C	2.62	0.43
3:C:459:PHE:HB3	3:C:498:VAL:HG22	2.00	0.43
3:C:492:ILE:O	3:C:497:LYS:HA	2.19	0.43
3:C:423:HIS:CD2	3:C:429:SER:HA	2.55	0.42
4:D:145:GLU:O	4:D:148:LYS:HB2	2.19	0.42
3:C:420:HIS:HD2	3:C:433:VAL:HA	1.84	0.42
3:C:503:LEU:CD2	3:C:511:ALA:HB2	2.49	0.42
3:C:504:GLU:HA	3:C:505:PRO:HD3	1.90	0.42
3:C:501:ILE:HD13	3:C:501:ILE:N	2.24	0.42
3:C:501:ILE:O	3:C:501:ILE:HG12	2.19	0.42
5:E:272:ASN:O	5:E:275:ALA:N	2.53	0.42
3:C:594:GLN:O	3:C:642:ILE:HG13	2.20	0.42
2:B:5002:DA:C4	2:B:5003:DC:C5	3.08	0.41
5:E:275:ALA:O	5:E:276:ALA:C	2.63	0.41
2:B:5013:DT:H2"	2:B:5014:DA:OP2	2.20	0.41
3:C:491:LYS:HD2	3:C:497:LYS:HD2	2.02	0.41
4:D:171:GLN:O	4:D:174:ASP:CB	2.66	0.41
3:C:401:LEU:CD2	4:D:180:GLN:NE2	2.84	0.41
3:C:448:TYR:OH	3:C:454:LEU:HD11	2.20	0.41
3:C:523:ASN:O	3:C:527:GLU:HG3	2.21	0.41
3:C:578:PRO:O	3:C:579:MET:HB3	2.20	0.41
3:C:608:LYS:HD3	3:C:608:LYS:HA	1.85	0.41
4:D:176:LYS:HB2	5:E:301:ASN:OD1	2.21	0.41
4:D:187:LEU:HA	4:D:187:LEU:HD23	1.79	0.41
3:C:506:LYS:H	3:C:506:LYS:HG3	1.49	0.41
1:A:4016:DA:OP1	4:D:144:ARG:NH2	2.54	0.41
3:C:533:THR:HG22	5:E:289:ARG:HB3	2.03	0.41
5:E:272:ASN:C	5:E:274:ILE:N	2.77	0.40
3:C:448:TYR:CZ	3:C:450:GLU:HB2	2.57	0.40
3:C:508:ASN:ND2	3:C:508:ASN:O	2.55	0.40
2:B:5011:DC:P	5:E:269:ARG:HH21	2.44	0.40
3:C:484:VAL:O	3:C:486:THR:N	2.54	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	
3	C	278/280 (99%)	237 (85%)	32 (12%)	9 (3%)	3	18
4	D	51/53 (96%)	45 (88%)	4 (8%)	2 (4%)	2	14
5	E	50/52 (96%)	39 (78%)	10 (20%)	1 (2%)	6	25
All	All	379/385 (98%)	321 (85%)	46 (12%)	12 (3%)	3	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	480	THR
3	C	590	VAL
3	C	527	GLU
3	C	629	ASP
3	C	635	PRO
4	D	191	GLU
5	E	268	LYS
3	C	409	GLU
3	C	485	THR
3	C	464	ASP
4	D	190	LYS
3	C	493	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	238/250 (95%)	213 (90%)	25 (10%)	6	26
4	D	47/47 (100%)	44 (94%)	3 (6%)	16	44
5	E	45/45 (100%)	45 (100%)	0	100	100
All	All	330/342 (96%)	302 (92%)	28 (8%)	10	35

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	402	SER
3	C	403	SER
3	C	408	TYR
3	C	426	THR
3	C	445	LEU
3	C	465	GLU
3	C	468	LEU
3	C	476	VAL
3	C	487	THR
3	C	491	LYS
3	C	501	ILE
3	C	507	ASN
3	C	520	LYS
3	C	542	VAL
3	C	546	PHE
3	C	548	VAL
3	C	579	MET
3	C	613	GLU
3	C	614	LYS
3	C	615	THR
3	C	624	MET
3	C	640	VAL
3	C	648	LYS
3	C	652	THR
3	C	674	THR
4	D	161	LEU
4	D	165	LEU
4	D	174	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	423	HIS
3	C	444	GLN
3	C	451	ASN
3	C	457	GLN
3	C	495	ASN
3	C	508	ASN
3	C	523	ASN
3	C	539	ASN
3	C	565	ASN
3	C	671	GLN
3	C	676	HIS
4	D	180	GLN
5	E	314	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	20/20 (100%)	0.47	0 100 100	29, 39, 68, 81	0
2	B	20/20 (100%)	0.46	1 (5%) 34 18	28, 46, 60, 70	0
3	C	280/280 (100%)	0.74	35 (12%) 8 5	20, 55, 112, 151	0
4	D	53/53 (100%)	0.76	5 (9%) 14 8	25, 56, 116, 138	0
5	E	52/52 (100%)	0.98	12 (23%) 2 1	24, 63, 116, 126	0
All	All	425/425 (100%)	0.75	53 (12%) 8 5	20, 53, 112, 151	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	631	ASP	9.1
3	C	485	THR	6.7
3	C	483	THR	6.5
5	E	268	LYS	5.5
3	C	630	LYS	4.8
3	C	629	ASP	4.7
4	D	143	ARG	4.4
3	C	633	SER	4.1
3	C	419	HIS	4.1
3	C	431	GLY	4.1
3	C	484	VAL	3.8
3	C	562	THR	3.8
5	E	269	ARG	3.8
3	C	480	THR	3.7
3	C	407	SER	3.7
3	C	481	GLY	3.6
3	C	632	LYS	3.4
5	E	284	LEU	3.3
3	C	406	GLY	3.2
5	E	270	MET	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	273	ARG	3.0
3	C	508	ASN	2.8
4	D	140	ARG	2.8
3	C	449	MET	2.7
5	E	272	ASN	2.7
2	B	5001	DA	2.7
3	C	507	ASN	2.7
3	C	430	ARG	2.6
5	E	278	LYS	2.6
3	C	399	TRP	2.5
3	C	447	GLY	2.5
3	C	451	ASN	2.4
5	E	310	MET	2.4
4	D	156	ASN	2.4
3	C	465	GLU	2.3
3	C	464	ASP	2.3
4	D	170	ASP	2.3
5	E	271	ARG	2.3
3	C	452	LYS	2.2
3	C	620	GLN	2.2
3	C	408	TYR	2.2
5	E	282	ARG	2.2
4	D	185	ASN	2.2
5	E	317	GLN	2.1
3	C	425	GLU	2.1
3	C	466	ARG	2.1
3	C	593	GLY	2.1
3	C	634	GLN	2.1
3	C	551	PRO	2.1
3	C	618	GLY	2.0
5	E	292	GLU	2.0
3	C	651	ARG	2.0
3	C	450	GLU	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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.