



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:04 PM UTC

PDB ID : 1GWQ / pdb_00001gwq
Title : HUMAN OESTROGEN RECEPTOR ALPHA LIGAND-BINDING DOMAIN IN COMPLEX WITH RALOXIFENE CORE AND TIF2 NRBOX2 PEPTIDE
Authors : Pike, A.C.W.; Brzozowski, A.M.
Deposited on : 2002-03-22
Resolution : 2.45 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

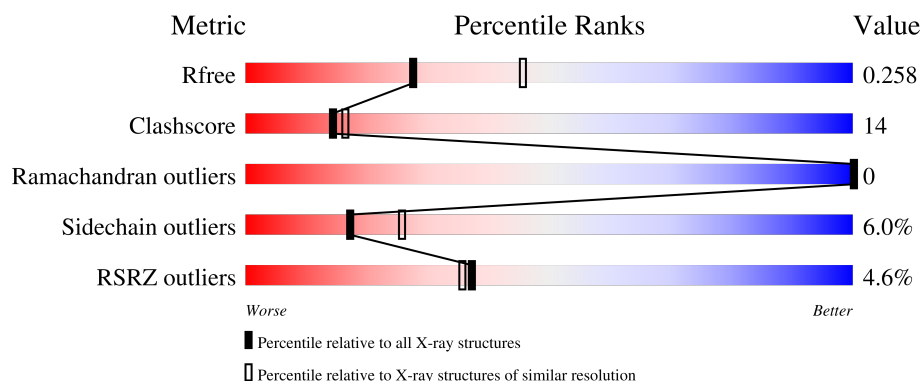
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	248	
1	B	248	
2	C	9	
2	D	9	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4192 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.

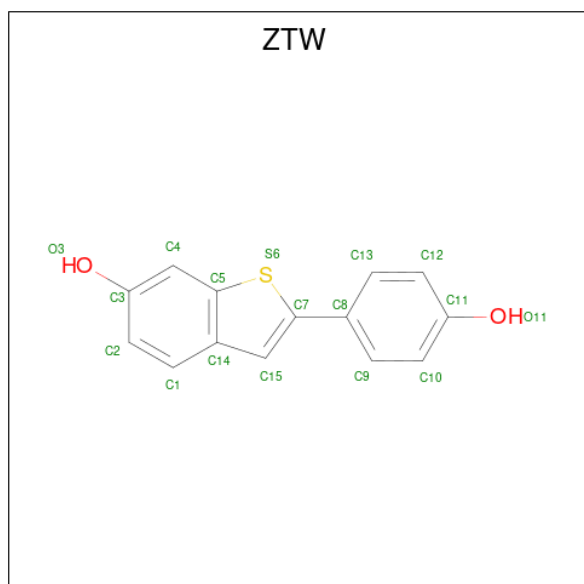
- Molecule 1 is a protein called OESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	6	0
			1952	1246	337	349	20			
1	B	242	Total	C	N	O	S	7	3	0
			1938	1240	334	345	19			

- Molecule 2 is a protein called NUCLEAR RECEPTOR COACTIVATOR 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			73	47	15	11			
2	D	9	Total	C	N	O	0	0	0
			76	48	15	13			

- Molecule 3 is RALOXIFENE CORE (CCD ID: ZTW) (formula: C₁₄H₁₀O₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			17	14	2	1		
3	B	1	Total	C	O	S	0	0
			17	14	2	1		

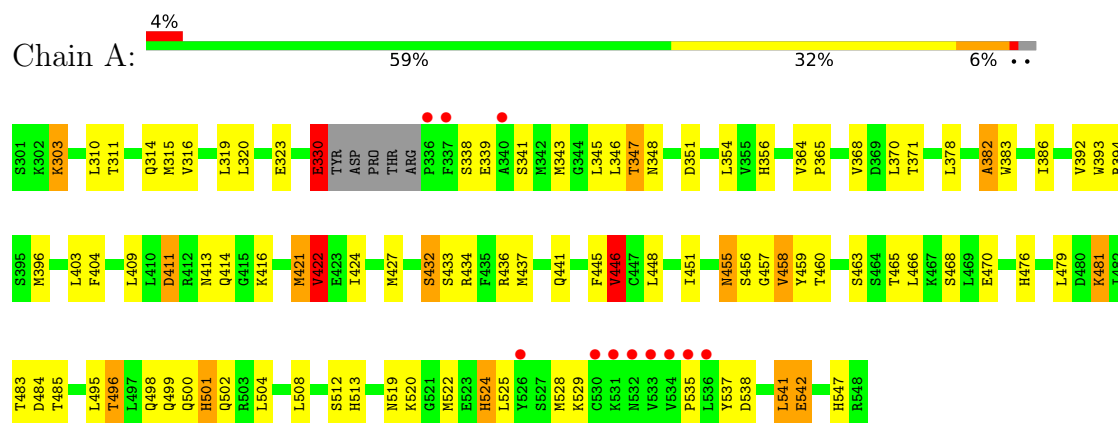
- Molecule 4 is water.

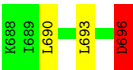
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	60	Total	O	0	0
			60	60		

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: OESTROGEN RECEPTOR





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.82Å 63.62Å 74.72Å 90.00° 98.34° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 20.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.45) 99.5 (20.00-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.206 , 0.269 0.203 , 0.258	Depositor DCC
R_{free} test set	977 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4192	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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

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

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	0/2019	1.98	63/2722 (2.3%)
1	B	0.77	1/1988 (0.1%)	2.05	64/2680 (2.4%)
2	C	0.63	0/73	1.62	0/96
2	D	0.46	0/76	1.30	1/100 (1.0%)
All	All	0.76	1/4156 (0.0%)	2.00	128/5598 (2.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	LEU	CB-CG	-5.27	1.43	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	436	ARG	CD-NE-CZ	37.07	176.30	124.40
1	A	436	ARG	CD-NE-CZ	24.38	158.53	124.40
1	A	411	ASP	CA-CB-CG	9.88	122.48	112.60
1	B	446	VAL	CB-CA-C	9.68	125.58	112.22
1	B	455	ASN	N-CA-C	9.38	121.58	111.36
1	A	445	PHE	O-C-N	-8.52	113.23	122.09
1	B	382	ALA	N-CA-C	8.42	123.74	113.38
1	A	458	VAL	CA-C-O	-8.13	111.87	120.57
1	A	422	VAL	CB-CA-C	-8.03	101.60	111.88
1	B	323	GLU	CA-C-N	8.02	128.64	120.38
1	B	323	GLU	C-N-CA	8.02	128.64	120.38
1	A	445	PHE	CA-C-O	7.99	129.44	120.90
1	A	348	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	B	422	VAL	CB-CA-C	-7.56	102.14	112.04
1	A	451	ILE	N-CA-C	-7.55	103.10	110.72
1	B	330	GLU	CB-CG-CD	7.40	125.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH2	7.36	125.83	119.20
1	A	484	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	320	LEU	CA-C-O	7.16	128.34	120.82
1	B	456	SER	N-CA-C	7.14	119.92	111.71
1	A	501[A]	HIS	CA-CB-CG	7.10	120.90	113.80
1	A	501[B]	HIS	CA-CB-CG	7.10	120.90	113.80
1	A	382	ALA	N-CA-C	7.03	122.03	113.38
1	B	352	ARG	NE-CZ-NH2	7.02	125.52	119.20
1	B	459	TYR	CA-CB-CG	-6.91	101.46	113.90
1	B	484	ASP	CA-CB-CG	6.90	119.50	112.60
1	B	498	GLN	OE1-CD-NE2	-6.84	115.75	122.60
1	B	512	SER	CA-C-O	-6.83	113.18	120.42
1	A	456	SER	CA-C-O	-6.77	112.45	120.10
1	A	463	SER	N-CA-C	6.66	119.06	109.14
1	B	436	ARG	NE-CZ-NH2	6.62	125.15	119.20
1	B	506	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	B	433	SER	O-C-N	6.60	129.22	122.09
1	B	346	LEU	CA-C-O	6.51	127.32	120.42
1	A	371	THR	N-CA-C	-6.47	101.98	110.53
1	B	515	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	A	348	ASN	CB-CG-ND2	6.45	126.08	116.40
1	A	441	GLN	CA-C-N	6.44	127.13	119.98
1	A	441	GLN	C-N-CA	6.44	127.13	119.98
1	B	538	ASP	N-CA-C	6.42	118.85	111.02
1	B	496	THR	N-CA-CB	-6.41	101.19	110.36
1	B	348	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	B	314	GLN	OE1-CD-NE2	6.39	128.99	122.60
1	B	411	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	364	VAL	CA-C-O	6.31	124.65	119.47
1	B	495	LEU	N-CA-CB	6.31	119.25	110.17
1	B	324	PRO	CB-CA-C	-6.30	103.24	110.92
1	A	394	ARG	O-C-N	6.25	129.54	122.22
1	B	347	THR	N-CA-CB	-6.25	100.91	110.16
1	B	412	ARG	CD-NE-CZ	6.22	133.10	124.40
1	A	414	GLN	CA-C-N	6.17	128.06	120.22
1	A	414	GLN	C-N-CA	6.17	128.06	120.22
1	A	356	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	A	483	THR	N-CA-C	-6.10	104.33	110.97
1	B	483	THR	CA-C-O	-6.08	114.43	120.82
1	B	441	GLN	CA-C-N	6.08	126.73	119.98
1	B	441	GLN	C-N-CA	6.08	126.73	119.98
1	B	501[A]	HIS	N-CA-CB	6.07	119.04	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	501[B]	HIS	N-CA-CB	6.07	119.04	110.12
1	A	311	THR	CA-C-N	6.07	128.33	120.44
1	A	311	THR	C-N-CA	6.07	128.33	120.44
1	A	364	VAL	N-CA-C	-6.06	103.42	108.63
1	A	483	THR	CA-C-O	-6.05	114.65	121.00
1	A	446	VAL	CB-CA-C	5.96	120.44	112.22
1	A	323	GLU	CA-C-N	5.95	126.51	120.38
1	A	323	GLU	C-N-CA	5.95	126.51	120.38
1	B	436	ARG	CA-C-O	5.94	126.72	120.42
1	A	303	LYS	N-CA-C	-5.92	102.71	110.53
1	B	368	VAL	CA-C-N	5.90	129.28	120.31
1	B	368	VAL	C-N-CA	5.90	129.28	120.31
2	D	696	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	512	SER	N-CA-CB	5.84	118.81	110.16
1	A	351	ASP	O-C-N	-5.84	116.06	122.07
1	A	476	HIS	CA-CB-CG	-5.84	107.96	113.80
1	B	448	LEU	CA-C-N	-5.80	111.49	120.31
1	B	448	LEU	C-N-CA	-5.80	111.49	120.31
1	B	483	THR	O-C-N	5.80	128.05	122.07
1	B	451	ILE	N-CA-C	-5.79	104.72	110.62
1	A	448	LEU	O-C-N	5.76	128.72	122.15
1	B	386	ILE	N-CA-CB	5.76	117.94	110.57
1	A	330	GLU	CB-CG-CD	5.71	122.30	112.60
1	A	396	MET	N-CA-CB	5.71	118.62	110.06
1	A	432	SER	CA-C-O	-5.68	114.49	120.63
1	B	438	MET	CA-C-O	5.67	126.37	119.11
1	B	371	THR	O-C-N	-5.64	116.58	122.96
1	A	413	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	470	GLU	CA-C-O	-5.62	114.91	120.82
1	B	478	VAL	N-CA-C	-5.61	105.05	110.72
1	A	396	MET	CA-CB-CG	5.60	125.30	114.10
1	B	536	LEU	CA-C-O	5.59	127.10	121.07
1	A	465	THR	CA-C-N	5.55	127.99	120.38
1	A	465	THR	C-N-CA	5.55	127.99	120.38
1	A	303	LYS	N-CA-CB	5.51	118.24	110.36
1	B	456	SER	CA-C-O	-5.50	113.89	120.10
1	A	421	MET	CA-C-O	-5.46	114.77	120.55
1	A	455	ASN	N-CA-C	5.45	120.02	112.45
1	B	393	TRP	CA-C-N	5.45	128.13	120.28
1	B	393	TRP	C-N-CA	5.45	128.13	120.28
1	B	358	ILE	CB-CA-C	5.42	119.45	112.14
1	B	476	HIS	CA-CB-CG	-5.40	108.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	A	436	ARG	CA-C-O	5.40	126.14	120.42
1	B	303	LYS	N-CA-C	-5.38	103.28	110.55
1	A	356	HIS	CB-CG-ND1	5.37	130.76	122.70
1	B	470	GLU	CA-C-O	-5.36	114.87	120.55
1	A	512	SER	N-CA-CB	5.33	118.05	110.16
1	A	524	HIS	CA-CB-CG	-5.33	108.47	113.80
1	B	440	LEU	CB-CA-C	-5.32	102.66	110.06
1	A	496	THR	N-CA-C	-5.30	103.89	110.41
1	A	378	LEU	O-C-N	-5.28	116.63	122.07
1	B	450	SER	CA-CB-OG	-5.27	100.55	111.10
1	A	446	VAL	N-CA-CB	-5.27	102.68	110.58
1	B	512	SER	CB-CA-C	-5.22	101.98	110.85
1	A	427	MET	N-CA-C	-5.21	105.52	111.14
1	B	446	VAL	N-CA-CB	-5.18	102.80	110.58
1	B	448	LEU	CA-C-O	-5.16	114.95	120.42
1	B	449	LYS	O-C-N	-5.16	115.92	122.27
1	A	393	TRP	CA-C-N	5.16	127.71	120.28
1	A	393	TRP	C-N-CA	5.16	127.71	120.28
1	A	448	LEU	CA-C-O	-5.11	115.00	120.42
1	A	370	LEU	CA-C-O	-5.09	116.19	121.99
1	B	467	LYS	CA-C-O	-5.09	115.48	120.82
1	A	457	GLY	CA-C-N	5.05	128.44	120.47
1	A	457	GLY	C-N-CA	5.05	128.44	120.47
1	B	444	GLU	N-CA-C	-5.03	105.71	111.14
1	B	512	SER	O-C-N	5.03	127.88	122.15
1	B	501[A]	HIS	CA-CB-CG	5.02	118.82	113.80
1	B	501[B]	HIS	CA-CB-CG	5.02	118.82	113.80

There are no chirality outliers.

There are no planarity outliers.

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	1952	0	1997	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1938	0	1991	70	0
2	C	73	0	75	0	0
2	D	76	0	77	2	0
3	A	17	0	10	4	0
3	B	17	0	10	5	0
4	A	59	0	0	0	0
4	B	60	0	0	0	0
All	All	4192	0	4160	116	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 14.

All (116) 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:501[B]:HIS:CE1	1:B:501[B]:HIS:CE1	1.83	1.65
1:A:501[B]:HIS:HE1	1:B:501[B]:HIS:CE1	1.06	1.62
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:HE1	1.23	1.33
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:ND1	2.24	1.04
1:A:519:ASN:HD22	1:B:519:ASN:ND2	1.61	0.99
1:A:519:ASN:ND2	1:B:519:ASN:HD22	1.61	0.98
1:A:519:ASN:HD22	1:B:519:ASN:HD22	0.91	0.90
1:B:496:THR:HG22	1:B:499:GLN:H	1.36	0.88
1:A:513[A]:HIS:CD2	1:B:459:TYR:HD2	1.92	0.86
1:A:501[B]:HIS:ND1	1:B:501[B]:HIS:ND1	2.25	0.83
1:A:501[B]:HIS:ND1	1:B:501[B]:HIS:CE1	2.45	0.82
1:A:421:MET:HE3	1:A:424:ILE:HB	1.65	0.79
1:B:347:THR:HG21	1:B:534:VAL:HG11	1.65	0.78
1:A:513[A]:HIS:NE2	1:B:459:TYR:HD2	1.83	0.77
1:B:421:MET:HE3	1:B:424:ILE:HB	1.65	0.76
1:A:347:THR:HG21	1:A:535:PRO:HD2	1.67	0.76
1:B:338:SER:H	1:B:341:SER:HB3	1.49	0.76
1:A:513[A]:HIS:CE1	1:B:459:TYR:CD2	2.76	0.74
1:A:513[A]:HIS:NE2	1:B:459:TYR:CD2	2.57	0.73
1:A:343:MET:O	1:A:347:THR:HB	1.88	0.73
1:B:525:LEU:HD13	3:B:600:ZTW:H4	1.76	0.68
1:A:496:THR:O	1:A:500:GLN:HG3	1.94	0.68
1:B:343:MET:O	1:B:347:THR:HB	1.94	0.68
1:A:392:VAL:HG13	1:A:432:SER:HA	1.75	0.68
1:A:513[A]:HIS:CE1	1:B:459:TYR:HD2	2.12	0.67
1:A:525:LEU:HD13	3:A:600:ZTW:H4	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513[A]:HIS:CD2	1:B:459:TYR:CD2	2.82	0.64
1:B:522:MET:HE2	1:B:547:HIS:CD2	2.33	0.62
1:B:524:HIS:NE2	1:B:528:MET:HE3	2.14	0.62
1:A:338:SER:H	1:A:341:SER:HB3	1.66	0.61
1:A:315:MET:HE1	1:A:365:PRO:HG2	1.82	0.61
1:B:319:LEU:CB	1:B:446:VAL:HG13	2.30	0.60
1:A:501[B]:HIS:CE1	1:B:501[B]:HIS:HD1	2.13	0.60
1:B:504:LEU:O	1:B:508:LEU:HG	2.02	0.60
1:B:421:MET:HE1	3:B:600:ZTW:H1	1.83	0.60
1:B:525:LEU:HD13	3:B:600:ZTW:C4	2.31	0.59
1:A:315:MET:CE	1:A:365:PRO:HG2	2.34	0.58
1:B:396:MET:SD	1:B:435:PHE:HB3	2.44	0.58
1:A:315:MET:HE1	1:A:365:PRO:HD2	1.86	0.58
1:A:315:MET:HE2	1:A:319:LEU:HD21	1.84	0.57
1:A:315:MET:HE1	1:A:365:PRO:CG	2.34	0.57
1:B:319:LEU:HB2	1:B:446:VAL:HG13	1.87	0.56
1:A:524:HIS:NE2	1:A:528:MET:HE3	2.21	0.55
1:A:495:LEU:HB3	1:A:499:GLN:HB2	1.89	0.55
1:B:315:MET:CE	1:B:319:LEU:HD21	2.37	0.55
1:B:342:MET:HE1	1:B:415:GLY:HA2	1.89	0.54
1:A:310:LEU:O	1:A:481:LYS:HE3	2.07	0.54
1:B:536:LEU:HD12	1:B:536:LEU:H	1.73	0.54
1:A:504:LEU:O	1:A:508:LEU:HG	2.08	0.54
1:B:392:VAL:HG13	1:B:432:SER:HA	1.89	0.53
1:A:538:ASP:O	1:A:542:GLU:HB2	2.08	0.53
1:A:319:LEU:CB	1:A:446:VAL:HG13	2.39	0.53
1:A:382:ALA:O	1:A:386:ILE:HG12	2.08	0.53
1:B:522:MET:HE2	1:B:547:HIS:CG	2.44	0.53
1:B:403:LEU:HD13	1:B:409:LEU:HD13	1.90	0.52
1:A:513[A]:HIS:CE1	1:B:459:TYR:CE2	2.97	0.52
1:A:421:MET:HE1	3:A:600:ZTW:H1	1.92	0.52
1:A:513[A]:HIS:CG	1:B:459:TYR:HD2	2.26	0.51
1:A:529:LYS:HE3	1:A:541:LEU:CD2	2.41	0.51
1:B:339:GLU:HG2	1:B:533:VAL:HG11	1.93	0.51
1:A:319:LEU:HB3	1:A:446:VAL:HG13	1.94	0.50
1:B:316:VAL:HG23	1:B:485:THR:CG2	2.40	0.50
1:B:393:TRP:O	1:B:396:MET:HG3	2.11	0.50
1:B:319:LEU:HB3	1:B:446:VAL:HG13	1.92	0.50
1:A:504:LEU:HD23	1:B:504:LEU:HD23	1.94	0.50
1:A:315:MET:HE1	1:A:365:PRO:CD	2.42	0.49
1:A:316:VAL:HG23	1:A:485:THR:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.93	0.49
1:B:496:THR:HB	1:B:499:GLN:OE1	2.13	0.49
1:B:421:MET:HE2	1:B:425:PHE:CE1	2.47	0.49
1:A:421:MET:HE1	3:A:600:ZTW:C1	2.43	0.49
1:A:529:LYS:HE3	1:A:541:LEU:HD21	1.95	0.49
1:B:315:MET:HE3	1:B:319:LEU:HD21	1.95	0.49
1:B:421:MET:HE1	3:B:600:ZTW:C1	2.43	0.49
1:B:347:THR:HG21	1:B:534:VAL:CG1	2.37	0.48
1:A:330:GLU:OE2	1:A:345:LEU:HD23	2.14	0.48
1:B:330:GLU:OE2	1:B:345:LEU:HD23	2.13	0.48
1:A:346:LEU:HD22	1:A:404:PHE:CD1	2.49	0.48
1:A:522:MET:HE3	1:A:547:HIS:CE1	2.50	0.47
1:B:496:THR:HG22	1:B:499:GLN:N	2.18	0.47
1:A:455:ASN:O	1:A:458:VAL:HG12	2.16	0.46
1:A:522:MET:HE3	1:A:547:HIS:CD2	2.51	0.46
1:B:357:MET:HE2	1:B:386:ILE:HB	1.97	0.46
1:B:338:SER:O	1:B:339:GLU:C	2.58	0.46
1:A:535:PRO:HB2	1:A:537:TYR:CE2	2.51	0.45
1:B:387:LEU:HB3	3:B:600:ZTW:C12	2.47	0.45
1:A:433:SER:O	1:A:437:MET:HG3	2.16	0.45
1:B:319:LEU:HB2	1:B:446:VAL:CG1	2.47	0.45
1:B:362:LYS:NZ	2:D:696:ASP:OXT	2.47	0.45
1:A:459:TYR:HD2	1:B:513[A]:HIS:CD2	2.35	0.45
1:B:362:LYS:NZ	2:D:693:LEU:O	2.47	0.45
1:A:524:HIS:CE1	1:A:528:MET:HE3	2.52	0.44
1:A:315:MET:CE	1:A:319:LEU:HD21	2.48	0.44
1:B:374:ASP:OD2	1:B:471:GLU:HG3	2.18	0.44
1:B:316:VAL:HG21	1:B:489:LEU:HD21	2.00	0.43
1:A:498:GLN:O	1:A:502:GLN:HG3	2.19	0.43
1:B:371:THR:O	1:B:372:LEU:C	2.61	0.43
1:A:347:THR:CG2	1:A:537:TYR:HE2	2.32	0.42
1:A:501[A]:HIS:CE1	1:B:487:ILE:HG21	2.53	0.42
1:A:525:LEU:HD13	3:A:600:ZTW:C4	2.46	0.42
1:B:329:SER:OG	1:B:330:GLU:N	2.52	0.42
1:A:522:MET:HE3	1:A:547:HIS:NE2	2.33	0.42
1:B:534:VAL:O	1:B:536:LEU:HD12	2.20	0.42
1:B:343:MET:HB3	1:B:534:VAL:HG22	2.00	0.42
1:A:319:LEU:HB2	1:A:446:VAL:HG13	2.01	0.42
1:A:479:LEU:HD23	1:A:479:LEU:HA	1.93	0.42
1:B:315:MET:HE3	1:B:319:LEU:HG	2.01	0.41
1:B:488:HIS:O	1:B:489:LEU:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD21	1:A:383:TRP:CE3	2.56	0.41
1:B:421:MET:HE3	1:B:424:ILE:CB	2.43	0.41
1:A:338:SER:O	1:A:339:GLU:C	2.63	0.41
1:A:347:THR:HG23	1:A:537:TYR:CE2	2.56	0.40
1:B:374:ASP:OD2	1:B:471:GLU:OE2	2.38	0.40
1:A:434:ARG:NE	1:B:459:TYR:OH	2.54	0.40
1:A:416:LYS:HG2	1:A:422:VAL:HG13	2.03	0.40
1:B:310:LEU:O	1:B:481:LYS:HE3	2.21	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	245/248 (99%)	243 (99%)	2 (1%)	0	100	100
1	B	241/248 (97%)	234 (97%)	7 (3%)	0	100	100
2	C	7/9 (78%)	7 (100%)	0	0	100	100
2	D	7/9 (78%)	7 (100%)	0	0	100	100
All	All	500/514 (97%)	491 (98%)	9 (2%)	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	223/224 (100%)	209 (94%)	14 (6%)	16	23
1	B	219/224 (98%)	209 (95%)	10 (5%)	24	36
2	C	7/9 (78%)	6 (86%)	1 (14%)	3	2
2	D	8/9 (89%)	6 (75%)	2 (25%)	0	0
All	All	457/466 (98%)	430 (94%)	27 (6%)	17	26

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LYS
1	A	330	GLU
1	A	347	THR
1	A	368	VAL
1	A	411	ASP
1	A	422	VAL
1	A	446	VAL
1	A	460	THR
1	A	466	LEU
1	A	468	SER
1	A	481	LYS
1	A	520	LYS
1	A	541	LEU
1	A	542	GLU
1	B	309	SER
1	B	347	THR
1	B	368	VAL
1	B	411	ASP
1	B	422	VAL
1	B	446	VAL
1	B	466	LEU
1	B	481	LYS
1	B	496	THR
1	B	542	GLU
2	C	690	LEU
2	D	690	LEU
2	D	696	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	375	GLN
1	A	398	HIS
1	A	439	ASN
1	A	519	ASN
1	B	356	HIS
1	B	439	ASN
1	B	455	ASN
1	B	516	HIS
2	D	691	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	ZTW	B	600	-	19,19,19	1.21	3 (15%)	27,27,27	1.47	4 (14%)
3	ZTW	A	600	-	19,19,19	1.23	2 (10%)	27,27,27	1.64	5 (18%)

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	ZTW	B	600	-	-	0/4/4/4	0/3/3/3
3	ZTW	A	600	-	-	0/4/4/4	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	ZTW	C5-S6	-3.31	1.67	1.74
3	A	600	ZTW	C7-S6	-2.92	1.68	1.75
3	A	600	ZTW	C5-S6	-2.41	1.69	1.74
3	B	600	ZTW	C1-C14	-2.13	1.37	1.41
3	B	600	ZTW	C7-S6	-2.01	1.70	1.75

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	ZTW	C5-S6-C7	5.46	98.14	91.12
3	A	600	ZTW	C5-S6-C7	4.23	96.56	91.12
3	A	600	ZTW	C10-C9-C8	-3.49	117.08	120.80
3	A	600	ZTW	C9-C10-C11	3.30	123.37	119.88
3	A	600	ZTW	C8-C7-S6	3.03	124.35	119.70
3	A	600	ZTW	C13-C8-C7	-2.81	116.44	121.12
3	B	600	ZTW	C8-C7-C15	2.35	134.66	128.43
3	B	600	ZTW	C9-C8-C7	-2.26	117.35	121.12
3	B	600	ZTW	C15-C7-S6	-2.20	107.29	111.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	ZTW	5	0
3	A	600	ZTW	4	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	243/248 (97%)	-0.12	11 (4%) 38 37	12, 29, 79, 100	6 (2%)
1	B	242/248 (97%)	-0.07	12 (4%) 34 32	13, 29, 90, 108	5 (2%)
2	C	9/9 (100%)	0.62	0 100 100	49, 57, 62, 62	0
2	D	9/9 (100%)	0.77	0 100 100	53, 66, 70, 79	0
All	All	503/514 (97%)	-0.07	23 (4%) 37 36	12, 30, 85, 108	11 (2%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	VAL	4.0
1	B	534	VAL	3.4
1	A	336	PRO	3.2
1	A	532	ASN	3.1
1	B	526	TYR	3.1
1	A	531	LYS	3.0
1	B	330	GLU	2.9
1	A	536	LEU	2.8
1	B	531	LYS	2.8
1	B	545	ASP	2.6
1	B	337	PHE	2.6
1	A	533	VAL	2.6
1	B	537	TYR	2.5
1	A	530	CYS	2.4
1	A	337	PHE	2.4
1	B	464	SER	2.4
1	B	535	PRO	2.2
1	A	535	PRO	2.2
1	B	527	SER	2.1
1	B	530	CYS	2.1
1	A	340	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	526	TYR	2.1
1	B	546	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	ZTW	B	600	17/17	0.85	0.14	41,50,55,56	0
3	ZTW	A	600	17/17	0.93	0.08	27,31,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.